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Thermomechanical polythermal ice-sheet model

Supervisor: Prof. RNDr. Zdeněk Martinec, DrSc.

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Abstrakt: Z hlediska fyzikálních dějů a procesů řídících pohyb a dynamiku pevninských polytermálních ledovců rozlišujeme dvě oblasti, oblast chladného ledu, kde je teplota pod bodem tání, a poté oblast, kde se led nachází právě na teplotě tání, což vede k přítomnosti nenulové frakce vody v kapalném skupenství. Těžištěm této práce je analýza a popis této druhé oblasti na základě konceptu racionální termodynamiky reagujících směsí. Pro směs voda-led jsou odvozeny zákony bilance hmotnosti, hybnosti, momentu hybnosti, energie a entropie. Následuje komplexní formulace fyzikálního modelu polytermálního pevninského ledovce dodáním patřičných okrajových a hraničních podmínek. Výsledkem je fyzikální model připravený k numerické implementaci. Získané rovnice jsou numericky řešeny pro stacionární 2-D případ a je provedeno srovnání výsledků ve standardní a nové formulaci.

Klíčová slova: polytermální ledovec, racionální termodynamika směsí

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Abstract: Based on the physical processes governing the motion and dynamics of polythermal ice sheets, we distinguish two regions; the cold region, where the ice temperature is below the melting point, and the temperate region, where the ice temperature is exactly equal to the melting point, leading to the presence of a water fraction. This work focuses on the analysis and description of the temperate zone on the basis of rational thermodynamics of reacting mixtures. The balance laws for the ice-water mixture, that is the mass balance, balance of linear and angular momenta, energy and entropy, are discussed. A physical model for a polythermal ice sheet is then established, including appropriate boundary and transition conditions. The resulting formulation is convenient for numerical implementation. Numerical examples are carried out for a stationary 2-D case and the results of the present and traditional formulations are compared.

Keywords: polythermal ice sheet, rational thermodynamics of mixtures

Chapter 1

Introduction

Glaciology studies behaviour of ice masses subject to various climatic and mechanical conditions, and is of a broad interdisciplinary character. There are many fields of science relating to glaciology, as for instance, geophysics, material science, crystallography, meteorology, oceanology, as well as fundamental chemistry and applied mathematics. Glaciology covers diverse temporal and spatial scales, describing processes ranging from ice crystal or flake growth, avalanches, to the flow of mountain glaciers and the advance and retreat of large ice shelves and ice sheets during glacial cycles. The subject of this work is mostly connected to the last subject, that is the modelling of physical processes in large ice sheets.

Ice sheets are land-based ice masses of continental size. The largest contemporary ice sheets are the Antarctic Ice Sheet (ice volume of 29.5×10^6 km^3 $\sim$ sea-level equivalent of 65 m, see Greve [6]), and the smaller Greenland Ice Sheet (2.8×10^6 km^3 $\sim$ 7m sea-level equivalent, [6]). However, significant areas of the Earth's surface have experienced extended glaciation during the past glacial cycles. During the Last Glacial Maximum, approximately 21,000 years ago, large parts of North America, northern Europe, the European Alps, and other areas in the world were covered by ice sheets, with a total ice volume of approximately 200×10^6 km^3 ([6]).

An intense effort has been focused on the modelling of the time evolution of large ice sheets during glacial cycles, with various physical processes included in the models, starting from the purely mechanical, to the thermo-mechanically coupled ones. This work focuses on polythermal ice sheets, where the so-called temperate zone is present, containing meltwater which affects the material behaviour, both mechanically and thermodynamically.

In the second chapter, we briefly review the traditional formulation for a polythermal ice sheet, the theoretical concepts and the equations that have been widely used for large-scale ice-sheet modelling.

Our aim is an alternative formulation of the temperate-ice region on the basis of rational thermodynamics of reacting mixtures. The basic concepts of this theory are outlined in the third chapter, including the formulation of the balance laws, exploitation of the entropy principle and an investigation of the equilibrium conditions.

In the fourth chapter, we apply the results of the mixture theory to the particular case of a 2-component ice-water mixture, being the subject of interest for the temperate-ice region. The material model is reduced by implementing partial linearization with respect to the equilibrium state and by constraining the model with an incompressibility condition. The balance equations are then simplified to a form convenient for numerical implementation.

In the fifth chapter, we consider a standard ice-sheet configuration and formulate the boundary and transition conditions for the field variables, within the framework of mixture theory.

In the sixth chapter, the equations describing temperate ice are solved numerically in a simple 2-D stationary case, and an elementary sensitivity study is performed to show a comparison between the traditional and the new formulation.

Chapter 2

Traditional formulation of glacier physics

2.1 Introduction

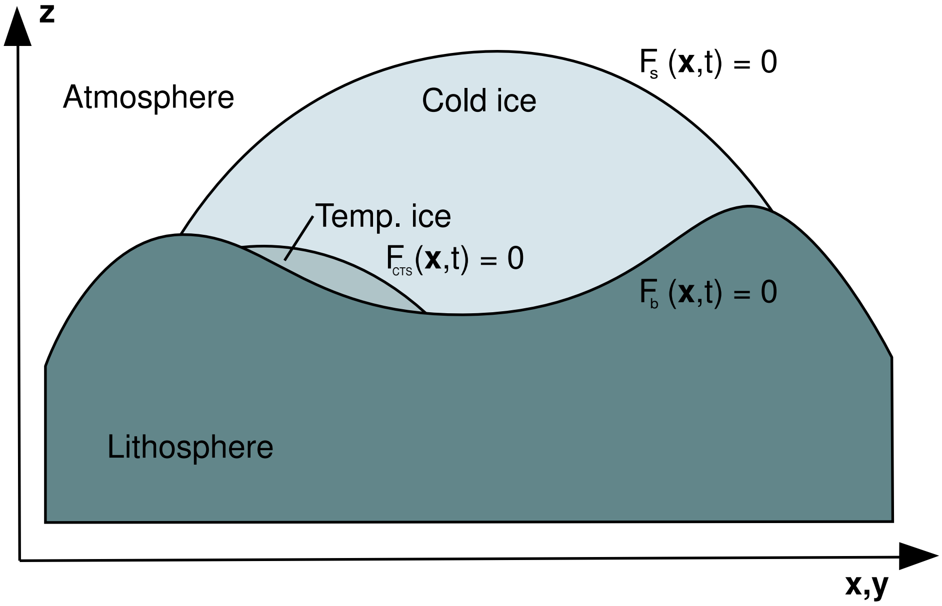

Figure 2.1: Sketch of a polythermal ice sheet resting on the lithospehere. Two distinct regions of an ice sheet are depicted - the cold-ice region containing no meltwater, and the temperate-ice region, with meltwater present. The dividing surfaces are represented by implicit equations $F_S(\vec{x},t) = 0$, $F_{CTS}(\vec{x},t) = 0$, and $F_B(\vec{x},t) = 0$, for the cold-ice – atmosphere boundary, cold-ice – temperate-ice boundary, and the ice–lithosphere boundary, respectively.

The physical processes governing the behaviour of an ice sheet are extremely complex however, for the purpose of large-scale modelling, we may confine ourselves to several important features. We distinguish two basic zones in a glacier; the *cold-ice zone*, where the ice temperature is below the pressure-melting point, and the *temperate-ice zone*, where the ice temperature is at the melting point and a certain amount of water is present, which significantly affects the thermal and mechanical behaviour of the glacier. The typical geometry of an ice sheet is depicted in Fig. 2.1.

In this chapter we summarize the traditional formulation of the field equations describing the thermo-mechanical behaviour in the cold-ice and temperate-ice zones.

2.2 Cold Ice Zone

In the cold-ice region, the ice is below the pressure melting-point and therefore no water is present. After neglecting the content of salt, debris, and other tracers, cold ice can be treated as a 1-component material. The continuum approach is adopted to describe both the thermal and the mechanical behaviour. According to the processes of interest, i.e. glacier flow on the decadal time scale, ice is described by a non-Newtonian, viscous, heat-conducting fluid. Moreover, the assumption of incompressibility is introduced, in good agreement with the density-variation observations across the cold-ice regions, (see Paterson [7]).

The continuum-mechanics description of a 1-component material includes *the local mass balance, the local balance of linear momentum* and the *local internal-energy balance* (see e.g. Martinec [2]):

$$\begin{aligned} \operatorname{div}\vec{v} &= 0\,, && (2.1)\\ \rho\dot{\vec{v}} &= -\operatorname{grad}\mathrm{p} \;+\; \operatorname{div}\overset{\circ}{\mathbf{T}} \;+\rho\,\vec{\mathrm{g}}_{\mathrm{a}}\,, && (2.2)\\ \rho\dot{\varepsilon} &= \mathbf{T}\cdot\mathbf{D} \;-\; \operatorname{div}\vec{q}\,, && (2.3) \end{aligned}$$

where $\vec{v}$ is *the ice velocity*, ρ denotes *the ice density*, the dot above $\vec{v}$ denotes *the material time derivative*, p *the pressure*, $\mathbf{T}$ *the Cauchy stress tensor* and $\overset{\circ}{\mathbf{T}}$ its *deviatoric part*, $\vec{g}_a$ is *the gravity acceleration*, ε is *the internal energy*,

$$\mathbf{D} = \{\operatorname{grad}\vec{v}\}^{sym.} \;=\; \frac{1}{2}\Big(\operatorname{grad}\vec{v} + (\operatorname{grad}\vec{v})^T\Big) \qquad (2.4)$$

the strain-rate tensor, and $\vec{q}$ *the heat flux*. We omit the angular momentum balance which constraints the Cauchy stress tensor to be symmetric, and the entropy balance, which provides constraints on the constitutive relations. However the choice of the constitutive relations as listed below ((2.5)–(2.8)) automatically satisfy both.

The constitutive relations adopted to complete the system of equations are

$$\begin{aligned} \mathbf{T} &= -p\mathbf{1} + \overset{\circ}{\mathbf{T}}\,, && (2.5)\\ \varepsilon &= c_V T\,, && (2.6)\\ \vec{q} &= -k(T)\operatorname{grad}T\,, && (2.7)\\ \mathbf{D} &= \mathcal{A}(T)\,d(\Sigma)\,\overset{\circ}{\mathbf{T}}\,, && (2.8) \end{aligned}$$

where c_V is *the specific heat at constant volume*[1] , $k(T)$ is the temperature-dependent *heat*

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[1] Hutter [4] claims that c_P, i.e. the specific heat at constant pressure, should be introduced instead of c_V, but we do not fully follow his argumentation, and keep c_V, according to Fowler and Larson [9].

conductivity of ice, Σ is *the effective shear stress* defined as

$$\Sigma = \sqrt{\frac{1}{2}\mathrm{tr}\{(\overset{\circ}{\mathbf{T}})^2\}}, \tag{2.9}$$

$\mathcal{A}(T)$ is *the rate factor*, and $d(\Sigma)$ *the creep response function* considered in the form

$$d(\Sigma) = \Sigma^{n-1} . \tag{2.10}$$

For n = 3, the stress-strain rate relation (2.8) represents *the Glen's flow law.* The temperature dependence of $\mathcal{A}(T)$ is usually assumed of the Arrhenius-type,

$$\mathcal{A}(T) = A \exp\left(-\frac{Q}{k_B T}\right) , \tag{2.11}$$

where Q is *the activation energy*, k_B *the Boltzmann's constant* and A a constant.

2.3 Temperate Ice Zone

Due to the slope of the Clausius-Clapeyron curve of the phase equilibrium between ice and water, high pressure in deep regions of large glaciers may lead to the presence of a non-zero water fraction. Such regions are called *temperate zones.* Although the mass fraction of water here is typically up to 5%, its presence significantly affects rheological and transport properties of the surrounding ice. The traditional way of describing the temperate-ice physics is as follows (Greve [6]).

Temperate ice may be described by two mass balances, one for the mixture as a whole and one for the water component. The linear momentum and energy balance are considered only for the mixture as a whole. Water is treated as a tracer component and its motion relative to the barycenter is described by a diffusion (Fickian) type of law. *The barycentric velocity* is introduced as

$$\vec{v}^B = \frac{1}{\rho}(\rho_1\vec{v}_1 + \rho_2\vec{v}_2) , \tag{2.12}$$

where ρ is *the mixture density*

$$\rho = \rho_1 + \rho_2 , \tag{2.13}$$

subscript (1) being for water and (2) for ice. *The water content* w is introduced as

$$w = \frac{\rho_1}{\rho} . \tag{2.14}$$

The diffusive water mass flux $\vec{j}$, describing the water motion relative to the motion of the barycenter is introduced as

$$\vec{j} = \rho_1(\vec{v}_1 - \vec{v}^B) = \rho w(\vec{v}_1 - \vec{v}^B) . \tag{2.15}$$

The mixture is assumed to be incompressible, since the total density variations do not exceed 1%. The mixture mass balance and the mixture momentum balance are then postulated as

$$\operatorname{div} \vec{v}^B = 0 \, , \tag{2.16}$$

$$\rho \dot{\vec{v}}^B = -\operatorname{grad} p + \operatorname{div} \overset{\circ}{\mathbf{T}} + \rho \vec{g}_a \, , \tag{2.17}$$

where again p denotes *the pressure*, $\mathbf{T}$ *the Cauchy stress tensor* and $\overset{\circ}{\mathbf{T}}$ its *deviatoric part*, and $\vec{g}_a$ *the gravity acceleration.* The mass balance for the water component is

$$\frac{\partial \rho_1}{\partial t} + \operatorname{div}(\rho_1 \vec{v}_1) = M \, , \tag{2.18}$$

which is under the assumption of mixture incompressibility equivalent to

$$\rho \dot{w} = -\operatorname{div} \vec{j} + M \, , \tag{2.19}$$

where M denotes *the water mass-production* term. Constitutive equations of the model are introduced as follows (see Hutter [4]):

$$\mathbf{T} = -p\mathbf{1} + \overset{\circ}{\mathbf{T}} \, , \tag{2.20}$$

$$\mathbf{D}^B = \mathcal{A}(T,w)\, d(\Sigma)\, \overset{\circ}{\mathbf{T}} \, , \tag{2.21}$$

$$\vec{j} = -\tilde{\nu} \operatorname{grad} w \, , \tag{2.22}$$

$$M = \frac{\mathbf{T} : \mathbf{D}^B}{L} \, , \tag{2.23}$$

where

$$\mathbf{D}^B = \{\operatorname{grad} \vec{v}^B\}^{sym.} = \frac{1}{2}\left(\operatorname{grad}\vec{v}^B + (\operatorname{grad}\vec{v}^B)^T\right) \tag{2.24}$$

is *the strain-rate tensor relative to the barycentric velocity*, $\mathcal{A}(T,w)$ is *the rate factor* (now dependent also on the water content w), $d(\Sigma)$ *the creep response function*, defined again as

$$d(\mathit{\Sigma}) = \Sigma^{n-1} \, , \tag{2.25}$$

with

$$\Sigma = \sqrt{\frac{1}{2}\operatorname{tr}\{(\overset{\circ}{\mathbf{T}})^2\}} \; ; \tag{2.26}$$

$\tilde{\nu}$ is *the diffusivity* and L *the latent heat of melting of ice.*

This has been the traditional approach to describe the temperate-zone physics. However, for example the constitutive equations are still a subject of discussion and from our point of view, the traditional formulation contains several problematic 'ad hoc' hypotheses. One example might be the stress-strain rate relation that is expressed by means of the gradient of the barycentric velocity, an assumption that may be difficult to justify. Moreover, the exact interpretation of the stress tensor is not clear, since the material is now a two-component mixture, hence two partial stress tensors are actually necessary. If the used tensor were the total stress tensor, which has the form (see e.g. Truesdell [14])

$$\mathbf{T} \ = \sum_{\alpha=1}^{2} (\mathbf{T}_\alpha + \rho_\alpha (\vec{v}_\alpha - \vec{v}^B) \otimes (\vec{v}_\alpha - \vec{v}^B)) \ ,$$

the presence of additional terms due to diffusion would require deeper analysis and justification before a stress-strain rate relation from the pure-ice case could be adopted.

In the following chapters, we will therefore attempt to formulate a thermo-mechanical temperate-ice model, strictly by means of rational thermodynamics of mixtures, that would involve the transport processes being related to water diffusion. We will adopt a fully-mixture concept, where the presented derivations will reveal the simplifications implicitly employed in the above formulation and will serve as a starting point for the possible generalization of the theoretical concept.

Therefore, the main focus of this thesis is the rational-thermodynamics theory of 2-component mixtures. A continuum theory describes a mixture as a superposition of continua components. The plausibility of this approach in the case of strictly separated media, as in our case, ice and water being two always separated phases, is discussed, for example, in Passman et al. [3], and is suitable for the large-scale ice-sheet modelling being considered in this work.

Chapter 3

Rational thermodynamics of mixtures

3.1 Introduction and basic principles

Since the rational thermodynamics of mixtures may not be a known theory to the reader, we outline it in this chapter following intensively the textbook by Samohýl [1].

The mixture theory is based on the continuum-mechanics approach. Its aim is to describe properties of a mixture and its components, formulate balance laws for them, and use the entropy and other constitutive principles to restrict the class of constitutive (response) functionals. The formulation of the mixture theory is based on the following three principles:

- All thermo-mechanical properties of a mixture are derivable from the properties of its components.
- The behaviour of a particular component is described as if it were isolated from the rest of the mixture, but includes all possible interactions with the rest of the mixture.
- The properties of a mixture are governed by the same principles as the properties of a one-component material.

According to the first principle, the properties of the components are first introduced as independent primitive quantities, from which the properties of the mixture are then derived. The second point gives a general idea as to how to formulate the balance laws for the components of a mixture, and the third principle constrains the mixture balance laws. They must be consistent with the balance laws for a 1-component material as follows. There should be a straightforward assignment between quantities appearing in a mixture balance law and in a 1-component material balance law and these quantities should coincide for a "1-component mixture". Hence, a 1-component material must be only a special case of a mixture.

3.2 Kinematics of a mixture

The α-component of a mixture is defined by its material body $\mathcal{B}_\alpha$, a set of particles $\{X_\alpha\}$. We express the configuration of this body by a mapping $\vec{\kappa}_\alpha$ (see e.g. Martinec [2]):

$$\left.\begin{array}{ll} \vec{\kappa}_\alpha : & \mathcal{B}_\alpha \rightarrow \mathrm{E}^3 \\ & X_\alpha \rightarrow \vec{X}_\alpha = \vec{\kappa}_\alpha(X_\alpha) \end{array}\right\} \alpha = 1, \ldots, n \ ,$$

where $\vec{\kappa}_\alpha$ represents *the reference configuration.*

The motion of the α-component particles is represented by a sufficiently smooth and invertible mapping $\vec{\chi}_\alpha$:

$$\vec{x}_\alpha = \vec{\chi}_\alpha(X_\alpha, t) = \vec{\chi}_\alpha(\vec{\kappa}_\alpha^{-1}((\vec{X}_\alpha, t), t) = \vec{\chi}_{\kappa\alpha}(\vec{X}_\alpha, t) \ , \qquad \alpha = 1, \ldots, n \ ,$$

where $\vec{x}_\alpha$ is the α-particle position in the present configuration.

We will assume that all the reference frames for the components coincide and also that all the present frames for the components coincide. However, the common reference frame (to which all the $\vec{X}_\alpha$ vectors are related) and the common present frame (to which we relate all the $\vec{x}_\alpha$ vectors) may differ.

The **mixture** is now defined as an intersection of the present configurations of all its components. Therefore, a material particle of a mixture at position $\vec{x}$ in the present configuration is composed of n component particles, all of them being present at the same position $\vec{x}_\alpha = \vec{x}, \ \alpha = 1, \ldots, n$.

All standard kinematic quantities can be defined for each mixture component. The most important are (see Martinec [2]) :

- *Deformation gradient:*

$$\mathbf{F}_{\kappa\alpha} = \mathrm{Grad}_{\kappa\alpha}\vec{\chi}_{\kappa\alpha}(\vec{X}_\alpha, t) = \frac{\partial\vec{\chi}_{\kappa\alpha}(\vec{X}_\alpha, t)}{\partial\vec{X}_\alpha} \ , \qquad (\mathbf{F}_{\kappa\alpha})^{iJ} = \frac{\partial \ \chi^i_{\kappa\alpha}(\vec{X}_\alpha, t)}{\partial \ X^J_\alpha} \ , \tag{3.1}$$

- *Second deformation gradient:*

$$\mathbf{G}_{\kappa\alpha} = \mathrm{Grad}_{\kappa\alpha}\mathbf{F}_{\kappa\alpha} = \frac{\partial\mathbf{F}_{\kappa\alpha}(\vec{X}_\alpha, t)}{\partial\vec{X}_\alpha} \ , \qquad (\mathbf{G}_{\kappa\alpha})^{iJK} = \frac{\partial^2\chi^i_{\kappa\alpha}(\vec{X}_\alpha, t)}{\partial X^J_\alpha \partial X^K_\alpha} \ , \tag{3.2}$$

- *Jacobian:*

$$J_{\kappa\alpha} = \det\mathbf{F}_{\kappa\alpha} \ ,$$

- *Cauchy polar decomposition of deformation gradient:*[1]

$$\mathbf{F}_{\kappa\alpha} = \mathbf{R}_{\kappa\alpha}\mathbf{U}_{\kappa\alpha} = \mathbf{V}_{\kappa\alpha}\mathbf{R}_{\kappa\alpha} \ , \tag{3.3}$$

$$(\mathbf{F}_{\kappa\alpha})^{iJ} = (\mathbf{R}_{\kappa\alpha})^{iK}(\mathbf{U}_{\kappa\alpha})^{KJ} = (\mathbf{V}_{\kappa\alpha})^{ik}(\mathbf{R}_{\kappa\alpha})^{kJ} \ ,$$

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[1] We are using the Einstein summation convention.

where $\mathbf{R}_{\kappa\alpha}$ is an orthogonal tensor and $\mathbf{V}_{\kappa\alpha}$, $\mathbf{U}_{\kappa\alpha}$ are positive definite and symmetric *stretch tensors*, i.e.:

$$\begin{aligned} &\mathbf{R}_{\kappa\alpha}\mathbf{R}^{\mathbf{T}}_{\kappa\alpha} \;=\; \mathbf{R}^{\mathbf{T}}_{\kappa\alpha}\mathbf{R}_{\kappa\alpha} \;=\; \mathbf{1}\ , \\ &\mathbf{V}_{\kappa\alpha} \;=\; \mathbf{V}^{T}_{\kappa\alpha}\ , \qquad\qquad \mathbf{U}_{\kappa\alpha} \;=\; \mathbf{U}^{T}_{\kappa\alpha}\ , \\ &\vec{a}\cdot\mathbf{V}_{\kappa\alpha}\cdot\vec{a} \;>\; 0\ ,\ \ \forall\,\vec{a}\ , \qquad \vec{a}\cdot\mathbf{U}_{\kappa\alpha}\cdot\vec{a} \;>\; 0\ ,\ \ \forall\,\vec{a}\ , \end{aligned}$$

- *Right and left Cauchy-Green tensors:*

$$\mathbf{C}_{\kappa\alpha} \;=\; (\mathbf{U}_{\kappa\alpha})^2\ , \qquad\qquad \mathbf{B}_{\kappa\alpha} \;=\; (\mathbf{V}_{\kappa\alpha})^2\ , \tag{3.4}$$

- *Temporal and spatial derivatives of a scalar, vector or tensor-valued field in the spatial description,* $\psi_\alpha \;=\; \psi_\alpha(\vec{x},t)$:

$$\frac{\partial\psi_\alpha}{\partial t} = \frac{\partial\psi_\alpha(\vec{x},t)}{\partial t}\ , \tag{3.5}$$

$$\frac{\partial\psi_\alpha}{\partial\vec{x}} = \mathrm{grad}\ \psi_\alpha\ . \tag{3.6}$$

The second equation (3.6) has the following meaning:

  - for ψ_α being a scalar quantity:

$$(\mathrm{grad}\ \psi_\alpha)^i = \frac{\partial\psi_\alpha}{\partial x^i}\ , \tag{3.7}$$

  - for ψ_α being a vector:

$$(\mathrm{grad}\ \psi_\alpha)^{ij} = \frac{\partial(\psi_\alpha)^i}{\partial x^j}\ , \tag{3.8}$$

  - for ψ_α being a second-order tensor:

$$(\mathrm{grad}\ \psi_\alpha)^{ijk} = \frac{\partial(\psi_\alpha)^{ij}}{\partial x^k}\ , \tag{3.9}$$

and likewise for higher-order tensors.

- Using the mapping $\vec{x} = \chi_{\kappa\alpha}(\vec{X}_\alpha,t)$ and the inverse mapping $\vec{X}_\alpha = \chi^{-1}_{\kappa\alpha}(\vec{x},t)$, we define:

  - *Material time derivative with respect to the* α*-component:*

$$\grave{\psi}_\alpha{}^{\alpha} \;=\; \frac{D_\alpha\psi_\alpha}{Dt} \;=\; \left.\frac{\partial\psi_\alpha(\vec{X}_\alpha,t)}{\partial t}\right|_{\vec{X}_\alpha}\ , \tag{3.10}$$

where the superscript in the first term and the subscript for D in the second term denote the differentiation at fixed $\vec{X}_\alpha$.
Using $\vec{X}_\alpha = \chi^{-1}_{\kappa\alpha}(\vec{x},t)$ and $\vec{x} = \chi_{\kappa\gamma}(\vec{X}_\gamma,t)$, it analogously holds:

$$\grave{\psi}_\alpha{}^{\gamma} \;=\; \frac{D_\gamma\psi_\alpha}{Dt} \;=\; \left.\frac{\partial\psi_\alpha(\vec{X}_\alpha,t)}{\partial t}\right|_{\vec{X}_\gamma} \;=\; \left.\frac{\partial\psi_\alpha(\chi^{-1}_{\kappa\alpha}(\chi_{\kappa\gamma}(\vec{X}_\gamma,t),t),t)}{\partial t}\right|_{\vec{X}_\gamma}\ , \tag{3.11}$$

  - *Referential gradient:*

$$\mathrm{Grad}\ \psi_\alpha \;=\; \frac{\partial \psi_\alpha(\vec{X}_\alpha, t)}{\partial \vec{X}_\alpha}\ , \tag{3.12}$$

- *α-component velocity:*

$$\vec{v}_\alpha \;=\; \left.\frac{\partial \vec{\chi}_{\kappa\alpha}(\vec{X}_\alpha, t)}{\partial t}\right|_{\vec{X}_\alpha}\ , \tag{3.13}$$

  thus for a field quantity expressed in spatial description $\psi(\vec{x}, t)$, we have:

$$\grave{\psi}^\alpha = \frac{\partial \psi}{\partial t} + \mathrm{grad}\psi \cdot \vec{v}_\alpha\ , \qquad \grave{\psi}^\alpha = \frac{\partial \psi}{\partial t} + v^i_\alpha \frac{\partial \psi}{\partial x^i}\ , \tag{3.14}$$

- *Spatial velocity gradient:*

$$\mathbf{L}_\alpha \;=\; \mathrm{grad}\ \vec{v}_\alpha\ , \qquad (\mathbf{L}_\alpha)^{ij} \;=\; \frac{\partial v^i_\alpha}{\partial x^j}\ , \tag{3.15}$$

  and its symmetric and antisymmetric parts:

  - *Strain-rate tensor:*

$$\mathbf{D}_\alpha \;\equiv\; \mathbf{L}^{sym.}_\alpha \;=\frac{1}{2}(\mathbf{L}_\alpha + \mathbf{L}^T_\alpha)\ , \tag{3.16}$$

  - *Spin:*

$$\mathbf{W}_\alpha \equiv\; \mathbf{L}^{antis.}_\alpha \;=\; \frac{1}{2}(\mathbf{L}_\alpha - \mathbf{L}^T_\alpha)\ . \tag{3.17}$$

It will be also convenient to introduce the following quantities:

- *Diffusion velocity relative to the k-th component $\vec{u}^{(k)}_\alpha$, $k \in (1, \ldots, n)$:*

$$\vec{u}^{(k)}_\alpha \;=\; \vec{v}_\alpha - \vec{v}_k\ , \qquad \alpha = 1, \ldots, n\ , \tag{3.18}$$

  if the superscript *(k)* is omitted, then the diffusion velocity is relative to the n-th component:

$$\vec{u}_\alpha \;=\; (\vec{v}_\alpha - \vec{v}_n) \qquad \Rightarrow \qquad \vec{u}_n \;=\; \vec{0}\ ; \tag{3.19}$$

- *Spin relative to the k-th component* $\mathbf{\Omega}^{(k)}_\alpha$, $k \in (1, \ldots, n)$:

$$\mathbf{\Omega}^{(k)}_\alpha \;=\; \mathbf{W}_\alpha - \mathbf{W}_k\ , \qquad \alpha = 1, \ldots, n\ , \tag{3.20}$$

  in particular, we also define spin relative to the n-th component $\mathbf{\Omega}_\alpha$,

$$\mathbf{\Omega}_\alpha \;=\; \mathbf{\Omega}^{(n)}_\alpha\ . \tag{3.21}$$

We will often use the **Reynold's transport theorem**; following Martinec [2]. Consider a material volume v intersected by a discontinuity surface $\sigma(t)$ across which a field variable

ψ_α, $\alpha \in (1, \ldots, n)$, undergoes a finite jump. Let the points of $\sigma(t)$ move with velocity $\vec{\nu}$. We can derive

$$\frac{D_\alpha}{Dt} \int_v \psi_\alpha \; dv = \int_{v \backslash \sigma(t)} \left(\frac{\partial \psi_\alpha}{\partial t} + \text{div} \; (\psi_\alpha \otimes \vec{v}_\alpha) \right) dv + \int_{\sigma(t)} [\psi_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \; da \; , \tag{3.22}$$

or, equivalently,

$$\frac{D_\alpha}{Dt} \int_v \psi_\alpha \; dv = \int_{v \backslash \sigma(t)} \left(\frac{D_\alpha \psi_\alpha}{Dt} + \psi_\alpha \; \text{div} \; \vec{v}_\alpha \right) dv + \int_{\sigma(t)} [\psi_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \; da \; , \tag{3.23}$$

where the symbol $\otimes$ denotes the tensor (dyadic) product and the square brackets denote the jump across the singular surface $\sigma(t)$, i.e. for an arbitrary field quantity ψ, $[\psi]_-^+ = \psi^+ - \psi^-$.

We will also use the modified Gauss theorem, which can be derived for a mixture in the same way as for a one-component material (Martinec [2]):

$$\int_{v \backslash \sigma(t)} \text{div} \; \psi_\alpha \; dv = \int_{\partial v} \psi_\alpha \cdot \vec{n} \; da - \int_{\sigma(t)} [\psi_\alpha]_-^+ \cdot \vec{n} \; da \; , \tag{3.24}$$

where ∂v is the boundary surface and $\sigma(t)$ the discontinuity surface.

In the following sections, we will derive the conservation laws or balance laws for mass, linear and angular momenta, energy and, finally, we will deal with the entropy inequality in mixtures. We will assume that the material volume can be intersected by a discontinuity surface $\sigma(t)$, where any of the material properties may undergo a finite jump.

3.3 Mass balance in a mixture

For each component α in the n-component mixture, we introduce a primitive scalar quantity

- *Mass density of the α-component* in the present configuration:

  $$\rho_\alpha = \rho_\alpha(\vec{x}, t) \geq 0 \; , \qquad\qquad \alpha = 1, \ldots, n \; ,$$

  such that the total mass of the α-component in material volume v is

  $$m_\alpha(v) = \int_v \rho_\alpha \; dv \; , \tag{3.25}$$

- *Volume rate of mass-change of the α-component:*

  $$r_\alpha = r_\alpha(\vec{x}, t) \; , \qquad \vec{x} \in v(t) \; , \qquad\qquad \alpha = 1, \ldots, n \; ,$$

- *Surface rate of mass-change of the α-component:*

  $$r_\alpha^S = r_\alpha^S(\vec{x}, t) \;, \qquad \vec{x} \in \sigma(t) \;, \qquad\qquad \alpha = 1, \ldots, n \;,$$

  such that the total mass change of the α-component, caused by reactions amongst the mixture components, in material volume v per unit time is

  $$\delta m_\alpha(v) = \int\limits_v r_\alpha \, dv \;+ \int\limits_{\sigma(t)} r_\alpha^S \, da \;.$$

We also distinguish between the *reacting components*:

$$r_\varphi \not\equiv 0 \;\text{ or }\; r_\varphi^S \not\equiv 0 \;, \qquad\qquad \varphi = 1, \ldots, m \;,$$

and the *non-reacting components*:

$$r_\omega \equiv 0 \;\text{ and }\; r_\omega^S \equiv 0 \;, \qquad\qquad \omega = m+1, \ldots, n \;.$$

The mass balance of the α-component of a mixture in material volume v is postulated to be:

$$\frac{D_\alpha}{Dt} \int\limits_v \rho_\alpha \, dv = \int\limits_v r_\alpha \, dv \;+ \int\limits_{\sigma(t)} r_\alpha^S \, da \;, \qquad\qquad \alpha = 1, \ldots, n \;, \tag{3.26}$$

and the mass balance of a mixture:

$$\sum_{\alpha=1}^{n} \left(\frac{D_\alpha}{Dt} \int\limits_v \rho_\alpha \, dv \right) = 0 \;. \tag{3.27}$$

Using (3.23), we obtain

$$\frac{D_\alpha}{Dt} \int\limits_v \rho_\alpha \, dv = \int\limits_{v \backslash \sigma(t)} \left(\grave{\rho}_\alpha^{\;\alpha} + \rho_\alpha \operatorname{div} \vec{v}_\alpha \right) dv + \int\limits_{\sigma(t)} [\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \, da \;,$$

which, with the use of (3.26), yields

$$\int\limits_{v \backslash \sigma(t)} \left(\grave{\rho}_\alpha^{\;\alpha} + \rho_\alpha \operatorname{div} \vec{v}_\alpha - r_\alpha \right) \, dv + \int\limits_{\sigma(t)} \left([\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \;-\; r_\alpha^S \right) \, da = 0 \;.$$

Since the material volume v was chosen arbitrarily, we can conclude that

$$\boxed{\begin{array}{lclcr} \grave{\rho}_\alpha^{\;\alpha} + \rho_\alpha \operatorname{div} \vec{v}_\alpha & = & r_\alpha & \text{in} & v \setminus \sigma(t) \;, \\ {[\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n}} & = & r_\alpha^S & \text{at} & \sigma(t) \;. \end{array}} \tag{3.28}$$

In addition, using (3.23) in (3.27), we arrive at

$$\int\limits_{v \backslash \sigma(t)} \sum_{\alpha=1}^{n} \left(\grave{\rho}_\alpha^{\;\alpha} + \rho_\alpha \operatorname{div} \vec{v}_\alpha \right) \, dv + \int\limits_{\sigma(t)} \sum_{\alpha=1}^{n} [\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \, da \;=\; 0 \;.$$

Since the material volume v was chosen arbitrarily, we conclude that

$$\boxed{\begin{array}{lcccr} \sum\limits_{\alpha=1}^{n} (\grave{\rho}_\alpha{}^{\alpha} + \rho_\alpha \operatorname{div} \vec{v}_\alpha\ ) & = & 0 & \text{in} & v \setminus \sigma(t)\ , \\ \sum\limits_{\alpha=1}^{n} [\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} & = & 0 & \text{at} & \sigma(t)\ . \end{array}} \tag{3.29}$$

By summation of the local mass balances and the boundary conditions expressed in (3.28) over α, we obtain

$$\sum_{\alpha=1}^{n} (\grave{\rho}_\alpha{}^{\alpha} + \rho_\alpha \operatorname{div} \vec{v}_\alpha\ - r_\alpha) \ = \ 0 \qquad \text{in} \qquad v \setminus \sigma(t)\ , \tag{3.30}$$

$$\sum_{\alpha=1}^{n} \Big([\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \ - \ r_\alpha^S \Big) \ = \ 0 \qquad \text{at} \qquad \sigma(t)\ . \tag{3.31}$$

Subtracting equations (3.30) and (3.31) from the equations in (3.29) yields

$$\boxed{\begin{array}{lcccr} \sum\limits_{\alpha=1}^{n} r_\alpha & = & 0 & \text{in} & v \setminus \sigma(t)\ , \\ \sum\limits_{\alpha=1}^{n} r_\alpha^S & = & 0 & \text{at} & \sigma(t)\ . \end{array}} \tag{3.32}$$

At this point, it is convenient to introduce:

- *Mass density of a mixture* ρ*:*

$$\rho \ = \ \sum_{\alpha=1}^{n} \rho_\alpha\ , \tag{3.33}$$

- *Mass fraction of the* α*-component* w_α*:*

$$w_\alpha \ = \ \frac{\rho_\alpha}{\rho}\ , \qquad \alpha = 1, \ldots, n\ , \tag{3.34}$$

consequently

$$\sum_{\alpha=1}^{n} w_\alpha = 1\ . \tag{3.35}$$

3.4 Linear momentum balance for a mixture

The linear momentum of the α-component of a mixture in material volume v is a vector quantity defined by

$$\vec{p}_\alpha(v) \ = \ \int_v \rho_\alpha \vec{v}_\alpha \, dv\ , \qquad \alpha = 1, \ldots, n\ ,$$

The linear-momentum balance for the α-component of a mixture is postulated to be:

$$\begin{aligned} \frac{D_\alpha}{Dt}\int\limits_v \rho_\alpha \vec{v}_\alpha \, dv &= \int\limits_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} \, da + \int\limits_v \rho_\alpha \vec{b}_\alpha \, dv + \int\limits_v \vec{k}_\alpha \, dv \\ &+ \int\limits_v r_\alpha \vec{v}_\alpha \, dv + \int\limits_{\sigma(t)} \vec{f}^S_\alpha \, da \, , \\ \alpha &= 1, \ldots, n \, , \end{aligned} \tag{3.36}$$

where

- $\int\limits_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} \, da$
  describes the total surface force exerted on the particular α-component at ∂v. The resulting force comes from the following types of interaction:
  - Interaction with the surroundings of the material volume v, i.e. the surface force exerted at the α-component from the outer side of the volume boundary ∂v (determined by the orientation of the normal vector $\vec{n}$). If the boundary ∂v is an internal boundary in a mixture, then this term consists of partial forces related to particular components of the surrounding mixture.
  - Interaction surface forces, which represent the surface interaction of the particular α-component with the remaining mixture components from the inner side of the volume v.

- $\int\limits_v \rho_\alpha \vec{b}_\alpha \, dv$
  describes the volume forces (e.g. gravity).

- $\int\limits_v \vec{k}_\alpha \, dv$
  describes the interaction volume forces – volume interaction with the rest of the mixture.

  The *interaction* and *inner surface forces* together with *the interaction volume forces* enable us to describe the mechanical interaction among the mixture components. For instance, for an ice-water mixture, these quantities model the volume-averaged force exerted by flowing water on the surrounding ice. Thus, despite the fact that the exact geometrical configuration of the water tunnels, cavities, etc., is not specified, this concept gives us a tool to handle the interactions in a volume-averaged sense, which is sufficient for certain time- and spatial-scales behaviour.

- $\int\limits_v r_\alpha \vec{v}_\alpha \, dv$
  Is the rate of change of linear momentum induced by composition changes, e.g. for a two-component ice-water mixture, both components are considered as continua moving with generally different velocities, if freezing of water or melting of ice occurs, it results in appropriate linear-momentum interchange between the components.

- $\int\limits_{\sigma(t)} \vec{f}_\alpha^S \, da$
  Is the linear-momentum surface-production term. We consider this term because we may identify a singular surface in a glacier where melting occurs. Thus, for particular mixture components, the surface behaves as a source of mass, linear and angular momenta, energy and entropy, respectively.

For the quantity φ_α of the α-component, using (3.23) and (3.28), we can write:

$$
\begin{aligned}
&\frac{D_\alpha}{Dt} \int\limits_{v} \rho_\alpha \varphi_\alpha \, dv \\
&= \int\limits_{v\backslash\sigma(t)} \left(\frac{D_\alpha(\rho_\alpha \varphi_\alpha)}{Dt} + \rho_\alpha \varphi_\alpha \operatorname{div} \vec{v}_\alpha \right) dv + \int\limits_{\sigma(t)} [\rho_\alpha \varphi_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \, da \\
&= \int\limits_{v\backslash\sigma(t)} \left\{ \varphi_\alpha \left(\grave{\rho}_\alpha^{\,\alpha} + \rho_\alpha \operatorname{div} \vec{v}_\alpha \right) + \rho_\alpha \grave{\varphi}_\alpha^{\,\alpha} \right\} \, dv + \int\limits_{\sigma(t)} [\rho_\alpha \varphi_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \, da \\
&= \int\limits_{v\backslash\sigma(t)} \varphi_\alpha r_\alpha \, dv \; + \int\limits_{v\backslash\sigma(t)} \rho_\alpha \grave{\varphi}_\alpha^{\,\alpha} \, dv \; + \int\limits_{\sigma(t)} [\rho_\alpha \varphi_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \, da \; .
\end{aligned}
\tag{3.37}
$$

Particularly for $\varphi_\alpha = \vec{v}_\alpha$, we obtain

$$
\frac{D_\alpha}{Dt} \int\limits_{v} \rho_\alpha \vec{v}_\alpha \, dv \; = \int\limits_{v\backslash\sigma(t)} \vec{v}_\alpha r_\alpha \, dv \; + \int\limits_{v\backslash\sigma(t)} \rho_\alpha \grave{\vec{v}}_\alpha^{\,\alpha} \, dv \; + \int\limits_{\sigma(t)} [\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \, da \; . \tag{3.38}
$$

Substituting this into (3.36) yields

$$
\begin{aligned}
\int\limits_{v\backslash\sigma(t)} \rho_\alpha \grave{\vec{v}}_\alpha^{\,\alpha} \, dv + \int\limits_{\sigma(t)} [\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \, da \quad &= \quad \int\limits_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} \, da + \int\limits_{v\backslash\sigma(t)} \rho_\alpha \vec{b}_\alpha \, dv \\
&\quad + \int\limits_{v\backslash\sigma(t)} \vec{k}_\alpha \, dv \; + \int\limits_{\sigma(t)} \vec{f}_\alpha^S \, da \, .
\end{aligned}
\tag{3.39}
$$

Applying the modified Gauss theorem (3.24) to the first integral on the right-hand side gives

$$
\begin{aligned}
\vec{0} \; = \; & \int\limits_{v\backslash\sigma(t)} \left(\rho_\alpha \grave{\vec{v}}_\alpha^{\,\alpha} - \operatorname{div} \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha - \vec{k}_\alpha \right) dv \\
& - \int\limits_{\sigma(t)} \left([\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \; + \; \vec{f}_\alpha^S \right) da \; .
\end{aligned}
\tag{3.40}
$$

Since the volume v was chosen arbitrarily, we conclude that

$$
\boxed{
\begin{array}{rcllr}
\rho_\alpha \grave{\vec{v}}_\alpha^{\,\alpha} & = & \operatorname{div} \mathbf{T}_\alpha \; + \; \rho_\alpha \vec{b}_\alpha \; + \; \vec{k}_\alpha & \text{in} & v \setminus \sigma(t) \; , \\
\vec{0} & = & [\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \; + \; \vec{f}_\alpha^S & \text{at} & \sigma(t) \; .
\end{array}
}
\tag{3.41}
$$

The balance of linear momentum of a mixture is postulated as

$$\sum_{\alpha=1}^{n} \frac{D_\alpha}{Dt} \int\limits_{v} \rho_\alpha \vec{v}_\alpha \; dv \;=\; \sum_{\alpha=1}^{n} \int\limits_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} \; da \;+\; \sum_{\alpha=1}^{n} \int\limits_{v \backslash \sigma(t)} \rho_\alpha \vec{b}_\alpha \; dv \; . \tag{3.42}$$

Again, applying (3.37) to the left-hand side and (3.24) to the first term on the right-hand side, we obtain

$$\begin{aligned} \vec{0} \;&=\; \int\limits_{v \backslash \sigma(t)} \sum_{\alpha=1}^{n} \left(\rho_\alpha \grave{\vec{v}}_\alpha{}^{\alpha} + r_\alpha \vec{v}_\alpha \; - \mathrm{div}\; \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha \right) \; dv \; + \\ &+ \; \int\limits_{\sigma(t)} \left[\sum_{\alpha=1}^{n} \left\{ \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu}) - \mathbf{T}_\alpha \right\} \right]_{-}^{+} \cdot \vec{n} \; da \; . \end{aligned} \tag{3.43}$$

Since the material volume v was arbitrary, we conclude that

$$\boxed{\begin{array}{lcllc} \vec{0} & = & \sum\limits_{\alpha=1}^{n} \left(\rho_\alpha \grave{\vec{v}}_\alpha{}^{\alpha} + r_\alpha \vec{v}_\alpha \; - \mathrm{div}\; \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha \right) & \text{in} & v \setminus \sigma(t) \; , \\ \vec{0} & = & \left[\sum\limits_{\alpha=1}^{n} \left\{ \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu}) - \mathbf{T}_\alpha \right\} \right]_{-}^{+} \cdot \vec{n} & \text{at} & \sigma(t) \; . \end{array}} \tag{3.44}$$

Summing up the balance laws and boundary conditions (3.41) over all components yields

$$\begin{array}{rcccc} \sum\limits_{\alpha=1}^{n} \left(\rho_\alpha \grave{\vec{v}}_\alpha{}^{\alpha} - \mathrm{div}\; \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha - \vec{k}_\alpha \right) & = & \vec{0} & \text{in} & v \setminus \sigma(t) \; , \\ \sum\limits_{\alpha=1}^{n} \left([\mathbf{T}_\alpha \; - \; \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]_{-}^{+} \cdot \vec{n} \; + \; \vec{f}_\alpha^{S} \right) & = & \vec{0} & \text{at} & \sigma(t) \; , \end{array}$$

which with the use of (3.44) implies

$$\boxed{\begin{array}{rcccc} \sum\limits_{\alpha=1}^{n} (\vec{k}_\alpha + r_\alpha \vec{v}_\alpha) & = & \vec{0} & \text{in} & v \setminus \sigma(t) \; . \\ \sum\limits_{\alpha=1}^{n} \vec{f}_\alpha^{S} & = & \vec{0} & \text{at} & \sigma(t) \; . \end{array}} \tag{3.45}$$

3.5 Angular momentum balance for a mixture

The angular momentum of the α-component of a mixture in material volume v relative to a spatial point $\vec{y}_0$ is defined as a second-order tensor

$$\mathbf{l}_\alpha(v) = \int\limits_{v} (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{v}_\alpha \; dv \; , \qquad\qquad \alpha = 1, \ldots, n \; ,$$

where $\vec{y}_0$ is assumed to be a constant vector and the operator $\wedge$ is defined by

$$\vec{a} \wedge \vec{b} \;=\; \vec{a} \otimes \vec{b} - \vec{b} \otimes \vec{a} \; , \qquad (\vec{a} \wedge \vec{b})^{ij} \;=\; (a^i b^j - a^j b^i) \; , \tag{3.46}$$

for two vectors and

$$(\vec{a} \wedge \mathbf{B})^{ijk} \;\equiv\; a^i A^{jk} - a^j A^{ik} \ ,$$

for a vector and a second-order tensor.

The angular momentum balance for the α-component in material volume v is postulated

$$\begin{aligned}
\frac{D_\alpha}{Dt} \int\limits_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{v}_\alpha \; dv \;&=\; \int\limits_{\partial v} (\vec{x} - \vec{y}_0) \wedge \mathbf{T}_\alpha \cdot \vec{n} \; da + \int\limits_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{b}_\alpha \; dv \\
&+\; \int\limits_v (\vec{x} - \vec{y}_0) \wedge (\vec{k}_\alpha + r_\alpha \vec{v}_\alpha) \; dv \;+\; \int\limits_{\sigma(t)} (\vec{x} - \vec{y}_0) \wedge \vec{f}^S_\alpha \; da \ , \\
\alpha \;&=\; 1, \ldots, n \ . \qquad (3.47)
\end{aligned}$$

By (3.37) we have

$$\begin{aligned}
\frac{D_\alpha}{Dt} \int\limits_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{v}_\alpha \; dv \;&=\; \int\limits_{v \setminus \sigma(t)} \rho_\alpha \left(\frac{D_\alpha (\vec{x} - \vec{y}_0)}{Dt} \wedge \vec{v}_\alpha + (\vec{x} - \vec{y}_0) \wedge {\grave{\vec{v}}_\alpha}{}^{\alpha} \right) \; dv \; + \\
+ \int\limits_{v \setminus \sigma(t)} r_\alpha (\vec{x} - \vec{y}_0) \wedge \vec{v}_\alpha \; dv \;&+\; \int\limits_{\sigma(t)} \left[(\rho_\alpha (\vec{x} - \vec{y}_0) \wedge \vec{v}_\alpha) \otimes (\vec{v}_\alpha - \vec{\nu}) \right]_-^+ \cdot \vec{n} \; da \ .
\end{aligned}$$

Since

$$\frac{D_\alpha (\vec{x} - \vec{y}_0)}{Dt} \wedge \vec{v}_\alpha = \vec{v}_\alpha \wedge \vec{v}_\alpha = \mathbf{0} \ ,$$

and applying the Gauss theorem[2] (3.24) on the first surface integral in (3.47), we have

$$\begin{aligned}
&\left[\int\limits_{\partial v} (\vec{x} - \vec{y}_0) \wedge \mathbf{T}_\alpha \cdot \vec{n} \; da \right]^{ij} \\
=\;& \int\limits_{\partial v} \left\{ (x^i - y_0^i) T_\alpha^{jk} - (x^j - y_0^j) T_\alpha^{ik} \right\} n^k \; da \\
=\;& \int\limits_{v \setminus \sigma(t)} \frac{\partial}{\partial x^k} \left\{ (x^i - y_0^i) T_\alpha^{jk} - (x^j - y_0^j) T_\alpha^{ik} \right\} \; dv \\
+\;& \int\limits_{\sigma(t)} \left[(x^i - y_0^i) T_\alpha^{jk} - (x^j - y_0^j) T_\alpha^{ik} \right]_-^+ n^k \; da \\
=\;& \left[\int\limits_{v \setminus \sigma(t)} (\mathbf{T}_\alpha^T - \mathbf{T}_\alpha) \;+\; (\vec{x} - \vec{y}_0) \wedge \operatorname{div} \mathbf{T}_\alpha \; dv \right]^{ij} + \left[\int\limits_{\sigma(t)} \left[(\vec{x} - \vec{y}_0) \wedge \mathbf{T}_\alpha \right]_-^+ \cdot \vec{n} \; da \right]^{ij} \ .
\end{aligned}$$

Equation (3.47) can be rewritten as follows:

$$\begin{aligned}
\mathbf{0} \;=\; \int\limits_{v \setminus \sigma(t)} (\mathbf{T}_\alpha - \mathbf{T}_\alpha^T) \; dv \;&+\; \int\limits_{v \setminus \sigma(t)} (\vec{x} - \vec{y}_0) \wedge \left\{ \rho_\alpha {\grave{\vec{v}}_\alpha}{}^{\alpha} - \operatorname{div} \mathbf{T}_\alpha - \vec{k}_\alpha - \rho_\alpha \vec{b}_\alpha \right\} \; dv \; + \\
&+\; \int\limits_{\sigma(t)} (\vec{x} - \vec{y}_0) \wedge \left(\left[\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu}) - \mathbf{T}_\alpha \right]_-^+ \cdot \vec{n} \;-\; \vec{f}^S_\alpha \right) \; da \ ,
\end{aligned}$$

---

[2] We have chosen the component description for the sake of brevity.

where in the last term on the right-hand side the continuity of $(\vec{x}-\vec{y}_0)$ at the singular surface $\sigma(t)$ has been considered. Inspecting the linear-momentum balance and the boundary condition (3.41), we can see that the second and the third integral vanish, hence we conclude that

$$\int\limits_{v\setminus\sigma(t)} (\mathbf{T}_\alpha - \mathbf{T}_\alpha^T)\; dv \;=\; \mathbf{0}\;. \tag{3.48}$$

Since the material volume v was chosen arbitrarily, we obtain

$$\boxed{\mathbf{T}_\alpha = \mathbf{T}_\alpha^T \qquad\qquad \text{in} \qquad\qquad v\setminus\sigma(t)\;.} \tag{3.49}$$

The balance of angular momentum of a mixture in material volume v is postulated in the following form:

$$\sum_{\alpha=1}^{n}\frac{D_\alpha}{Dt}\int\limits_{v}(\vec{x}-\vec{y}_0)\wedge\rho_\alpha\vec{v}_\alpha\; dv \;=\; \sum_{\alpha=1}^{n}\int\limits_{\partial v}(\vec{x}-\vec{y}_0)\wedge\mathbf{T}_\alpha\cdot\vec{n}\; da + \sum_{\alpha=1}^{n}\int\limits_{v}(\vec{x}-\vec{y}_0)\wedge\rho_\alpha\vec{b}_\alpha\; dv\;. \tag{3.50}$$

Applying (3.37), we derive

$$\begin{aligned}\sum_{\alpha=1}^{n}\frac{D_\alpha}{Dt}\int\limits_{v}(\vec{x}-\vec{y}_0)\wedge\rho_\alpha\vec{v}_\alpha\; dv \;&=\; \int\limits_{v\setminus\sigma(t)}(\vec{x}-\vec{y}_0)\wedge\left(\sum_{\alpha=1}^{n}\rho_\alpha\grave{\vec{v}}_\alpha^{\;\alpha}\right) dv \;+\\ +\int\limits_{v\setminus\sigma(t)}(\vec{x}-\vec{y}_0)\wedge\left(\sum_{\alpha=1}^{n}r_\alpha\vec{v}_\alpha\right) dv \;&+\; \int\limits_{\sigma(t)}\left[(\vec{x}-\vec{y}_0)\wedge\sum_{\alpha=1}^{n}\{\rho_\alpha\vec{v}_\alpha\otimes(\vec{v}_\alpha-\vec{\nu})\}\right]_-^+\cdot\vec{n}\; da\;.\end{aligned}$$

Following the procedure for a one-component body, we obtain

$$\begin{aligned}\sum_{\alpha=1}^{n}\int\limits_{\partial v}(\vec{x}-\vec{y}_0)\wedge\mathbf{T}_\alpha\cdot\vec{n}\; da \;=\; &\int\limits_{v\setminus\sigma(t)}\sum_{\alpha=1}^{n}(\mathbf{T}_\alpha^T-\mathbf{T}_\alpha)\; dv + \int\limits_{v\setminus\sigma(t)}(\vec{x}-\vec{y}_0)\wedge\operatorname{div}\,(\sum_{\alpha=1}^{n}\mathbf{T}_\alpha)\; dv \;+\\ &+\int\limits_{\sigma(t)}\left[(\vec{x}-\vec{y}_0)\wedge\;\sum_{\alpha=1}^{n}\mathbf{T}_\alpha\right]_-^+\cdot\vec{n}\; da\;.\end{aligned} \tag{3.51}$$

After substituting this into (3.50) and rearranging the terms, we arrive at

$$\begin{aligned}\int\limits_{v\setminus\sigma(t)}\sum_{\alpha=1}^{n}(\mathbf{T}_\alpha-\mathbf{T}_\alpha^T)\; dv \;+\; &\int\limits_{v\setminus\sigma(t)}(\vec{x}-\vec{y}_0)\wedge\sum_{\alpha=1}^{n}\left\{\rho_\alpha\grave{\vec{v}}_\alpha^{\;\alpha}+r_\alpha\vec{v}_\alpha\;-\operatorname{div}\,\mathbf{T}_\alpha-\rho_\alpha\vec{b}_\alpha\right\}\; dv \;+\\ +\; &\int\limits_{\sigma(t)}(\vec{x}-\vec{y}_0)\wedge\left[\sum_{\alpha=1}^{n}\rho_\alpha\vec{v}_\alpha\otimes(\vec{v}_\alpha-\vec{\nu})-\mathbf{T}_\alpha\right]_-^+\cdot\vec{n}\; da \;=\; \mathbf{0}\;,\end{aligned}$$

where we have used the continuity of $(\vec{x}-\vec{y}_0)$ across the singular surface $\sigma(t)$. In view of (3.44), we finally obtain the angular momentum balance for a mixture

$$\int\limits_{v\setminus\sigma(t)}\sum_{\alpha=1}^{n}(\mathbf{T}_\alpha-\mathbf{T}_\alpha^T)\; dv \;=\; \mathbf{0}\;, \tag{3.52}$$

but this is a trivial result of the angular momentum balance for components (3.49).

3.6 Energy balance of a mixture

To formulate the energy-balance principle, we first introduce the following quantities:

- *Internal energy* ε_α
- *Partial heat flux* $\vec{q}_\alpha$
- *Internal heating* Q_α
- *Volume interaction energy* e_α
- *Surface energy production* e^S_α

The energy balance for the α-component of a mixture in material volume v is postulated as

$$\begin{aligned}\frac{D_\alpha}{Dt}\int\limits_v \rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,{\vec{v}_\alpha}^2)\;dv \quad &= \quad \int\limits_{\partial v} \vec{v}_\alpha \cdot \mathbf{T}_\alpha \cdot \vec{n}\;da \;+\; \int\limits_v \rho_\alpha \vec{b}_\alpha \cdot \vec{v}_\alpha\;dv \;+\; \int\limits_v \vec{k}_\alpha \cdot \vec{v}_\alpha\;dv \\ &- \quad \int\limits_{\partial v} \vec{q}_\alpha \cdot \vec{n}\;da \;+\; \int\limits_v Q_\alpha\;dv \;+\; \int\limits_v r_\alpha(\varepsilon_\alpha + \frac{1}{2}\,{\vec{v}_\alpha}^2)\;dv \\ &+ \quad \int\limits_v e_\alpha\;dv \;+\; \int\limits_{\sigma(t)} e^S_\alpha\;da\;, \qquad \alpha = 1,\ldots,n\;. \end{aligned} \tag{3.53}$$

The terms additionally appeared in (3.53) compared to the energy balance of a one-component material (see e.g. Samohýl [1]) are as follows:

- $\int\limits_{v\setminus\sigma(t)} \vec{k}_\alpha \cdot \vec{v}_\alpha\;dv$
  is the power produced by the interaction volume force $\vec{k}_\alpha$,
- $\int\limits_{v\setminus\sigma(t)} e_\alpha\;dv$
  is the volume interaction power,
- $\int\limits_{\sigma(t)} e^S_\alpha\;da$
  is the energy production at the singular surface $\sigma(t)$, related to the production of the particular component of a mixture at the singular surface $\sigma(t)$,
- $\int\limits_{v\setminus\sigma(t)} r_\alpha(\varepsilon_\alpha + \frac{1}{2}\,{\vec{v}_\alpha}^2)\;dv$
  is the rate of energy change due to compositional changes.

In the handling of (3.53), we proceed in a way analogous to the previous balance laws. First, we make use of the formula (3.37) and rewrite the time derivative of the left-hand side of (3.53) as:

$$\begin{aligned}\frac{D_\alpha}{Dt}\int\limits_v \rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,{\vec{v}_\alpha}^2)\;dv \quad &= \quad \int\limits_{v\setminus\sigma(t)} \rho_\alpha(\grave{\varepsilon}_\alpha{}^{\alpha} + \vec{v}_\alpha \cdot \grave{\vec{v}}_\alpha{}^{\alpha})\;dv \;+\; \int\limits_{v\setminus\sigma(t)} r_\alpha(\varepsilon_\alpha + \frac{1}{2}\,{\vec{v}_\alpha}^2)\;dv \;+ \\ &+ \quad \int\limits_{\sigma(t)} \Big[\rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,{\vec{v}_\alpha}^2)(\vec{v}_\alpha - \vec{\nu})\Big]^+_- \cdot \vec{n}\;da\;. \end{aligned} \tag{3.54}$$

We now use the Gauss theorem (3.24) and express the surface integral as[3]

$$\begin{aligned}\int\limits_{\partial v} \vec{v}_\alpha \cdot \mathbf{T}_\alpha \cdot \vec{n}\; da \;&=\; \int\limits_{\partial v} v^i_\alpha T^{ij}_\alpha n^j\; da \;=\; \int\limits_{v\backslash\sigma(t)} \frac{\partial}{\partial x^j}(v^i_\alpha T^{ij}_\alpha)\; dv \;+\; \int\limits_{\sigma(t)} \Big[v^i_\alpha T^{ij}_\alpha\Big]^+_- n^j\; da \\ &= \int\limits_{v\backslash\sigma(t)} \frac{\partial v^i_\alpha}{\partial x^j} T^{ij}_\alpha\; dv \;+\; \int\limits_{v\backslash\sigma(t)} v^i_\alpha \frac{\partial T^{ij}_\alpha}{\partial x^j}\; dv \;+\; \int\limits_{\sigma(t)} \Big[v^i_\alpha T^{ij}_\alpha\Big]^+_- n^j\; da \\ &= \int\limits_{v\backslash\sigma(t)} \mathbf{L}_\alpha : \mathbf{T}_\alpha\; dv \;+\; \int\limits_{v\backslash\sigma(t)} \vec{v}_\alpha \cdot \mathrm{div}\; \mathbf{T}_\alpha\; dv \;+\; \int\limits_{\sigma(t)} [\vec{v}_\alpha \cdot \mathbf{T}_\alpha]^+_- \cdot \vec{n}\; da\;,\end{aligned} \tag{3.55}$$

where $\mathbf{L}_\alpha = \mathrm{grad}\; \vec{v}_\alpha$ is the velocity gradient and the symbol $:$ denotes the double-dot product of second-order tensors:

$$\mathbf{A} : \mathbf{B} \;\equiv\; A^{ij}\; B^{ij}. \tag{3.56}$$

Analogously, from the Gauss theorem (3.24), we obtain

$$\int\limits_{\partial v} \vec{q}_\alpha \cdot \vec{n}\; da \;=\; \int\limits_{v\backslash\sigma(t)} \mathrm{div}\; \vec{q}_\alpha\; dv \;+\; \int\limits_{\sigma(t)} [q_\alpha]^+_- \cdot \vec{n}\; da\;. \tag{3.57}$$

Substituting (3.54), (3.55) and (3.57) into (3.53) yields

$$\begin{aligned} 0 \;&=\; \int\limits_{v\backslash\sigma(t)} \Big\{\rho_\alpha \grave{\varepsilon}_\alpha{}^{\alpha} - \mathbf{T}_\alpha : \mathbf{L}_\alpha + \mathrm{div}\; \vec{q}_\alpha - Q_\alpha - e_\alpha + \vec{v}_\alpha \cdot (\rho_\alpha \grave{\vec{v}}_\alpha{}^{\alpha} - \mathrm{div}\; \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha - \vec{k}_\alpha)\Big\}\; dv \\ &+\; \int\limits_{\sigma(t)} \left(\Big[\rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\; \vec{v}_\alpha^{\,2})(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha + \vec{q}_\alpha\Big]^+_- \cdot \vec{n} \;-\; e^S_\alpha\right)\; da\;. \end{aligned}$$

With the help of the linear momentum balance of the α-component (3.41), this equation further reduces to

$$\begin{aligned} 0 \;&=\; \int\limits_{v\backslash\sigma(t)} \{\rho_\alpha \grave{\varepsilon}_\alpha{}^{\alpha} - \mathbf{T}_\alpha : \mathbf{L}_\alpha + \mathrm{div}\; \vec{q}_\alpha - Q_\alpha - e_\alpha\}\; dv \\ &+\; \int\limits_{\sigma(t)} \left(\Big[\rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\; \vec{v}_\alpha^{\,2})(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha + \vec{q}_\alpha\Big]^+_- \cdot \vec{n} \;-\; e^S_\alpha\right)\; da\;. \end{aligned}$$

Since the material volume v was chosen arbitrarily, we conclude that

$$\boxed{\begin{array}{rcllr} \rho_\alpha \grave{\varepsilon}_\alpha{}^{\alpha} &=& \mathbf{T}_\alpha : \mathbf{D}_\alpha - \mathrm{div}\; \vec{q}_\alpha + Q_\alpha + e_\alpha & \text{in} & v \setminus \sigma(t)\;, \\ e^S_\alpha &=& \Big[\rho_\alpha(\varepsilon_\alpha + \tfrac{1}{2}\; \vec{v}_\alpha^{\,2})(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha + \vec{q}_\alpha\Big]^+_- \cdot \vec{n} & \text{at} & \sigma(t)\;, \end{array}} \tag{3.58}$$

---

[3] To make the derivation transparent, we use the componental description.

where we have used the symmetry of the Cauchy stress tensor to write

$$\mathbf{T}_\alpha : \mathbf{L}_\alpha \;=\; \mathbf{T}_\alpha : (\mathbf{L}_\alpha^{sym.} + \mathbf{L}_\alpha^{antis.}) = \mathbf{T}_\alpha : \mathbf{L}_\alpha^{sym.} = \mathbf{T}_\alpha : \mathbf{D}_\alpha \; . \tag{3.59}$$

Now we postulate the energy balance of a mixture

$$\begin{aligned}\sum_{\alpha=1}^{n} \frac{D_\alpha}{Dt} \int_v \rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha^{\,2})\; dv \;\; &= \;\; \sum_{\alpha=1}^{n} \int_{\partial v} \vec{v}_\alpha \cdot\; \mathbf{T}_\alpha \cdot \vec{n}\; da \;+ \sum_{\alpha=1}^{n} \int_v \vec{v}_\alpha \cdot \rho_\alpha \vec{b}_\alpha \; dv \;- \\ &- \int_{\partial v} \vec{q} \cdot \vec{n}\; da \;+\; \int_v Q\; dv \;,\end{aligned} \tag{3.60}$$

where we have defined

- *Total heat flux* $\vec{q}$

$$\vec{q} \;=\; \sum_{\alpha=1}^{n} \vec{q}_\alpha \;, \tag{3.61}$$

- *Total internal heating* Q

$$Q \;=\; \sum_{\alpha=1}^{n} Q_\alpha \;. \tag{3.62}$$

Similarly to (3.54), the left-hand side of (3.60) may be rewritten as

$$\begin{aligned}\sum_{\alpha=1}^{n} \frac{D_\alpha}{Dt} \int_v \rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha^{\,2})\; dv \;&=\; \int_{v\backslash\sigma(t)} \sum_{\alpha=1}^{n} \rho_\alpha(\grave{\varepsilon}_\alpha^{\;\alpha} + \vec{v}_\alpha \cdot \grave{\vec{v}}_\alpha^{\;\alpha})\; dv \;+ \\ + \int_{v\backslash\sigma(t)} \sum_{\alpha=1}^{n} r_\alpha(\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha^{\,2})\; dv \;&+ \int_{\sigma(t)} \sum_{\alpha=1}^{n} \Big[\rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha^{\,2})(\vec{v}_\alpha - \vec{\nu})\Big]_-^+ \cdot \vec{n}\; da \;.\end{aligned} \tag{3.63}$$

With the help of (3.55) and (3.59), the surface integral on the right-hand side of (3.60) is

$$\begin{aligned}\sum_{\alpha=1}^{n} \int_{\partial v} \vec{v}_\alpha \cdot\; \mathbf{T}_\alpha \cdot \vec{n}\; da \;\; &= \;\; \int_{v\backslash\sigma(t)} \sum_{\alpha=1}^{n} (\mathbf{D}_\alpha : \mathbf{T}_\alpha)\; dv \;+\; \int_{v\backslash\sigma(t)} \sum_{\alpha=1}^{n} (\vec{v}_\alpha \cdot \mathrm{div}\; \mathbf{T}_\alpha)\; dv \;+ \\ &+ \int_{\sigma(t)} \sum_{\alpha=1}^{n} [\vec{v}_\alpha \cdot \mathbf{T}_\alpha]_-^+ \cdot \vec{n}\; da \;.\end{aligned} \tag{3.64}$$

Also, from the Gauss theorem (3.24), we have

$$\int_{\partial v} \vec{q} \cdot \vec{n}\; da \;=\; \int_{v\backslash\sigma(t)} \mathrm{div}\; \vec{q}\; dv \;+\; \int_{\sigma(t)} [q]_-^+ \cdot \vec{n}\; da \;. \tag{3.65}$$

Substituting (3.63), (3.64) and (3.65) into (3.60) gives

$$\begin{aligned} 0 \;=\; \int_{v\backslash\sigma(t)} \left(\sum_{\alpha=1}^{n} \Big\{ \rho_\alpha \grave{\varepsilon}_\alpha^{\;\alpha} - \mathbf{T}_\alpha : \mathbf{D}_\alpha + \vec{v}_\alpha \cdot (\rho_\alpha \grave{\vec{v}}_\alpha^{\;\alpha} - \mathrm{div}\; \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha) \Big\} + \mathrm{div}\; \vec{q} - Q \right) dv \;+ \\ \int_{v\backslash\sigma(t)} \sum_{\alpha=1}^{n} \Big\{ r_\alpha(\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha^{\,2}) \Big\}\; dv \;+\; \int_{\sigma(t)} \Bigg[\sum_{\alpha=1}^{n} \Big\{ \rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha^{\,2})(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha \Big\} + \vec{q} \Bigg]_-^+ \cdot \vec{n}\; da \;. \end{aligned}$$

The term in parenthesis standing at $\vec{v}_\alpha\cdot$ in the first volume integral is equal to $\vec{k}_\alpha$ due to the linear momentum balance (3.41). Finally, postulating, that this result is valid for any arbitrary material volume v, we get

$$\boxed{\begin{array}{rclll} 0 & = & \sum\limits_{\alpha=1}^{n}\left\{\rho_\alpha \grave{\varepsilon}_\alpha{}^\alpha - \mathbf{T}_\alpha : \mathbf{D}_\alpha + \vec{v}_\alpha\cdot\vec{k}_\alpha + r_\alpha\varepsilon_\alpha + \tfrac{1}{2}\, r_\alpha \vec{v}_\alpha{}^2\right\} + \operatorname{div}\vec{q} - Q & \text{in} & v\setminus\sigma(t)\ , \\ 0 & = & \left[\sum\limits_{\alpha=1}^{n}\left\{\rho_\alpha(\varepsilon_\alpha + \tfrac{1}{2}\,\vec{v}_\alpha{}^2)(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha\cdot\mathbf{T}_\alpha\right\} + \vec{q}\right]_-^+ \cdot\vec{n} & \text{at} & \sigma(t)\ . \end{array}}$$

(3.66)

By summation of (3.58), we obtain

$$\begin{aligned} 0 &= \sum_{\alpha=1}^{n}\left\{\rho_\alpha \grave{\varepsilon}_\alpha{}^\alpha - \mathbf{T}_\alpha : \mathbf{D}_\alpha + \operatorname{div}\vec{q}_\alpha - Q_\alpha - e_\alpha\right\}, \\ 0 &= \sum_{\alpha=1}^{n}\left(\left[\rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha{}^2)(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha\cdot\mathbf{T}_\alpha + \vec{q}_\alpha\right]_-^+ \cdot\vec{n} \;-\; e_\alpha^S\right)\ . \end{aligned}$$

Subtracting these equation from (3.66) and with the use of (3.61) and (3.62) yields

$$\sum_{\alpha=1}^{n}\left\{e_\alpha + \vec{v}_\alpha\cdot\vec{k}_\alpha + r_\alpha\varepsilon_\alpha + \frac{1}{2}\, r_\alpha\vec{v}_\alpha{}^2\right\} = 0 \qquad \text{in} \qquad v\setminus\sigma(t)\ , \tag{3.67}$$

$$\sum_{\alpha=1}^{n} e_\alpha^S = 0 \qquad \text{at} \qquad \sigma(t)\ . \tag{3.68}$$

For the following, we express the first equation in terms of the diffusion velocity (3.19) ($\vec{u}_\alpha = \vec{v}_\alpha - \vec{v}_n$) as:

$$\begin{aligned} &\sum_{\alpha=1}^{n}\vec{v}_\alpha\cdot\vec{k}_\alpha + \frac{1}{2}\sum_{\alpha=1}^{n} r_\alpha\vec{v}_\alpha{}^2 \\ &= \sum_{\alpha=1}^{n}(\vec{v}_n + \vec{u}_\alpha)\cdot\vec{k}_\alpha + \frac{1}{2}\sum_{\alpha=1}^{n} r_\alpha\,(\vec{v}_n{}^2 + 2\vec{v}_n\cdot\vec{u}_\alpha + \vec{u}_\alpha{}^2) \\ &= \vec{v}_n\cdot\sum_{\alpha=1}^{n}(\vec{k}_\alpha + r_\alpha\,\underbrace{\vec{u}_\alpha}_{\vec{v}_\alpha-\vec{v}_n}) + \sum_{\alpha=1}^{n}\vec{u}_\alpha\cdot\vec{k}_\alpha + \frac{1}{2}\,\vec{v}_n{}^2\sum_{\alpha=1}^{n} r_\alpha + \frac{1}{2}\sum_{\alpha=1}^{n} r_\alpha\vec{u}_\alpha{}^2 \\ &= \vec{v}_n\cdot\sum_{\alpha=1}^{n}(\vec{k}_\alpha + r_\alpha\vec{v}_\alpha) - \frac{1}{2}\,\vec{v}_n{}^2\sum_{\alpha=1}^{n} r_\alpha + \sum_{\alpha=1}^{n}\vec{u}_\alpha\cdot\vec{k}_\alpha + \frac{1}{2}\sum_{\alpha=1}^{n} r_\alpha\vec{u}_\alpha{}^2 \\ &= \sum_{\alpha=1}^{n}\vec{u}_\alpha\cdot\vec{k}_\alpha + \frac{1}{2}\sum_{\alpha=1}^{n} r_\alpha\vec{u}_\alpha{}^2 \\ &= \sum_{\beta=1}^{n-1}\vec{u}_\beta\cdot\vec{k}_\beta + \frac{1}{2}\sum_{\beta=1}^{n-1} r_\beta\vec{u}_\beta{}^2\ , \end{aligned} \tag{3.69}$$

where we have used the constraints $\sum\limits_{\alpha=1}^{n} r_\alpha = 0$, $\sum\limits_{\alpha=1}^{n}(\vec{k}_\alpha + r_\alpha\vec{v}_\alpha) = \vec{0}$, $\vec{u}_n = \vec{0}$, according to (3.32), (3.45) and (3.19), respectively.

To conclude, the energy-balance of a mixture can be rewritten as

$$\boxed{\begin{array}{lll} 0 = \sum\limits_{\alpha=1}^{n} \{e_\alpha + r_\alpha \varepsilon_\alpha\} + \sum\limits_{\beta=1}^{n-1} \left\{\vec{u}_\beta \cdot \vec{k}_\beta + \frac{1}{2}\, r_\beta \vec{u}_\beta^{\,2}\right\} & \text{in} & v \setminus \sigma(t)\ , \\ 0 = \sum\limits_{\alpha=1}^{n} e_\alpha^S & \text{at} & \sigma(t)\ . \end{array}} \tag{3.70}$$

3.7 Entropy balance in a mixture

In this section, we will introduce several new quantities:

- *entropy density* s_α,
- *absolute temperature* T,

and postulate the entropy balance (the Clausius-Duham) inequality of a mixture in material volume v as follows

$$\sum_{\alpha=1}^{n} \frac{D_\alpha}{Dt} \int_v \rho_\alpha s_\alpha \, dv \geq -\int_{\partial v} \frac{1}{T}\, \vec{q} \cdot \vec{n}\, da + \int_{v \setminus \sigma(t)} \frac{Q}{T}\, dv\ . \tag{3.71}$$

Making use of (3.37) and the Gauss theorem (3.24), we arrive at

$$0 \leq \int_{v\setminus\sigma(t)} \left\{ \sum_{\alpha=1}^{n} \rho_\alpha \grave{s}_\alpha{}^\alpha + \sum_{\alpha=1}^{n} r_\alpha s_\alpha + \operatorname{div}\left(\frac{\vec{q}}{T}\right) - \frac{Q}{T} \right\} dv \ +$$

$$+ \int_{\sigma(t)} \left[\sum_{\alpha=1}^{n} \rho_\alpha s_\alpha (\vec{v}_\alpha - \vec{\nu}) + \frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n}\, da\ . \tag{3.72}$$

Since the material volume v was chosen arbitrarily, we may conclude that

$$\sum_{\alpha=1}^{n} \rho_\alpha \grave{s}_\alpha{}^\alpha + \sum_{\alpha=1}^{n} r_\alpha s_\alpha + \operatorname{div}\left(\frac{\vec{q}}{T}\right) - \frac{Q}{T} \ \geq\ 0 \qquad \text{in} \qquad v \setminus \sigma(t)\ , \tag{3.73}$$

$$\left[\sum_{\alpha=1}^{n} \rho_\alpha s_\alpha (\vec{v}_\alpha - \vec{\nu}) + \frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n} \ \geq\ 0 \qquad \text{at} \qquad \sigma(t)\ . \tag{3.74}$$

We now employ the energy balance of a mixture (3.66) and the formula (3.69) to express

$$\operatorname{div} \vec{q} - Q = -\sum_{\alpha=1}^{n} \rho_\alpha \grave{\varepsilon}_\alpha{}^\alpha - \sum_{\alpha=1}^{n} r_\alpha \varepsilon_\alpha + \sum_{\alpha=1}^{n} \mathbf{D}_\alpha : \mathbf{T}_\alpha - \sum_{\beta=1}^{n-1} \vec{u}_\beta \cdot \vec{k}_\beta - \frac{1}{2} \sum_{\beta=1}^{n-1} r_\beta \vec{u}_\beta^{\,2}\ .$$

Substituting this expression into the entropy inequality (3.73) yields

$$0 \ \leq\ \frac{1}{T} \left\{ -\sum_{\alpha=1}^{n} \rho_\alpha \grave{\varepsilon}_\alpha{}^\alpha - \sum_{\alpha=1}^{n} r_\alpha \varepsilon_\alpha + \sum_{\alpha=1}^{n} \mathbf{D}_\alpha : \mathbf{T}_\alpha - \sum_{\beta=1}^{n-1} \vec{u}_\beta \cdot \vec{k}_\beta - \frac{1}{2} \sum_{\beta=1}^{n-1} r_\beta \vec{u}_\beta^{\,2} \right\} +$$

$$+ \sum_{\alpha=1}^{n} \rho_\alpha \grave{s}_\alpha{}^\alpha + \sum_{\alpha=1}^{n} r_\alpha s_\alpha - \frac{1}{T^2} \operatorname{grad} T \cdot \vec{q} \qquad \text{in} \qquad v \setminus \sigma(t)\ . \tag{3.75}$$

Multiplying this inequality with $-T$ and introducing a new field variable

- *Free energy of the α-component*

$$f_\alpha \;=\; \varepsilon_\alpha - T s_\alpha \;, \qquad\qquad \alpha = 1, \ldots, n \;, \tag{3.76}$$

gives the Clausius-Duham inequality in the following form

$$\boxed{\begin{aligned} 0 \quad \geq \quad & \sum_{\alpha=1}^{n} \rho_\alpha \grave{f}_\alpha{}^{\alpha} + \sum_{\alpha=1}^{n} r_\alpha f_\alpha + \sum_{\alpha=1}^{n} \rho_\alpha s_\alpha \grave{T}^{\alpha} + T^{-1}\mathrm{grad}\, T \cdot \vec{q} - \sum_{\alpha=1}^{n} \mathbf{D}_\alpha : \mathbf{T}_\alpha \\ + \quad & \sum_{\beta=1}^{n-1} \vec{k}_\beta \cdot \vec{u}_\beta + \frac{1}{2} \sum_{\beta=1}^{n-1} r_\beta \vec{u}_\beta^{\,2} \qquad\qquad \text{in} \qquad v \setminus \sigma(t) \;. \end{aligned}} \tag{3.77}$$

3.8 Constitutive equations of a mixture

Note: It is not the aim of this section to provide an exhaustive description of the constitutive theory of mixtures, since it would require much more effort and moreover it is not a subject of this text. However, the basic concepts have to be outlined to enable the following derivations. This section, more than any other in this chapter, would probably require further reading, e.g. the textbook by Samohýl [1]).

The independent balance laws listed above, namely the mass balance of the components and the mixture, the linear-momenta balance of the components and the mixture, the angular-momenta balance of the components, and the balance of energy of the mixture, together with the entropy inequality, do not suffice to determine the thermo-mechanical behaviour of the mixture[4]. The missing equations should specify the material class by adding relationships among the kinematic, mechanical and thermal field variables. This task is handled by the *constitutive theory.*

A *process* is defined as a set of all the fields that appear in the theory:

$$\chi_\alpha(X_\alpha, t),\; \rho_\alpha(X_\alpha, t),\; T(X_\alpha, t), \tag{3.78}$$

$$r_\alpha(\vec{x}, t),\; \varepsilon_\alpha(\vec{x}, t),\; s_\alpha(\vec{x}, t),\; \vec{q}(\vec{x}, t),\; \vec{k}_\alpha(\vec{x}, t),\; \mathbf{T}_\alpha(\vec{x}, t), \tag{3.79}$$

$$Q(\vec{x}, t),\; \vec{b}_\alpha(\vec{x}, t), \qquad\qquad \alpha \;=\; 1, \ldots, n \;. \tag{3.80}$$

A *thermodynamic process* is such a process that satisfies the mass balance of the reacting components, the linear-momenta balance of the components, and the energy balance of the mixture. The validity of the remaining balance laws will be ensured in the following principles of the constitutive theory, namely in the principle of determinism and in the

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[4] The angular momentum balance of the mixture (of non-polar components) follows from the balance of its components, it is therefore not independent. The energy balance for components need not be considered, if all the components have the same temperature. Then the entropy inequality does not constrain interaction energies e_α, and variables $\vec{q}_\alpha$ and Q_α appear in the rest of balance laws only in $\vec{q}$, and Q, respectively (see Samohýl [1]).

entropy principle.

The constitutive theory is based on several axioms, that are listed below.

- **The principle of determinism**
  This postulates that *the constitutive (response) functionals*:
  $$r_\alpha,\ \varepsilon_\alpha,\ s_\alpha,\ \vec{q},\ \vec{k}_\alpha,\ \mathbf{T}_\alpha, \qquad \alpha = 1,\ldots,n\ , \tag{3.81}$$
  at a given location $\vec{x}$ and at the present instant t, depend upon the *thermo-kinetic process*, i.e. fields of motion (relative to the configuration κ_γ), density of the components and temperature:
  $$\vec{\chi}_{\kappa\gamma}(\vec{X}_\gamma,\tau),\ \rho_\gamma(\vec{X}_\gamma,\tau),\ T(\vec{X}_\gamma,\tau)\ , \qquad \tau \le t,\ \gamma = 1,\ldots,n\ , \tag{3.82}$$
  for which the mass balance of the non-reacting components and the mixture, the linear-momentum balance of the mixture and the angular-momenta balance of the components are satisfied.

- **The principle of local action**
  states, that the responses (3.81) for a material particle at $\vec{x}$ are most affected by the values of fields (3.82) is the closest neighborhood of $\vec{x}$.

- **The principle of differential memory**
  states that the responses (3.81) are most affected by the values of fields (3.82) at the present time and in the nearest past.

The last two principles enable us to reduce the functional form of (3.81) to a function of the Taylor expansion series of the fields (3.82). The order of the expansion specifies a particular material class.

- **The principle of equipresence**
  states that the set of independent variables, i.e. the set of appropriate Taylor expansion terms of (3.82), is the same for all response functionals (3.81) unless other constitutive principles constrain that.

In particular, we are interested in the material class called *a mixture of non-simple materials with differential memory*:
$$\{r_\psi, \varepsilon_\alpha, s_\alpha, \vec{q}, \vec{k}_\beta, \mathbf{T}_\alpha\} = \mathcal{F}_\kappa[\vec{x}, \mathbf{F}_{\kappa\gamma}, \mathbf{G}_{\kappa\gamma}, \mathbf{L}_\gamma, \vec{v}_\gamma, \rho_\varphi, \vec{h}_\varphi, T, \vec{g}, X_\gamma, t]\ ,$$
$$\psi = 1,\ldots,m-1;\quad \varphi = 1,\ldots,m;\quad \beta = 1,\ldots,n-1;\quad \alpha,\gamma = 1,\ldots,n\ ,$$
where we denoted:

- $\vec{x}$ ... *present position of the material particle,*
- $\mathbf{F}_{\kappa\gamma}$ ... *deformation gradient – see (3.1),*
- $\mathbf{G}_{\kappa\gamma}$ ... *second deformation gradient – see (3.2),*
- $\mathbf{L}_\gamma$ ... *velocity gradient – see (3.15),*
- $\vec{v}_\gamma$ ... *velocity of a material particle,*
- ρ_φ ... *density of a reacting component,*
- $\vec{h}_\varphi$ ... *density gradient of a reacting component,*

$$\vec{h}_\varphi = \text{grad}\ \rho_\varphi(\vec{x},t)\ , \tag{3.83}$$

- T ... *absolute temperature,*
- $\vec{g}$ ... *temperature gradient,*

$$\vec{g} \;=\; \mathrm{grad}\, T(\vec{x}, t) \ , \tag{3.84}$$

- X_γ ... *material particle,*
- t ... *present time,*
- m ... *number of reacting components, i.e.* $r_\epsilon \not\equiv 0$ *for* $\epsilon \in (1 \dots m)$.

- **The principle of objectivity**
  states that the shape of constitutive functionals $\mathcal{F}_\kappa$ does not depend on a change of the present frame. The general relation of two Cartesian frames can be expressed as[5]:

$$\vec{x}^* \;=\; \vec{c}(t) + \mathbf{Q}(t)\vec{\chi}_\alpha(\vec{X}_\alpha, t) \ , \tag{3.85}$$

and

$$t^* \;=\; t + b \ , \tag{3.86}$$

where $\mathbf{Q}$ is a member of the group of all orthogonal second-order tensors (*Orth*)

$$\mathbf{Q}(t) \in Orth : \qquad \mathbf{Q}(t)\mathbf{Q}^T(t) = \mathbf{Q}^T(t)\mathbf{Q}(t) = \mathbf{1} \ . \tag{3.87}$$

The velocity then transforms as

$$\vec{v}^*_\alpha \;=\; \mathbf{Q}(t)\vec{v}_\alpha + \dot{\vec{c}} + \mathbf{\Lambda}(\vec{x}^* - \vec{c}) \ , \qquad \text{with} \qquad \mathbf{\Lambda} = \dot{\mathbf{Q}}\mathbf{Q}^T \ . \tag{3.88}$$

The principle of objectivity asserts that

$$\begin{aligned} &\{r_\psi, \varepsilon_\alpha, s_\alpha, \mathbf{Q}\vec{q}, \mathbf{Q}\vec{k}_\beta, \mathbf{Q}\mathbf{T}_\alpha\mathbf{Q}^T\} \;= \\ &\mathcal{F}_\kappa[\vec{c} + \mathbf{Q}\vec{x}, \mathbf{Q}\mathbf{F}_{\kappa\gamma}, \mathbf{Q}\mathbf{G}_{\kappa\gamma}, \mathbf{Q}\mathbf{L}_\gamma\mathbf{Q}^T + \mathbf{\Lambda}, \mathbf{Q}\vec{v}_\gamma + \dot{\vec{c}} + \mathbf{\Lambda}\mathbf{Q}\vec{x}, \rho_\varphi, \mathbf{Q}\vec{h}_\varphi, T, \mathbf{Q}\vec{g}, X_\gamma, t + b] \ , \end{aligned}$$

for any arbitrary scalar b, vectors $\vec{c}$ and $\dot{\vec{c}}$, orthogonal tensor $\mathbf{Q}$ and antisymmetric tensor $\mathbf{\Lambda}$. It can be shown, see Samohýl [1], that this constraint reduces the dependence of the constitutive functionals to the following form

$$\{r_\psi, \varepsilon_\alpha, s_\alpha, \vec{q}, \vec{k}_\beta, \mathbf{T}_\alpha\} = \mathcal{F}_\kappa[\mathbf{F}_{\kappa\gamma}, \mathbf{G}_{\kappa\gamma}, \mathbf{D}_\gamma, \mathbf{\Omega}_\delta, \vec{u}_\delta, \rho_\varphi, \vec{h}_\varphi, T, \vec{g}, X_\gamma] \ , \tag{3.89}$$

$$\psi = 1, \dots, m-1; \quad \varphi = 1, \dots, m; \quad \beta, \delta = 1, \dots, n-1; \quad \alpha, \gamma = 1, \dots, n \ ,$$

satisfying

$$\begin{aligned} &\{r_\psi, \varepsilon_\alpha, s_\alpha, \mathbf{Q}\vec{q}, \mathbf{Q}\vec{k}_\beta, \mathbf{Q}\mathbf{T}_\alpha\mathbf{Q}^T\} \;= \\ &\mathcal{F}_\kappa[\mathbf{Q}\mathbf{F}_{\kappa\gamma}, \mathbf{Q}\mathbf{G}_{\kappa\gamma}, \mathbf{Q}\mathbf{D}_\gamma\mathbf{Q}^T, \mathbf{Q}\mathbf{\Omega}_\delta\mathbf{Q}^T, \mathbf{Q}\vec{u}_\delta, \rho_\varphi, \mathbf{Q}\vec{h}_\varphi, T, \mathbf{Q}\vec{g}, X_\gamma] \ , \end{aligned} \tag{3.90}$$

for any orthogonal tensor $\mathbf{Q}$.

Analogously to one-component materials, we can deal with the changes of the reference configuration and introduce the **symmetry groups** of a mixture:

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[5] Vectors are considered here as triplets of coordinates related to a "static" frame.

- *for a reacting component*, $\epsilon \in (1, \ldots, m)$, we define the symmetry group $\mathcal{G}_{\kappa\epsilon}$

$$(\mathbf{H}, \mathbf{J}) \in \mathcal{G}_{\kappa\epsilon} \Longleftrightarrow \mathcal{F}_{\kappa}[\mathbf{F}_{\kappa\epsilon}, \mathbf{G}_{\kappa\epsilon}, \Theta_{\epsilon}, X_{\epsilon}] = \mathcal{F}_{\kappa}[(\mathbf{F}_{\kappa\epsilon}, \mathbf{G}_{\kappa\epsilon}) \circ (\mathbf{H}, \mathbf{J}), \Theta_{\epsilon}, X_{\epsilon}] \ , \qquad (3.91)$$

where $\mathbf{H}$ is a regular second-order tensor and $\mathbf{J}$ is a third-order tensor symmetric in last two indices. For the sake of brevity, we have denoted

$$\Theta_{\epsilon} = [\mathbf{F}_{\kappa\gamma\neq\epsilon}, \mathbf{G}_{\kappa\gamma\neq\epsilon}, \mathbf{D}_{\gamma}, \mathbf{\Omega}_{\delta}, \vec{u}_{\delta}, \rho_{\varphi}, \vec{h}_{\varphi}, T, \vec{g}, X_{\gamma\neq\epsilon}] \ ,$$

$$\gamma = 1, \ldots, n; \quad \delta = 1, \ldots, n-1; \quad \varphi = 1, \ldots, m \ .$$

The group $\mathcal{G}_{\kappa\epsilon}$ is a subgroup of a group of all ordered couples $(\mathbf{P}, \mathbf{K})$ of arbitrary regular second-order tensors $\mathbf{P}$ and arbitrary third-order tensors $\mathbf{K}$, symmetric in the last two indices with the group operation $\circ$ defined as

$$(\mathbf{P}_3, \mathbf{K}_3) \ = \ (\mathbf{P}_2, \mathbf{K}_2) \circ (\mathbf{P}_1, \mathbf{K}_1) \ ,$$

with

$$\mathbf{P}_3 \ = \ \mathbf{P}_2\mathbf{P}_1, \qquad\qquad \mathbf{K}_3 \ = \ \mathrm{C}(\mathbf{K}_2 \otimes \mathbf{P}_1 \otimes \mathbf{P}_1) + \mathbf{P}_2\mathbf{K}_1 \ .$$

The contracting operator C is defined as

$$\mathrm{C}(\mathbf{A} \otimes \mathbf{B} \otimes \mathbf{D})^{ijk} = A^{ilm} B^{lj} D^{mk} \ .$$

The inverse is defined as

$$(\mathbf{P}, \mathbf{K})^{-1} \ = \ (\mathbf{P}^{-1}, \mathbf{K}^{-1}) \ , \qquad \text{with} \qquad \mathbf{K}^{-1} \ = \ -\mathbf{P}^{-1} C(\mathbf{K} \otimes \mathbf{P}^{-1} \otimes \mathbf{P}^{-1}) \ . \quad (3.92)$$

- *for a non-reacting component* $\epsilon \in (m+1, \ldots, n)$, the definition of the symmetry group is the same as for a reacting component, i.e.

$$(\mathbf{H}, \mathbf{J}) \in \mathcal{G}_{\kappa\varepsilon} \Longleftrightarrow \mathcal{F}_{\kappa}[\mathbf{F}_{\kappa\varepsilon}, \mathbf{G}_{\kappa\varepsilon}, \Theta_{\varepsilon}, X_{\varepsilon}] = \mathcal{F}_{\kappa}[(\mathbf{F}_{\kappa\varepsilon}, \mathbf{G}_{\kappa\varepsilon}) \circ (\mathbf{H}, \mathbf{J}), \Theta_{\varepsilon}, X_{\varepsilon}] \ , \qquad (3.93)$$

but, in addition, the tensors $\mathbf{H}$ and $\mathbf{J}$ must satisfy the relationships

$$|\ \det\mathbf{H}\ | = \ 1 \qquad \ldots \qquad \mathbf{H} \text{ is } \textit{unimodular} \ ,$$

and

$$\mathrm{tr}(\mathbf{H}^{-1}\mathbf{J}) + \vec{a}_{\kappa\varepsilon}(\mathbf{H} - \mathbf{1}) = \vec{0} \ , \qquad (3.94)$$

where

$$\vec{a}_{\kappa\varepsilon} = \rho_{\kappa\varepsilon}^{-1} \mathrm{Grad}_{\kappa\varepsilon}\rho_{\kappa\varepsilon} \ , \qquad (3.95)$$

coming from the constraint on the set of reference configurations representing the material symmetry of non-reacting components:

$$\rho_{\kappa\epsilon} = \rho_{\lambda\epsilon} \ , \qquad \mathrm{Grad}_{\kappa\epsilon}\rho_{\kappa\epsilon} = \mathrm{Grad}_{\lambda\epsilon}\rho_{\lambda\epsilon} \ , \qquad \epsilon \in (m+1, \ldots, n) \ ,$$

which states that we are investigating the symmetry properties only in reference configurations with the same referential density and the density gradient (at the given material point).

Thus, for any component ϵ of a mixture, reacting or non-reacting, we have defined a symmetry group $\mathcal{G}_{\kappa\varepsilon}$ with respect to the reference configuration κ_ε. When the reference configuration is changed to λ_ε, the symmetry group changes according to Noll's rule:

$$\mathcal{G}_{\lambda\epsilon} = (\mathbf{P}_\epsilon, \mathbf{K}_\epsilon) \circ \mathcal{G}_{\kappa\epsilon} \circ (\mathbf{P}_\epsilon, \mathbf{K}_\epsilon)^{-1} \ .$$

- **The entropy principle**

  The balance of entropy introduces additional constraints on the constitutive functionals.

  The entropy principle, according to the interpretation of Coleman and Noll, asserts that the constitutive functionals are such that the reduced entropy inequality (3.77) is satisfied for all *admissible thermodynamic processes*, that is thermodynamic processes taking place in a mixture of non-simple materials with differential memory and constitutive equations (3.89), (3.90). This implies that the following balance laws are satisfied: the mass balance of reacting and non-reacting components and the mixture, linear-momenta balance of components and the mixture, angular-momenta balance of components and the energy balance of the mixture. We will moreover assume that the mixture possesses a homogeneous reference.

The reduced entropy inequality for the non-simple material with differential memory has the form:

$$\begin{aligned}
0 \ \geq \quad & \sum_{\alpha=1}^{n}\sum_{\gamma=1}^{n}\rho_\alpha\frac{\partial f_\alpha}{\partial \mathbf{F}_\gamma} : \grave{\mathbf{F}}^{\alpha}_{\gamma} + \sum_{\alpha=1}^{n}\sum_{\gamma=1}^{n}\rho_\alpha\frac{\partial f_\alpha}{\partial \mathbf{G}_\gamma} : \grave{\mathbf{G}}^{\alpha}_{\gamma} + \sum_{\alpha=1}^{n}\sum_{\gamma=1}^{n}\rho_\alpha\frac{\partial f_\alpha}{\partial \mathbf{D}_\gamma} : \grave{\mathbf{D}}^{\alpha}_{\gamma} \\
+ \ & \sum_{\alpha=1}^{n}\sum_{\delta=1}^{n-1}\rho_\alpha\frac{\partial f_\alpha}{\partial \boldsymbol{\Omega}_\delta} : \grave{\boldsymbol{\Omega}}^{\alpha}_{\delta} + \sum_{\alpha=1}^{n}\sum_{\delta=1}^{n-1}\rho_\alpha\frac{\partial f_\alpha}{\partial \vec{u}_\delta} \cdot \grave{\vec{u}}_{\delta}{}^{\alpha} + \sum_{\alpha=1}^{n}\sum_{\varphi=1}^{m}\rho_\alpha\frac{\partial f_\alpha}{\partial \rho_\varphi}\ \grave{\rho}^{\alpha}_{\varphi} \\
+ \ & \sum_{\alpha=1}^{n}\sum_{\varphi=1}^{m}\rho_\alpha\frac{\partial f_\alpha}{\partial \vec{h}_\varphi} \cdot \grave{\vec{h}}^{\alpha}_{\varphi} + \sum_{\alpha=1}^{n}\rho_\alpha\frac{\partial f_\alpha}{\partial \vec{g}} \cdot \grave{\vec{g}}^{\alpha} + \sum_{\alpha=1}^{n}\rho_\alpha\left(\frac{\partial f_\alpha}{\partial T} + s_\alpha\right)\grave{T}^{\alpha} \\
+ \ & \sum_{\psi=1}^{m-1}(f_\psi - f_m)r_\psi + \frac{1}{T}\ \vec{q}\cdot\vec{g} - \sum_{\alpha=1}^{n}\mathbf{T}_\alpha : \mathbf{D}_\alpha + \sum_{\beta=1}^{n-1}\vec{k}_\beta\cdot\vec{u}_\beta \\
+ \ & \frac{1}{2}\sum_{\psi=1}^{m-1}(\vec{u}_\psi^{\,2} - \vec{u}_m^{\,2})r_\psi \ .
\end{aligned}$$

This inequality can then be rewritten by expanding the material time derivatives $\grave{\psi}^{\gamma}_{\alpha}$, where ψ_α stands for $\mathbf{F}_\alpha, \mathbf{G}_\alpha, \mathbf{D}_\alpha, \boldsymbol{\Omega}_\alpha, \vec{u}_\alpha, \rho_\alpha, \vec{h}_\alpha$, respectively, to a form, containing only the time derivatives of the form $\grave{\psi}^{\alpha}_{\alpha}$ (i.e. $\gamma = \alpha$). The resulting inequality is very complicated and for the sake of brevity we omit it (see Samohýl [1]).

Several new quantities are introduced:

– *Specific free energy of a mixture*

$$f \ = \ \sum_{\alpha=1}^{n}\frac{\rho_\alpha}{\rho}f_\alpha \ , \tag{3.96}$$

- *Specific entropy of a mixture*

$$s \;=\; \sum_{\alpha=1}^{n} \frac{\rho_\alpha}{\rho} s_\alpha \;, \tag{3.97}$$

- *Chemical potential g_φ and quantity $\vec{p}_\varphi$*

$$g_\varphi \;=\; \frac{\partial(\rho f)}{\partial \rho_\varphi} \;, \qquad \vec{p}_\varphi \;=\; \frac{\partial(\rho f)}{\partial \vec{h}_\varphi} \;, \qquad \varphi = 1, \ldots, m \;. \tag{3.98}$$

The rewritten entropy inequality (Samohýl [1]) depends on several independent variables only linearly, but the entropy principle asserts that the inequality is satisfied for all admissible thermodynamic processes, i.e. for any arbitrary choice of the independent variables. Therefore, the coefficients standing at these "linear" variables must vanish. Namely:

- at $\frac{\partial T}{\partial t}$:

$$\frac{\partial f}{\partial T} = -s \;, \tag{3.99}$$

- at $\frac{\partial \vec{g}}{\partial t}$:

$$\frac{\partial f}{\partial \vec{g}} = \vec{0} \;, \tag{3.100}$$

- at $(\grave{\vec{v}}^{\delta}_{\delta} - \grave{\vec{v}}^{n}_{n})$:

$$\frac{\partial f}{\partial \vec{u}_\delta} = \vec{0} \;, \qquad \delta = 1, \ldots, n-1 \;, \tag{3.101}$$

- at $(\grave{\mathbf{F}})^{\gamma}_{\gamma}$:

$$\frac{\partial f}{\partial \mathbf{D}_\gamma} = \mathbf{0} \;, \qquad \frac{\partial f}{\partial \mathbf{\Omega}_\delta} = \mathbf{0} \;, \qquad \gamma = 1, \ldots, n; \;\; \delta = 1, \ldots, n-1 \;. \tag{3.102}$$

Hence, the specific free energy of a mixture depends only upon

$$f = f(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T) \;, \qquad \gamma = 1, \ldots, n; \;\; \varphi = 1, \ldots, m \;, \tag{3.103}$$

in addition, according to (3.98) g_ν, $\vec{p}_\nu$ may be written as:

$$\begin{gathered} g_\nu = g_\nu(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T) \;, \qquad \vec{p}_\nu = \vec{p}_\nu(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T) \;, \\ \gamma = 1, \ldots, n \;, \qquad \nu, \varphi = 1, \ldots, m \;, \end{gathered} \tag{3.104}$$

and due to (3.99) also

$$s = s(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T) \;, \qquad \gamma = 1, \ldots, n; \;\; \varphi = 1, \ldots, m \;, \tag{3.105}$$

Since the definition of the free energy f (3.96), with the use of (3.76), gives

$$f = \varepsilon - Ts \;, \tag{3.106}$$

we can immediately write

$$\varepsilon = \varepsilon(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T) \;, \qquad \gamma = 1, \ldots, n; \;\; \varphi = 1, \ldots, m \;. \tag{3.107}$$

- at grad $\vec{g}$:

  $$A^{ij} + A^{ji} = 0 \ , \tag{3.108}$$

  where

  $$A^{ij} \ = \ \sum_{\delta=1}^{n-1} \rho_\delta \frac{\partial f_\delta}{\partial g^i} u_\delta^j + \sum_{\psi=1}^{m-1} (p_\psi^j - p_m^j) \frac{\partial r_\psi}{\partial g^i} \ ,$$

- at Grad $\vec{d}_\varphi$:

  $$N_\varphi^{ij} + N_\varphi^{ji} = 0 \ , \qquad\qquad \varphi = 1, \ldots, m \ , \tag{3.109}$$

  where

  $$N_\varphi^{ij} \ = \ \sum_{\alpha=1}^{n} \rho_\alpha \frac{\partial f_\alpha}{\partial h_\varphi^i} u_\alpha^j - p_\varphi^i u_\varphi^j + \sum_{\psi=1}^{m-1} (p_\psi^j - p_m^j) \frac{\partial r_\psi}{\partial h_\varphi^i} \ , \qquad\qquad \varphi = 1, \ldots, m \ ,$$

- at $\grave{\mathbf{G}}_\gamma^{\gamma\ \ iJK}$:

  $$C_\gamma^{iJK} + C_\gamma^{iKJ} = 0 \ , \qquad\qquad \gamma = 1, \ldots, n \ , \tag{3.110}$$

  with

  $$\begin{aligned} C_\gamma^{iJK} \ = \ & \frac{\partial(\rho f)}{\partial G_\gamma^{iJK}} - \sum_{\varphi=1}^{m} \delta_{\gamma\varphi} \rho_\varphi p_\varphi^k {F_\varphi^{-1}}^{Ji} {F_\varphi^{-1}}^{Kk} \ + \ {F_\gamma^{-1}}^{Jj} {F_\gamma^{-1}}^{Kk} \left\{ \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^k \frac{\partial f_\alpha}{\partial D_\gamma^{ij}} \right. \\ & \left. + \ \sum_{\delta=1}^{n-1} (\delta_{\gamma\delta} - \delta_{\gamma n}) \sum_{\alpha=1}^{n} \rho_\alpha u_\alpha^k \frac{\partial f_\alpha}{\partial \Omega_\delta^{ij}} \ + \ \sum_{\psi=1}^{m-1} (p_\psi^k - p_m^k) \left[\frac{\partial r_\psi}{\partial D_\gamma^{ij}} + \sum_{\delta=1}^{n-1} (\delta_{\gamma\delta} - \delta_{\gamma n}) \frac{\partial r_\psi}{\partial \Omega_\delta^{ij}} \right] \right\} \ , \end{aligned}$$

- at Grad $\mathbf{G}_\gamma$:

  $$D_\gamma^{iJKL} = D_\gamma^{iKJL} \ , \qquad D_\gamma^{i\underline{JJJ}} = 0 \ , \qquad D_\gamma^{i\underline{JJ}K} + 2D_\gamma^{i\underline{J}K\underline{J}} = 0 \ ,$$
  $$D_\gamma^{i123} + D_\gamma^{i231} + D_\gamma^{i312} = 0 \ , \quad \gamma = 1, \ldots, n; \ \ i, J, K = 1, 2, 3 \ , \tag{3.111}$$

  where we do not sum over the underlined superscripts, and where

  $$D_\gamma^{iJKL} \ = \ \sum_{\alpha=1}^{n} \rho_\alpha \frac{\partial f_\alpha}{\partial G_\gamma^{iJK}} (u_\alpha^j - u_\gamma^j) {F_\gamma^{-1}}^{Lj} + \sum_{\psi=1}^{m-1} (p_\psi^k - p_m^k) \frac{\partial r_\psi}{\partial G_\gamma^{iJK}} {F_\gamma^{-1}}^{Lk} \ . \tag{3.112}$$

Due to the previous results, the dependence of the entropy inequality on $\mathbf{W}_n$ reduces to the linear dependence, hence we obtain an additional constraint

$$K^{ij} = K^{ji} \ , \tag{3.113}$$

for

$$K^{ij} = \sum_{\gamma=1}^{n} \sum_{\alpha=1}^{n} \rho_\alpha \frac{\partial f_\alpha}{\partial F_\gamma^{iJ}} F_\gamma^{jJ} \ + \ \sum_{\gamma=1}^{n} \frac{\partial(\rho f)}{\partial G_\gamma^{iJK}} G_\gamma^{jJK} - \sum_{\varphi=1}^{m} p_\varphi^j h_\varphi^i \ .$$

The rest of the entropy inequality can be rearranged into the following form:

$$\begin{aligned}
0 \quad \geq\ & \sum_{\alpha=1}^{n}\sum_{\gamma=1}^{n}\rho_\alpha\left[\frac{\partial f_\alpha}{\partial F_\gamma^{iJ}}F_\gamma^{jJ}+\frac{\partial f_\alpha}{\partial G_\gamma^{iJK}}G_\gamma^{jJK}\right](D_\gamma^{ij}+\Omega_\gamma^{ij}) \ - \ \sum_{\varphi=1}^{m}p_\varphi^j h_\varphi^i(D_\varphi^{ij}+\Omega_\varphi^{ij})\\
&+\sum_{\alpha=1}^{n}\sum_{\gamma=1}^{n}\rho_\alpha\frac{\partial f_\alpha}{\partial F_\gamma^{iJ}}G_\gamma^{iJK}{F_\gamma^{-1}}^{Kj}(u_\alpha^j-u_\gamma^j) \ + \ \sum_{\delta=1}^{n-1}\sum_{\alpha=1}^{n}\rho_\alpha\frac{\partial f_\alpha}{\partial u_\delta^i}u_\alpha^j(D_\delta^{ij}-D_n^{ij}+\Omega_\delta^{ij})\\
&+\sum_{\varphi=1}^{m}\sum_{\alpha=1}^{n}\rho_\alpha\frac{\partial f_\alpha}{\partial\rho_\varphi}u_\alpha^i h_\varphi^i \ - \ \sum_{\varphi=1}^{m}(u_\varphi^i h_\varphi^i+\rho_\varphi D_\varphi^{ii})(g_\varphi-f_\varphi) \ - \ \sum_{\varphi=1}^{m}p_\varphi^i h_\varphi^i D_\varphi^{kk}\\
&+\sum_{\psi=1}^{m-1}(p_\psi^k-p_m^k)\left\{\sum_{\gamma=1}^{n}\frac{\partial r_\psi}{\partial F_\gamma^{iJ}}G_\gamma^{iJL}{F_\gamma^{-1}}^{Lk} \ + \ \sum_{\delta=1}^{n-1}\frac{\partial r_\psi}{\partial u_\delta^i}(D_\delta^{ik}-D_n^{ik}+\Omega_\delta^{ik})\right.\\
&\left.+\sum_{\varphi=1}^{m}\frac{\partial r_\psi}{\partial\rho_\varphi}h_\varphi^k \ + \ \frac{\partial r_\psi}{\partial T}g^k\right\} \ + \ \sum_{\alpha=1}^{n}\rho_\alpha\left(\frac{\partial f_\alpha}{\partial T}+s_\alpha\right)u_\alpha^j g^j \ + \ \sum_{\psi=1}^{m-1}(g_\psi-g_m)r_\psi\\
&+\frac{1}{T}\,q^i g^i \ - \sum_{\alpha=1}^{n}T_\alpha^{ij}D_\alpha^{ij}+\sum_{\beta=1}^{n-1}k_\beta^i u_\beta^i \ + \ \frac{1}{2}\sum_{\psi=1}^{m-1}(u_\psi^i u_\psi^i-u_m^i u_m^i)r_\psi \ . \qquad (3.114)
\end{aligned}$$

All results of this section further simplify for fluids with their exceptional symmetry.

3.9 Mixtures of reacting and non-reacting fluids

Fluids are defined by their symmetry groups:

- *Reacting fluid* $\epsilon\in(1,\ldots,m)$,
  where the symmetry group consists of all pairs $(\mathbf{H},\mathbf{J})$, where $\mathbf{H}$ is an arbitrary regular second-order tensor and $\mathbf{J}$ is an arbitrary third-order tensor symmetric in last two indices.
- *Non-reacting fluid* $\epsilon\in(m+1,\ldots,n)$,
  where the symmetry group consists of pairs $(\mathbf{H},\mathbf{J})$, where $\mathbf{H}$ is an arbitrary unimodular ($|\det\mathbf{H}|=1$) second-order tensor and $\mathbf{J}$ is a third-order tensor that fulfils (3.94).

Thus, for a reacting component, we can choose $\mathbf{H}=\mathbf{F}_{\kappa\epsilon}^{-1}$ and $\mathbf{J}=\mathbf{G}_{\kappa\epsilon}^{-1}$, defined by (3.92), and then obtain

$$(\mathbf{F}_{\kappa\epsilon},\mathbf{G}_{\kappa\epsilon})\circ(\mathbf{H},\mathbf{J})=(\mathbf{1},\mathbf{0}) \ ,$$

where $(\mathbf{1},\mathbf{0})$ is the unit element of the group g. According to the definition of the symmetry group (3.91), we obtain

$$\mathcal{F}_\kappa[(\mathbf{F}_{\kappa\epsilon},\mathbf{G}_{\kappa\epsilon}),\Theta_\epsilon,X_\epsilon]=\mathcal{F}_\kappa[(\mathbf{1},\mathbf{0}),\Theta_\epsilon,X_\epsilon]=\mathcal{F}_\kappa[\Theta_\epsilon] \ . \qquad (3.115)$$

The possibility to omit the dependence on X_ϵ in the last equality results from the fact that the first equality in (3.115) is valid for any reference configuration. We can in fact choose a *homogeneous* configuration where the dependence upon X_ϵ vanishes (see Samohýl [1]).

For a non-reacting component, we choose

$$\mathbf{H} = J_{\kappa\epsilon}^{1/3}\mathbf{F}_{\kappa\epsilon}^{-1} \ ,$$

and

$$\begin{aligned}\mathbf{J} = -J_{\kappa\epsilon}^{2/3}\mathbf{F}_{\kappa\epsilon}^{-1}C(\mathbf{G}_{\kappa\epsilon} \otimes \mathbf{F}_{\kappa\epsilon}^{-\mathbf{1}} \otimes \mathbf{F}_{\kappa\epsilon}^{-\mathbf{1}}) \ + \ \frac{1}{2}J_{\kappa\epsilon}^{-1/3}[\mathbf{F}_{\kappa\epsilon} \otimes \mathrm{grad}\ J_{\kappa\epsilon}]^{sym.} \\ + \ \frac{1}{2}J_{\kappa\epsilon}^{1/3}[\mathbf{F}_{\kappa\epsilon}^{-1} \otimes \vec{k}_{\kappa\epsilon}]^{sym.} - \ \frac{1}{2}J_{\kappa\epsilon}^{2/3}[\mathbf{F}_{\kappa\epsilon}{}^{-1} \otimes \vec{k}_{\kappa\epsilon} \cdot \mathbf{F}_{\kappa\epsilon}^{-1}]^{sym.} \ ,\end{aligned}$$

where the superscript *sym.* for a third-order tensor means symmetrization in the last two indices:

$$(\mathbf{A}^{sym.})^{ijk} \equiv \ \frac{1}{2}(A^{ijk} + A^{ikj}) \ . \qquad (3.116)$$

It can be shown (Samohýl [1]) that the tensors **H** and **J** satisfy condition (3.94). Applying the definition of the symmetry group (3.93) yields

$$\begin{aligned}\mathcal{F}_{\epsilon} = \mathcal{F}_{\kappa\epsilon}[(\mathbf{F}_{\kappa\epsilon}, \mathbf{G}_{\kappa\epsilon}), \Theta_{\epsilon}, X_{\epsilon}] \\ = \ \mathcal{F}_{\kappa\epsilon}\left[\left(\frac{\rho_{\kappa\epsilon}}{\rho_{\epsilon}}\right)^{1/3}\mathbf{1}, \frac{1}{2}\rho_{\kappa\epsilon}\left(\frac{\rho_{\kappa\epsilon}}{\rho_{\epsilon}}\right)^{1/3}\left\{\mathbf{1} \otimes \left(\mathrm{Grad}_{\kappa\epsilon}\rho_{\kappa\epsilon} - \left(\frac{\rho_{\kappa\epsilon}}{\rho_{\epsilon}}\right)^{4/3}\vec{h}_{\epsilon}\right)\right\}^{sym.}, \Theta_{\epsilon}, X_{\epsilon}\right] \\ = \ \mathcal{F}(\rho_{\varepsilon}, \vec{h}_{\varepsilon}, \Theta_{\varepsilon}) \ .\end{aligned}$$

The last equality results from the fact that the previous formula can be derived for any reference configuration κ, particulary for the homogeneous reference, where the dependence on X_{ε} vanishes.

As a result, the constitutive equations of a mixture of reacting and non-reacting components have the following form:

$$\{r_{\psi}, f_{\alpha}, s_{\alpha}, \vec{q}, \vec{k}_{\beta}, \mathbf{T}_{\alpha}\} = \hat{\mathcal{F}}[\rho_{\gamma}, \vec{h}_{\gamma}, \mathbf{D}_{\gamma}, \mathbf{\Omega}_{\delta}, \vec{u}_{\delta}, T, \vec{g}] \ , \qquad (3.117)$$

$$\psi = 1, \ldots, m-1; \qquad \beta, \delta = 1, \ldots, n-1; \qquad \alpha, \gamma = 1, \ldots, n \ ,$$

where we replaced ε_{α} with f_{α}, since they are uniquely connected by the definition (3.76).

The principle of objectivity has in the case of fluid mixtures the following form:

$$\{r_{\psi}, f_{\alpha}, s_{\alpha}, \mathbf{Q}\vec{q}, \mathbf{Q}\vec{k}_{\beta}, \mathbf{Q}\mathbf{T}_{\alpha}\mathbf{Q}^{T}\} = \hat{\mathcal{F}}[\rho_{\gamma}, \mathbf{Q}\vec{h}_{\gamma}, \mathbf{Q}\mathbf{D}_{\gamma}\mathbf{Q}^{T}, \mathbf{Q}\mathbf{\Omega}_{\delta}\mathbf{Q}^{T}, \mathbf{Q}\vec{u}_{\delta}, T, \mathbf{Q}\vec{g}] \ , \qquad (3.118)$$

for any second-order orthogonal tensor **Q**.

We can now rewrite the results (3.99) - (3.114) of the entropy principle for the case of fluid mixtures, where we obtain:

$$f = f(\rho_{\gamma}, \vec{h}_{\gamma}, T) \ , \qquad \gamma = 1, \ldots, n \ , \qquad (3.119)$$

$$\frac{\partial f}{\partial T} = -s \ . \qquad (3.120)$$

For all components, we define the *chemical potential* g_α and the *vector* $\vec{p}_\alpha$:

$$g_\alpha = \frac{\partial(\rho f)}{\partial \rho_\alpha}\ , \qquad \vec{p}_\alpha = \frac{\partial(\rho f)}{\partial \vec{h}_\alpha}\ , \qquad \alpha = 1, \dots, n\ . \tag{3.121}$$

And find that

$$s = s(\rho_\gamma, \vec{h}_\gamma, T)\ , \qquad g_\alpha = g_\alpha(\rho_\gamma, \vec{h}_\gamma, T)\ , \qquad \vec{p}_\alpha = \vec{p}_\alpha(\rho_\gamma, \vec{h}_\gamma, T)\ , \qquad \alpha, \gamma = 1, \dots, n\ . \tag{3.122}$$

$$\mathbf{0} = \left[\sum_{\delta=1}^{n-1} \rho_\delta \frac{\partial f_\delta}{\partial \vec{g}} \otimes \vec{u}_\delta + \sum_{\psi=1}^{m-1} \frac{\partial r_\psi}{\partial \vec{g}} \otimes (\vec{p}_\psi - \vec{p}_m)\right]^{sym.}\ , \tag{3.123}$$

$$\mathbf{0} = \left[\sum_{\delta=1}^{n-1} \rho_\delta \frac{\partial f_\delta}{\partial \vec{h}_\gamma} \otimes \vec{u}_\delta - \vec{p}_\gamma \otimes \vec{u}_\gamma + \sum_{\psi=1}^{m-1} \frac{\partial r_\psi}{\partial \vec{h}_\gamma} \otimes (\vec{p}_\psi - \vec{p}_m)\right]^{sym.}\ , \qquad \gamma = 1, \dots, n\ , \tag{3.124}$$

$$\begin{aligned}\mathbf{0} = {} & \Bigg[\sum_{\delta=1}^{n-1} \rho_\delta \frac{\partial f_\delta}{\partial \mathbf{D}_\gamma} \otimes \vec{u}_\delta + \sum_{\psi=1}^{m-1} \frac{\partial r_\psi}{\partial \mathbf{D}_\gamma} \otimes (\vec{p}_\psi - \vec{p}_m) + \sum_{\delta=1}^{n-1} (\delta_{\gamma\delta} - \delta_{\gamma n}) \Bigg(\sum_{\alpha=1}^{n} \rho_\alpha \frac{\partial f_\alpha}{\partial \mathbf{\Omega}_\delta} \otimes \vec{u}_\alpha \\ & + \sum_{\psi=1}^{m-1} \frac{\partial r_\psi}{\partial \mathbf{\Omega}_\delta} \otimes (\vec{p}_\psi - \vec{p}_m)\Bigg) - \rho_\gamma \mathbf{1} \otimes \vec{p}_\gamma\Bigg]^{sym.}\ , \qquad \gamma = 1, \dots, n\ ,\end{aligned} \tag{3.125}$$

$$\mathbf{0} = \sum_{\gamma=1}^{n} (\vec{p}_\gamma \otimes \vec{h}_\gamma - \vec{h}_\gamma \otimes \vec{p}_\gamma)\ , \tag{3.126}$$

with the entropy inequality in a mixture of fluids reading as:

$$\begin{aligned} 0 \geq {} & \sum_{\gamma=1}^{n}\sum_{\alpha=1}^{n} \rho_\alpha \frac{\partial f_\alpha}{\partial \rho_\gamma} \vec{h}_\gamma \cdot \vec{u}_\alpha - \sum_{\gamma=1}^{n} (g_\gamma - f_\gamma) \vec{h}_\gamma \cdot \vec{u}_\gamma - \sum_{\gamma=1}^{n} \rho_\gamma (g_\gamma - f_\gamma) \mathrm{tr}\ \mathbf{D}_\gamma \\ & - \sum_{\gamma=1}^{n} \vec{p}_\gamma \cdot \vec{h}_\gamma \mathrm{tr}\ \mathbf{D}_\gamma - \sum_{\gamma=1}^{n} \vec{h}_\gamma \cdot (\mathbf{D}_\gamma + \mathbf{\Omega}_\gamma) \vec{p}_\gamma + \sum_{\delta=1}^{n-1}\sum_{\alpha=1}^{n} \rho_\alpha \frac{\partial f_\alpha}{\partial \vec{u}_\delta} \cdot (\mathbf{D}_\delta - \mathbf{D}_n + \mathbf{\Omega}_\delta) \vec{u}_\alpha \\ & + \sum_{\psi=1}^{m-1} (\vec{p}_\psi - \vec{p}_m) \cdot \left[\sum_{\gamma=1}^{n} \frac{\partial r_\psi}{\partial \rho_\gamma} \vec{h}_\gamma + \frac{\partial r_\psi}{\partial T} \vec{g} + \sum_{\delta=1}^{n-1} \frac{\partial r_\psi}{\partial \vec{u}_\delta} \cdot (\mathbf{D}_\delta - \mathbf{D}_n + \mathbf{\Omega}_\delta)\right] \\ & + \sum_{\psi=1}^{m-1} (g_\psi - g_m) r_\psi + \sum_{\alpha=1}^{n} \rho_\alpha \left(\frac{\partial f_\alpha}{\partial T} + s_\alpha\right) \vec{u}_\alpha \cdot \vec{g} + \frac{1}{T} \vec{q} \cdot \vec{g} - \sum_{\alpha=1}^{n} \mathrm{tr}\ \mathbf{T}_\alpha \mathbf{D}_\alpha \\ & + \sum_{\beta=1}^{n-1} \vec{k}_\beta \cdot \vec{u}_\beta + \frac{1}{2} \sum_{\psi=1}^{m-1} (\vec{u}_\psi^{\,2} - \vec{u}_m^{\,2}) r_\psi\ . \end{aligned} \tag{3.127}$$

3.10 Equilibrium in a mixture of fluids

In the next chapter, we will inspect the constitutive equations of a two-component reacting mixture of fluids. One of the assumptions in our derivations will be that the mixture is not too distant from the thermodynamic equilibrium. First, let us therefore define it properly.

An equilibrium is defined as a thermodynamic process with a zero entropy production. This means that there is an equality in the reduced entropy inequality (3.127). To satisfy that, we will consider equilibrium as a process for which it holds that

$$\mathbf{D}^+_\gamma = \mathbf{0} \ , \qquad \mathbf{\Omega}^+_\delta = \mathbf{0} \ , \qquad \vec{u}^+_\delta = \vec{0} \ , \qquad \vec{g}^+ = \vec{0} \ , \tag{3.128}$$

$$\sum_{\psi=1}^{m-1} \sum_{\gamma=1}^{n} \left(\frac{\partial r_\psi}{\partial \rho_\gamma} \right)^+ (\vec{p}^+_\psi - \vec{p}^+_m) \cdot \vec{h}^+_\gamma = 0 \ , \tag{3.129}$$

$$\sum_{\psi=1}^{m-1} (g^+_\psi - g^+_m) r^+_\psi = 0 \ , \qquad\qquad \gamma = 1, \ldots, n; \ \delta = 1, \ldots, n-1 \ , \tag{3.130}$$

where the equilibrated quantities are denoted by the symbol $+$. By this choice, the equality in (3.127) is ensured.
Let the symbol Ξ denote the right-hand side of the entropy inequality (3.127),

$$\Xi = \Xi(\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_\delta, \vec{u}_\delta, T, \vec{g}).$$

According to the definition of equilibrium, Ξ is maximal in equilibrium. Thus we can write

$$\frac{d}{d\lambda} \ \Xi(\rho^+_\gamma + \lambda \alpha_\gamma, \vec{h}^+_\gamma + \lambda \vec{\gamma}_\gamma, \lambda \mathbf{D}_\gamma, \lambda \mathbf{\Omega}_\delta, \lambda \vec{u}_\delta, T^+ + \lambda \beta, \lambda \vec{g}) \Big|_{\lambda=0} \ = \ 0 \ , \tag{3.131}$$

$$\frac{d^2}{d\lambda^2} \ \Xi(\rho^+_\gamma + \lambda \alpha_\gamma, \vec{h}^+_\gamma + \lambda \vec{\gamma}_\gamma, \lambda \mathbf{D}_\gamma, \lambda \mathbf{\Omega}_\delta, \lambda \vec{u}_\delta, T^+ + \lambda \beta, \lambda \vec{g}) \Big|_{\lambda=0} \ \leq \ 0 \ , \tag{3.132}$$

for a real parameter λ, and arbitrary but fixed quantities

$$\alpha_\gamma, \vec{\gamma}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_\delta, \vec{u}_\delta, \beta, \vec{g}, \qquad\qquad \gamma = 1, \ldots, n; \ \delta = 1, \ldots, n-1 \ ,$$

and equilibrated

$$\rho^+_\gamma, \ \vec{h}^+_\gamma, \ T^+ \ ,$$

that satisfy (3.129) and (3.130).

We will consider only the extremal condition (3.131). Applying it to the reduced entropy inequality (3.127) yields:

$$\begin{aligned}
0 \ = \ & \sum_{\alpha=1}^{n} \sum_{\gamma=1}^{n} \rho^+_\alpha \left(\frac{\partial f_\alpha}{\partial \rho_\gamma} \right)^+ \vec{h}^+_\gamma \cdot \vec{u}_\alpha \ - \ \sum_{\alpha=1}^{n} (g^+_\alpha - f^+_\alpha) \vec{h}^+_\alpha \cdot \vec{u}_\alpha + \sum_{\beta=1}^{n-1} \vec{k}^+_\beta \cdot \vec{u}_\beta \\
- \ & \sum_{\gamma=1}^{n} \rho^+_\gamma (g^+_\gamma - f^+_\gamma) \mathrm{tr}\, \mathbf{D}_\gamma \ - \ \sum_{\gamma=1}^{n} \vec{p}^+_\gamma \cdot \vec{h}^+_\gamma \mathrm{tr}\, \mathbf{D}_\gamma \ - \ \sum_{\gamma=1}^{n} \vec{p}^+_\gamma \cdot \mathbf{D}_\gamma \vec{h}^+_\gamma \\
+ \ & \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} \sum_{\delta=1}^{n-1} (\delta_{\delta\gamma} - \delta_{\gamma n}) \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+ \cdot \mathbf{D}_\gamma (\vec{p}^+_\psi - \vec{p}^+_m) \ - \ \sum_{\gamma=1}^{n} \mathrm{tr}\, (\mathbf{T}^+_\gamma \mathbf{D}_\gamma) \\
- \ & \sum_{\delta=1}^{n-1} \vec{h}^+_\delta \cdot \mathbf{\Omega}_\delta \vec{p}^+_\delta \ + \ \sum_{\delta=1}^{n-1} \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+ \cdot \mathbf{\Omega}_\delta (\vec{p}^+_\psi - \vec{p}^+_m) \ + \ \frac{1}{T^+} \ \vec{q}^+ \cdot \vec{g}
\end{aligned}$$

$$
\begin{aligned}
&+ \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial T}\right)^{+} (\vec{p}_\psi^{+} - \vec{p}_m^{+}) \cdot \vec{g} \;+\; \sum_{\gamma=1}^{n} \vec{h}_\gamma^{+} \cdot \Bigg\{ \sum_{\psi=1}^{m-1} \Bigg[\sum_{\eta=1}^{n} \left(\frac{\partial(\vec{p}_\psi - \vec{p}_m)}{\partial \rho_\eta}\right)^{+} \alpha_\eta \\
&+ \sum_{\eta=1}^{n} \left(\frac{\partial(\vec{p}_\psi - \vec{p}_m)}{\partial \vec{h}_\eta}\right)^{+} \cdot \vec{\gamma}_\eta \;+\; \left(\frac{\partial(\vec{p}_\psi - \vec{p}_m)}{\partial T}\right)^{+} \beta \Bigg] \left(\frac{\partial r_\psi}{\partial \rho_\gamma}\right)^{+} \\
&+ \sum_{\psi=1}^{m-1} (\vec{p}_\psi^{+} - \vec{p}_m^{+}) \Bigg[\sum_{\eta=1}^{n} \left(\frac{\partial^2 r_\psi}{\partial \rho_\eta \partial \rho_\gamma}\right)^{+} \alpha_\eta \;+\; \sum_{\eta=1}^{n} \left(\frac{\partial^2 r_\psi}{\partial \vec{h}_\eta \partial \rho_\gamma}\right)^{+} \cdot \vec{\gamma}_\eta \;+\; \left(\frac{\partial^2 r_\psi}{\partial T \partial \rho_\gamma}\right)^{+} \beta \\
&+ \sum_{\eta=1}^{n} \left(\frac{\partial^2 r_\psi}{\partial \mathbf{D}_\eta \partial \rho_\gamma}\right)^{+} : \mathbf{D}_\eta \;+\; \sum_{\delta=1}^{n-1} \left(\frac{\partial^2 r_\psi}{\partial \mathbf{\Omega}_\delta \partial \rho_\gamma}\right)^{+} : \mathbf{\Omega}_\delta \;+\; \sum_{\delta=1}^{n-1} \left(\frac{\partial^2 r_\psi}{\partial \vec{u}_\delta \partial \rho_\gamma}\right)^{+} \cdot \vec{u}_\delta \\
&+ \left(\frac{\partial^2 r_\psi}{\partial \vec{g} \partial \rho_\gamma}\right)^{+} \cdot \vec{g} \Bigg]\Bigg\} \;+\; \sum_{\psi=1}^{m-1} \sum_{\gamma=1}^{n} \left(\frac{\partial r_\psi}{\partial \rho_\gamma}\right)^{+} (\vec{p}_\psi^{+} - \vec{p}_m^{+}) \cdot \vec{\gamma}_\gamma \;+\; \sum_{\psi=1}^{m-1} \Bigg\{ \Bigg[\sum_{\eta=1}^{n} \left(\frac{\partial(g_\psi - g_m)}{\partial \rho_\eta}\right)^{+} \alpha_\eta \\
&+ \sum_{\eta=1}^{n} \left(\frac{\partial(g_\psi - g_m)}{\partial \vec{h}_\eta}\right)^{+} \cdot \vec{\gamma}_\eta \;+\; \sum_{\eta=1}^{n} \left(\frac{\partial(g_\psi - g_m)}{\partial T}\right)^{+} \beta \Bigg] r_\psi^{+} \\
&+ (g_\psi^{+} - g_m^{+}) \Bigg[\sum_{\eta=1}^{n} \left(\frac{\partial r_\psi}{\partial \rho_\eta}\right)^{+} \alpha_\eta \;+\; \sum_{\eta=1}^{n} \left(\frac{\partial r_\psi}{\partial \vec{h}_\eta}\right)^{+} \cdot \vec{\gamma}_\eta \;+\; \sum_{\eta=1}^{n} \left(\frac{\partial r_\psi}{\partial \mathbf{D}_\eta}\right)^{+} : \mathbf{D}_\eta \\
&+ \sum_{\delta=1}^{n-1} \left(\frac{\partial r_\psi}{\partial \mathbf{\Omega}_\delta}\right)^{+} : \mathbf{\Omega}_\delta \;+ \sum_{\delta=1}^{n-1} \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta}\right)^{+} \cdot \vec{u}_\delta \;+\; \left(\frac{\partial r_\psi}{\partial T}\right)^{+} \beta \;+\; \left(\frac{\partial r_\psi}{\partial \vec{g}}\right)^{+} \cdot \vec{g} \Bigg]\Bigg\} \;.
\end{aligned}
$$

Since $\alpha_\eta, \vec{\gamma}_\alpha, \mathbf{D}_\gamma, \mathbf{\Omega}_\delta, \vec{u}_\delta, \beta, \vec{g}$, are arbitrary constants, we obtain the following seven constraints:
The terms at α_η must vanish

$$
\begin{aligned}
0 \;=\;& \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \rho_\gamma}\right)^{+} \left(\frac{\partial(\vec{p}_\psi - \vec{p}_m)}{\partial \rho_\eta}\right)^{+} \cdot \vec{h}_\gamma^{+} \;+\; \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \rho_\eta}\right)^{+} (\vec{p}_\psi^{+} - \vec{p}_m^{+}) \cdot \vec{h}_\gamma^{+} \\
+\;& \sum_{\psi=1}^{m-1} (g_\psi^{+} - g_m^{+}) \left(\frac{\partial r_\psi}{\partial \rho_\eta}\right)^{+} \;+\; \sum_{\psi=1}^{m-1} \left(\frac{\partial(g_\psi - g_m)}{\partial \rho_\eta}\right)^{+} r_\psi^{+} \;, \qquad \eta = 1, \ldots, n \;.
\end{aligned}
\tag{3.133}
$$

The terms at $\vec{\gamma}_\eta$ must vanish:

$$
\begin{aligned}
\vec{0} \;=\;& \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \rho_\eta}\right)^{+} (\vec{p}_\psi^{+} - \vec{p}_m^{+}) \;+\; \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \rho_\gamma}\right)^{+} \vec{h}_\gamma^{+} \cdot \left(\frac{\partial(\vec{p}_\psi - \vec{p}_m)}{\partial \vec{h}_\eta}\right)^{+} \\
+\;& \sum_{\psi=1}^{m-1} (g_\psi^{+} - g_m^{+}) \left(\frac{\partial r_\psi}{\partial \vec{h}_\eta}\right)^{+} \;+\; \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} [(\vec{p}_\psi^{+} - \vec{p}_m^{+}) \cdot \vec{h}_\gamma^{+}] \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \vec{h}_\eta}\right)^{+} \\
+\;& \sum_{\psi=1}^{m-1} \left(\frac{\partial(g_\psi - g_m)}{\partial h_\eta}\right)^{+} r_\psi^{+} \;, \qquad \eta = 1, \ldots, n \;.
\end{aligned}
\tag{3.134}
$$

The terms at $\mathbf{D}_\gamma$ must vanish after symmetrization:

$$
\mathbf{0} \;=\; \Bigg[\sum_{\alpha=1}^{n} \sum_{\psi=1}^{m-1} [(\vec{p}_\psi^{+} - \vec{p}_m^{+}) \cdot \vec{h}_\alpha^{+}] \left(\frac{\partial^2 r_\psi}{\partial \rho_\alpha \partial \mathbf{D}_\gamma}\right)^{+} \;+\; \sum_{\psi=1}^{m-1} (g_\psi^{+} - g_m^{+}) \left(\frac{\partial r_\psi}{\partial \mathbf{D}_\gamma}\right)^{+}
$$

$$
\begin{aligned}
& - \quad \rho_\gamma^+ (g_\gamma^+ - f_\gamma^+) \mathbf{1} \; - \; (\vec{p}_\gamma^{\,+} \cdot \vec{h}_\gamma^+) \mathbf{1} \; - \; \vec{h}_\gamma^+ \otimes \vec{p}_\gamma^{\,+} \\
& + \quad \left. \sum_{\psi=1}^{m-1} \sum_{\delta=1}^{n-1} (\delta_{\delta\gamma} - \delta_{\gamma n}) \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+ \otimes (\vec{p}_\psi^{\,+} - \vec{p}_m^{\,+}) \; - \; \mathbf{T}_\gamma^+ \right]^{sym.} , \qquad \gamma = 1, \ldots, n \; .
\end{aligned} \tag{3.135}
$$

The terms at $\mathbf{\Omega}_\delta$ must vanish after antisymmetrization:

$$
\begin{aligned}
\mathbf{0} \; = \; & \left[\sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+ \otimes (\vec{p}_\psi^{\,+} - \vec{p}_m^{\,+}) \; - \; \vec{h}_\delta^+ \otimes \vec{p}_\delta^{\,+} + \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} ((\vec{p}_\psi^{\,+} - \vec{p}_m^{\,+}) \cdot \vec{h}_\gamma^+) \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \mathbf{\Omega}_\delta} \right)^+ \right. \\
& + \left. \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \mathbf{\Omega}_\delta} \right)^+ \right]^{antis.} , \qquad \delta = 1, \ldots, n-1 \; .
\end{aligned} \tag{3.136}
$$

The terms at $\vec{u}_\delta$ must vanish:

$$
\begin{aligned}
\vec{0} \; = \; & \sum_{\gamma=1}^{n} \rho_\delta^+ \left(\frac{\partial f_\delta}{\partial \rho_\gamma} \right)^+ \vec{h}_\gamma^+ \; - \; (g_\delta^+ - f_\delta^+) \vec{h}_\delta^+ \; + \; \vec{k}_\delta^+ \; + \; \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} ((\vec{p}_\psi^{\,+} - \vec{p}_m^{\,+}) \cdot \vec{h}_\gamma^+) \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \vec{u}_\delta} \right)^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+ , \qquad \delta = 1, \ldots, n-1 \; .
\end{aligned} \tag{3.137}
$$

The term at β must vanish:

$$
\begin{aligned}
0 \; = \; & \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} \left(\frac{\partial (\vec{p}_\psi - \vec{p}_m)}{\partial T} \right)^+ \cdot \vec{h}_\gamma^+ \left(\frac{\partial r_\psi}{\partial \rho_\gamma} \right)^+ \; + \; \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial T} \right)^+ (\vec{p}_\psi^{\,+} - \vec{p}_m^{\,+}) \cdot \vec{h}_\gamma^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial T} \right)^+ \; + \; \sum_{\psi=1}^{m-1} \left(\frac{\partial (g_\psi - g_m)}{\partial T} \right)^+ r_\psi^+ \; .
\end{aligned} \tag{3.138}
$$

Finally, the term at $\vec{g}$ must vanish:

$$
\begin{aligned}
\vec{0} \; = \; & \frac{1}{T^+} \, \vec{q}^{\,+} \; + \; \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial T} \right)^+ (\vec{p}_\psi^{\,+} - \vec{p}_m^{\,+}) \; + \; \sum_{\gamma=1}^{n} \sum_{\psi=1}^{m-1} ((\vec{p}_\psi^{\,+} - \vec{p}_m^{\,+}) \cdot \vec{h}_\gamma^+) \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \vec{g}} \right)^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{g}} \right)^+ \; .
\end{aligned} \tag{3.139}
$$

We will in addition assume that the rate of mass change converges to zero in equilibrium,

$$
r_\psi^+ \; = \; r_\psi(\rho_\gamma^+, \vec{h}_\gamma^+, \mathbf{0}, \mathbf{0}, \vec{0}, T^+, \vec{0}) \; = \; 0 \; , \qquad \psi = 1, \ldots, m-1 \; , \tag{3.140}
$$

i.e. that no reactions take place in equilibrium, and that the density gradient in equilibrium is equal to zero,

$$
\vec{h}_\gamma^+ \; = \; \vec{0} \; , \qquad \gamma = 1, \ldots, n \; . \tag{3.141}
$$

As a result of these assumptions, conditions (3.129) and (3.130) are satisfied automatically.

With an assumption (justified later by the choice of a particular material model) that the free energy of the mixture f is independent of the density gradient,

$$\vec{p}_\gamma \;=\; \frac{\partial(\rho f)}{\partial \vec{h}_\gamma} \;\equiv\; \vec{0}\;, \tag{3.142}$$

the equilibrium conditions (3.133) – (3.139) reduce to the form:

$$0 \;=\; \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \rho_\alpha}\right)^+ \;, \qquad \alpha = 1, \dots, n\;, \tag{3.143}$$

$$\vec{0} \;=\; \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{h}_\alpha}\right)^+ \;, \qquad \alpha = 1, \dots, n\;, \tag{3.144}$$

$$\mathbf{0} \;=\; \left[\sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \mathbf{D}_\gamma}\right)^+ \;-\; \rho_\gamma^+ (g_\gamma^+ - f_\gamma^+)\mathbf{1} \;-\; \mathbf{T}_\gamma^+\right]^{sym.} \;, \qquad \gamma = 1, \dots, n\;, \tag{3.145}$$

$$\mathbf{0} \;=\; \left[\sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \mathbf{\Omega}_\delta}\right)^+\right]^{antis.} \;, \qquad \delta = 1, \dots, n-1\;, \tag{3.146}$$

$$\vec{0} \;=\; \vec{k}_\delta^+ \;+\; \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta}\right)^+ \;, \qquad \delta = 1, \dots, n-1\;, \tag{3.147}$$

$$0 \;=\; \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial T}\right)^+ \;, \tag{3.148}$$

$$\vec{0} \;=\; \frac{1}{T^+}\,\vec{q}^{\,+} \;+\; \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{g}}\right)^+ \;. \tag{3.149}$$

Note that the above analysis should be completed by inspecting the equilibrium conditions at singular surfaces in the mixture, since the reduced entropy inequality (3.127) used in this section corresponds only to the volume part of the entropy production in (3.72), while the surface entropy production at singular surfaces in the mixture is not considered. We could, in analogy with the procedure above also assume particular functional dependence of the surface production terms, namely r_α^S, $\vec{f}_\alpha^S$, e_α^S, and attempt to derive constraints corresponding to the zero surface-entropy production that must hold in equilibrium. Instead of this, we only assert that in equilibrium no reactions amongst the components take place and thus all the surface-production functionals are zero:

$$r_\alpha^{S+} = 0\;, \qquad \vec{f}_\alpha^{S+} = \vec{0}\;, \qquad e_\alpha^{S+} = 0\;, \qquad\qquad \alpha = 1 \dots n\;. \tag{3.150}$$

Chapter 4

Application to the water-ice mixture

4.1 Introduction

In this chapter we will apply the approach of rational thermodynamics to the water-ice mixture in the temperate-ice region of a glacier.

Despite water being distinctly separate from ice, since both are different phases of the same material, and are separated by a singular surface of phase equilibrium, in our approach we consider these two phases as mixed continua, both present at each point of the mixture at the same time. The phase interface between ice and water is not considered in this concept. The theory that justifies our approach is a **theory of multi-phase mixtures** discussed, for example, in Passman et al. [3].

4.2 The material model

Both components, water ($\alpha = 1$) and ice ($\alpha = 2$), are treated as non-simple fluids of the constitutive model (3.117):

$$\{r_1, f_\alpha, s_\alpha, \vec{q}, \vec{k}_1, \mathbf{T}_\alpha\} = \hat{\mathcal{F}}[\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}] \ , \tag{4.1}$$

$$\alpha, \gamma = 1, 2 \ .$$

For further simplifications of this constitutive model, several assumptions are introduced. Guided by the need to keep the material model as simple as possible, and to implement the expected features of the mixture, e.g. the nonlinear stress – strain-rate relationship, we will confine ourselves to the following model. The constitutive functionals

$$\{r_1, f_\alpha, s_\alpha, \vec{q}, \vec{k}_1\} \ , \qquad \alpha = 1, 2 \ , \tag{4.2}$$

will be linearized in the vicinity of equilibrium, defined by eq. (3.128) – (3.149), in variables $\{\vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, \vec{g}\}$, without imposing any restrictions on the functional dependence on the remaining variables, ρ_γ, T.

The stress-tensor functionals $\mathbf{T}_\alpha$ will not be linearized, since the constitutive relation for the stress in pure ice is nonlinear with respect to $\mathbf{D}$ and T. We expect this behaviour to persist in the mixture. Thus a simplification by truncating the Taylor expansion series, as in the case of constitutive functionals $\{r_1, f_\alpha, s_\alpha, \vec{q}, \vec{k}_1\}$ may be incorrect for $\mathbf{T}_\alpha$.

We now make use of the *principle of objectivity* (3.118), that states:

$$\{r_1, f_\alpha, s_\alpha, \mathbf{Q}\vec{q}, \mathbf{Q}\vec{k}_1, \mathbf{Q}\mathbf{T}_\alpha\mathbf{Q}^T\} = \hat{\mathcal{F}}[\rho_\gamma, \mathbf{Q}\vec{h}_\gamma, \mathbf{Q}\mathbf{D}_\gamma\mathbf{Q}^T, \mathbf{Q}\mathbf{\Omega}_1\mathbf{Q}^T, \mathbf{Q}\vec{u}_1, T, \mathbf{Q}\vec{g}] \ , \qquad (4.3)$$

for any orthogonal tensor $\mathbf{Q}$, $\alpha, \gamma = 1, 2$. This principle asserts that the constitutive relations (4.1) are *isotropic functions* of their variables:

A scalar a, a vector $\vec{a}$ or a tensor (second-order) $\mathbf{A}$ are isotropic functions of scalars y_α, vectors $\vec{y}_\beta$ and second-order tensors $\mathbf{Y}_\gamma$ respectively, if they satisfy:

$$\begin{aligned} a &= a(y_\alpha, \vec{y}_\beta, \mathbf{Y}_\gamma) = a(y_\alpha, \mathbf{Q}\vec{y}_\beta, \mathbf{Q}\mathbf{Y}_\gamma\mathbf{Q}^T) \ , && (4.4)\\ \vec{a} &= \vec{a}(y_\alpha, \vec{y}_\beta, \mathbf{Y}_\gamma) = \mathbf{Q}^T\vec{a}(y_\alpha, \mathbf{Q}\vec{y}_\beta, \mathbf{Q}\mathbf{Y}_\gamma\mathbf{Q}^T) \ , && (4.5)\\ \mathbf{A} &= \mathbf{A}(y_\alpha, \vec{y}_\beta, \mathbf{Y}_\gamma) = \mathbf{Q}^T\mathbf{A}(y_\alpha, \mathbf{Q}\vec{y}_\beta, \mathbf{Q}\mathbf{Y}_\gamma\mathbf{Q}^T)\mathbf{Q} \ , && (4.6) \end{aligned}$$

for any orthogonal second-order tensor $\mathbf{Q}$. We now introduce **the representation theorem for linear isotropic functions**, (Samohýl [1]):
If an isotropic scalar a, an isotropic vector $\vec{a}$ or an isotropic second-order tensor $\mathbf{A}$, depend linearly on r vectors $\vec{y}_\beta$, $(\beta = 1, \ldots, r)$, and s second-order tensors $\mathbf{Y}_\gamma$, $(\gamma = 1, \ldots, s)$, it is sufficient and necessary to represent them in the forms

$$\begin{aligned} a &= a_0 + \sum_{\gamma=1}^{s} \vartheta_\gamma \mathrm{tr}\, \mathbf{Y}_\gamma \ , && (4.7)\\ \vec{a} &= \sum_{\beta=1}^{r} \zeta_\beta \vec{y}_\beta \ , && (4.8)\\ \mathbf{A} &= \tau\mathbf{1} + \sum_{\gamma=1}^{s} \alpha_\gamma (\mathrm{tr}\, \mathbf{Y}_\gamma)\mathbf{1} + \sum_{\gamma=1}^{s} (\eta_\gamma \mathbf{Y}_\gamma + \xi_\gamma \mathbf{Y}^T) \ , && (4.9) \end{aligned}$$

where a_0, ϑ_γ, ζ_β, τ, α_γ, η_γ, and ξ_γ are scalar constants.

The linearization of the constitutive equations (4.2) with respect to $\{\vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, \vec{g}\}$, with the use of objectivity (4.3), and employing the representation theorem for linear isotropic functions (4.7) and (4.8) gives the constitutive equations in the following form,

$$\begin{aligned} r_1 &= r_1^{(0)}(\rho_\gamma, T) + r_1^{(1)}(\rho_\gamma, T)\, \mathrm{tr}\mathbf{D}_1 + r_1^{(2)}(\rho_\gamma, T)\, \mathrm{tr}\mathbf{D}_2, && (4.10)\\ f_\alpha &= f_\alpha^{(0)}(\rho_\gamma, T) + f_\alpha^{(1)}(\rho_\gamma, T)\, \mathrm{tr}\mathbf{D}_1 + f_\alpha^{(2)}(\rho_\gamma, T)\, \mathrm{tr}\mathbf{D}_2, && (4.11)\\ s_\alpha &= s_\alpha^{(0)}(\rho_\gamma, T) + s_\alpha^{(1)}(\rho_\gamma, T)\, \mathrm{tr}\mathbf{D}_1 + s_\alpha^{(2)}(\rho_\gamma, T)\, \mathrm{tr}\mathbf{D}_2, && (4.12)\\ \vec{q} &= -\, k(\rho_\gamma, T)\vec{g} - \lambda(\rho_\gamma, T)\vec{u}_1 + \sum_{\psi=1}^{2} \chi_\psi(\rho_\gamma, T)\vec{h}_\psi \ , && (4.13)\\ \vec{k}_1 &= -\, \xi(\rho_\gamma, T)\vec{g} - \nu(\rho_\gamma, T)\vec{u}_1 + \sum_{\psi=1}^{2} \omega_\psi(\rho_\gamma, T)\vec{h}_\psi \ , && (4.14) \end{aligned}$$

while the stress tensors $\mathbf{T}_\alpha$ are represented by nonlinear functionals as

$$\mathbf{T}_\alpha = \mathbf{T}_\alpha(\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \ , \qquad (4.15)$$

$$\alpha, \gamma = 1, 2 \ .$$

4.3 Equilibrium in the water-ice mixture

We have simplified our material model by partial linearization. To learn more about its properties, we will inspect the equilibrium in the model more closely.

In the previous chapter, the equilibrium in a two-component mixture of non-simple fluids is defined as a process, for which it holds:

$$\mathbf{D}_\gamma^+ = \mathbf{0}\ , \qquad \mathbf{\Omega}_1^+ = \mathbf{0}\ , \qquad \vec{u}_1^+ = \vec{0}\ , \qquad \vec{g}^+ = \vec{0}\ , \tag{4.16}$$

$$\sum_{\psi=1}^{2} \left(\frac{\partial r_1}{\partial \rho_\gamma}\right)^+ (\vec{p}_1^+ - \vec{p}_2^+) \cdot \vec{h}_\gamma^+ = 0\ , \tag{4.17}$$

$$(g_1^+ - g_2^+) r_1^+ = 0\ , \tag{4.18}$$

$$\gamma = 1, 2\ .$$

We assumed in (3.140) that:

$$r_1^+ \ = \ r_1(\rho_\gamma^+, \vec{0}, \mathbf{0}, \mathbf{0}, \vec{0}, T^+, \vec{0}) \ = \ 0\ ,$$

and by (3.141) that:

$$\vec{h}_\gamma^+ \ = \ \vec{0}\ , \qquad \gamma = 1, 2\ .$$

As a consequence of these two postulates, (4.17) and (4.18) are satisfied identically.

According to (4.11), the free energies f_α are independent of the density gradients $\vec{h}_\gamma$. The same holds for the free energy f of a mixture, because of its definition (3.96). Consequently, (3.121), yields

$$\vec{p}_\gamma \ \equiv \ \vec{0}\ , \qquad \gamma = 1, 2\ , \tag{4.19}$$

and the equilibrium conditions (3.133)-(3.139) can be reduced to the form (3.143)-(3.149). In the case of a 2-component mixture, they become:

$$0 \ = \ (g_1^+ - g_2^+) \left(\frac{\partial r_1}{\partial \rho_\alpha}\right)^+ , \qquad \alpha = 1, 2\ , \tag{4.20}$$

$$\vec{0} \ = \ (g_1^+ - g_2^+) \left(\frac{\partial r_1}{\partial \vec{h}_\alpha}\right)^+ , \qquad \alpha = 1, 2\ , \tag{4.21}$$

$$\mathbf{0} \ = \ (g_1^+ - g_2^+) \left(\frac{\partial r_1}{\partial \mathbf{D}_\alpha}\right)^+ \ - \ \rho_\alpha^+ (g_\alpha^+ - f_\alpha^+) \mathbf{1} \ - \ \mathbf{T}_\alpha^+\ , \qquad \alpha = 1, 2\ , \tag{4.22}$$

$$\mathbf{0} \ = \ (g_1^+ - g_2^+) \left(\frac{\partial r_1}{\partial \mathbf{\Omega}_1}\right)^+ , \tag{4.23}$$

$$\vec{0} \ = \ \vec{k}_1^+ \ + \ (g_1^+ - g_2^+) \left(\frac{\partial r_1}{\partial \vec{u}_1}\right)^+ , \tag{4.24}$$

$$0 \ = \ (g_1^+ - g_2^+) \left(\frac{\partial r_1}{\partial T}\right)^+ , \tag{4.25}$$

$$\vec{0} \ = \ \frac{1}{T^+}\, \vec{q}^+ \ + \ (g_1^+ - g_2^+) \left(\frac{\partial r_1}{\partial \vec{g}}\right)^+ . \tag{4.26}$$

We have omitted the superscripts *sym.* and *antis.* in (4.22) and (4.23), respectively, since (4.22) is already symmetric (see (3.49)) and (4.23) is antisymmetric due to the antisymmetry of $\mathbf{\Omega_1}$.

Equations (4.10)-(4.15) imply that (4.21) and (4.23) are satisfied automatically, since r_1 does not depend on $\vec{h}_1$, nor $\mathbf{\Omega_1}$. Moreover, r_1 does not depend on $\vec{u}_1$ and $\vec{g}$, hence equations (4.24) and (4.26), yield

$$\vec{k}_1^+ \;=\; \vec{0} \;, \qquad \text{and} \qquad \vec{q}^{\,+} \;=\; \vec{0} \;.$$

If we assume that either

$$\left(\frac{\partial r_1}{\partial \rho_\alpha}\right)^+ \;\neq\; 0 \;, \qquad \text{or} \qquad \left(\frac{\partial r_1}{\partial T}\right)^+ \;\neq\; 0 \;,$$

then (4.20) or (4.25) imply that

$$g_1^+ \;=\; g_2^+ . \tag{4.27}$$

This result was expected as g_1 and g_2 are *chemical potentials* of the two phases. Finally, (4.22) states that

$$\mathbf{T}_\alpha^+ \;=\; -\rho_\alpha^+ (g_\alpha^+ - f_\alpha^+)\mathbf{1} \;, \tag{4.28}$$

hence the Cauchy stress tensor in equilibrium reduces to an isotropic tensor.

4.4 Further reductions by the entropy principle

In this section we employ the entropy principle to simplify the constitutive model. Inspecting (3.123)-(3.126) we see that they are satisfied identically due to (4.10)–(4.15), (4.19), except (3.125) which now reads

$$\mathbf{0} \;=\; \left[\rho_1 \frac{\partial f_1}{\partial \mathbf{D}_1} \otimes \vec{u}_1\right]^{sym.} , \qquad \mathbf{0} \;=\; \left[\rho_1 \frac{\partial f_1}{\partial \mathbf{D}_2} \otimes \vec{u}_1\right]^{sym.} . \tag{4.29}$$

According to (4.11), we have

$$f_1 \;=\; f_1^{(0)}(\rho_\gamma, T) \;+\; f_1^{(1)}(\rho_\gamma, T)\;\mathrm{tr}\mathbf{D}_1 + \; f_1^{(2)}(\rho_\gamma, T)\;\mathrm{tr}\mathbf{D}_2 \;, \tag{4.30}$$

hence, the differentiation of f_1 with respect to $\mathbf{D}_1$ reads

$$\begin{aligned} \left(\frac{\partial f_1}{\partial \mathbf{D_1}}\right)_{ij} \;&=\; \frac{\partial f_1}{\partial D_{1ij}} \\ &=\; f_1^{(1)}(\rho_\gamma, T)\delta_{ij} \;. \end{aligned} \tag{4.31}$$

Then, according to (3.116), the first condition in (4.29) reads

$$\frac{1}{2}\rho_1 f_1^{(1)} \left(\delta_{ij} u_{1k} + \delta_{ik} u_{1j}\right) \;=\; 0 \;, \qquad\qquad \forall\; i, j, k = 1, 2, 3 \;. \tag{4.32}$$

Provided that $\vec{u}_1 \not\equiv \vec{0}$, we can always achieve by a suitable choice of the coordinate system the relationship

$$u_{11} \neq 0,\ u_{12} = u_{13} = 0\ .$$

In particular for $i = j = 3, k = 1$, we obtain:

$$\rho_1 f_1^{(1)} \ \equiv\ 0\ . \tag{4.33}$$

For a non-zero water-density ρ_1 we immediately find

$$f_1^{(1)}(\rho_\gamma, T) \ =\ 0\ . \tag{4.34}$$

Provided that the function $f_1^{(1)}(\rho_\gamma, T)$ is a continuous function of its arguments, we extend $f_1^{(1)}$ for $\rho_1 = 0$ by the limit

$$f_1^{(1)}(\rho_1 = 0, \rho_2, T) \ =\ \lim_{\rho_1 \to 0} f_1^{(1)}(\rho_\gamma, T) \ =\ 0\ ,$$

and thus obtain

$$f_1^{(1)}(\rho_\gamma, T) \ \equiv\ 0\ . \tag{4.35}$$

The second condition in (4.29) can be analyzed in exactly the same way to obtain (under the same assumptions of continuity of $f_1^{(2)}(\rho_\gamma, T)$)

$$f_1^{(2)}(\rho_\gamma, T) \ \equiv\ 0\ . \tag{4.36}$$

To conclude, eq. (4.29) yields

$$f_1 \ =\ f_1(\rho_\gamma, T), \tag{4.37}$$

where we have omitted the superscript $^{(0)}$.

Let us recall (3.119), which implies that

$$\frac{\partial f}{\partial \mathbf{D}_\gamma} \ \equiv\ \mathbf{0}\ , \qquad\qquad \gamma = 1, 2\ ,$$

where f is the free energy of mixture, defined by (3.96) as $\rho f = \rho_1 f_1 + \rho_2 f_2$. Having shown that f_1 is independent of $\mathbf{D}_\gamma$, we see that

$$\frac{\partial f_2}{\partial \mathbf{D}_\gamma} \equiv\ \mathbf{0}\ , \qquad\qquad \gamma = 1, 2\ . \tag{4.38}$$

Due to (4.11) for $\alpha = 2$,

$$f_2 \ =\ f_2^{(0)}(\rho_\gamma, T) \ +\ f_2^{(1)}(\rho_\gamma, T)\ \mathrm{tr}\mathbf{D}_1 +\ f_2^{(2)}(\rho_\gamma, T)\ \mathrm{tr}\mathbf{D}_2\ ,$$

and the constraint (4.38), we have

$$f_2^{(1)} \ \equiv\ 0\ , \tag{4.39}$$

$$f_2^{(2)} \ \equiv\ 0\ , \tag{4.40}$$

and, consequently,

$$f_2 \;=\; f_2(\rho_\gamma, T)\ , \tag{4.41}$$

where the superscript $^{(0)}$ has been omitted.

The reduced entropy inequality (3.127) has the following form:

$$\begin{aligned}
0 \;\geq\; & \left(\rho_1 \frac{\partial f_1}{\partial \rho_1} - (g_1 - f_1) + \omega_1\right) \vec{h}_1 \cdot \vec{u}_1 \;+\; \left(\rho_1 \frac{\partial f_1}{\partial \rho_2} + \omega_2\right) \vec{h}_2 \cdot \vec{u}_1 \\
+ \; & \left\{\rho_1 \left(\frac{\partial f_1}{\partial T} + s_1^{(0)} + s_1^{(1)}\ \mathrm{tr}\mathbf{D}_1 + s_1^{(2)}\ \mathrm{tr}\mathbf{D}_2\right) - \frac{\lambda}{T} - \xi\right\} \vec{g} \cdot \vec{u}_1 \;+\; \frac{\chi_1}{T} \vec{h}_1 \cdot \vec{g} \;+\; \frac{\chi_2}{T} \vec{h}_2 \cdot \vec{g} \\
+ \; & \left(\frac{1}{2}\left(r_1^{(0)} + r_1^{(1)}\ \mathrm{tr}\mathbf{D}_1 + r_1^{(2)}\ \mathrm{tr}\mathbf{D}_2\right) \;-\nu\right) \vec{u}_1^2 \;-\; \frac{k}{T} \vec{g}^2 \;-\; \rho_1 (g_1 - f_1) \mathrm{tr}\mathbf{D}_1 \\
- \; & \rho_2 (g_2 - f_2) \mathrm{tr}\mathbf{D}_2 \;+\; (g_1 - g_2)(r_1^{(0)} + r_1^{(1)}\ \mathrm{tr}\mathbf{D}_1 + r_1^{(2)}\ \mathrm{tr}\mathbf{D}_2) \;-\; \mathbf{T}_1 : \mathbf{D}_1 \;-\; \mathbf{T}_2 : \mathbf{D}_2\ .
\end{aligned} \tag{4.42}$$

This inequality must hold for any values of the independent variables, particularly for any arbitrary $\vec{h}_1$, $\vec{h}_2$, $\vec{u}_1$, $\vec{g}$, $\mathbf{D}_1$, $\mathbf{D}_2$. We now consider various combinations of these variables:

- for $\vec{h}_1$ arbitrary, $\vec{h}_2 = \vec{u}_1 = \vec{g} = \vec{0}$, $\mathbf{D}_1 = \mathbf{D}_2 = \mathbf{0}$:

  $$0 \;\geq\; (g_1 - g_2) r_1^{(0)}\ . \tag{4.43}$$

  This confirms the expected "direction" of the reaction from higher to lower chemical potential.

- for $\vec{u}_1$ arbitrary, $\vec{h}_1 = \vec{h}_2 = \vec{g} = \vec{0}$, $\mathbf{D}_1 = \mathbf{D}_2 = \mathbf{0}$:

  $$0 \;\geq\; \left(\frac{1}{2} r_1^{(0)} - \nu\right) \vec{u}_1^2 \;+\; (g_1 - g_2) r_1^{(0)}. \tag{4.44}$$

  Since the second term is independent of $\vec{u}_1$, we find that the term in parenthesis must always be non-positive:

  $$\frac{1}{2} r_1^{(0)} - \nu \;\leq\; 0\ , \qquad \text{or} \qquad \frac{1}{2} r_1^{(0)} \;\leq\; \nu\ . \tag{4.45}$$

- for $\vec{g}$ arbitrary, $\vec{h}_1 = \vec{h}_2 = \vec{u}_1 = \vec{0}$, $\mathbf{D}_1 = \mathbf{D}_2 = \mathbf{0}$:

  $$0 \;\geq\; -\frac{k}{T}\, \vec{g}^2 \;+\; (g_1 - g_2) r_1^{(0)}. \tag{4.46}$$

  Since the second term does not depend on $\vec{g}$, and since T is a positive quantity, it must hold that

  $$k \;\geq\; 0\ . \tag{4.47}$$

- for $\vec{h}_1,\ \vec{u}_1$ arbitrary, $\vec{h}_2 = \vec{g} = \vec{0}$, $\mathbf{D}_1 = \mathbf{D}_2 = \mathbf{0}$:

$$0 \ \geq \ \left(\rho_1 \frac{\partial f_1}{\partial \rho_1} - (g_1 - f_1) + \omega_1\right) \vec{h}_1 \cdot \vec{u}_1 \ + \ \left(\frac{1}{2} r_1^{(0)} - \nu\right) \vec{u}_1^2 \ + \ (g_1 - g_2) r_1^{(0)}. \quad (4.48)$$

Since the last two terms are independent of $\vec{h}_1$, the term in the first parenthesis must vanish:

$$\rho_1 \frac{\partial f_1}{\partial \rho_1} - (g_1 - f_1) + \omega_1 \ \equiv \ 0 \quad (4.49)$$

- for $\vec{h}_1,\ \vec{g}$ arbitrary, $\vec{h}_2 = \vec{u}_1 = \vec{0}$, $\mathbf{D}_1 = \mathbf{D}_2 = \mathbf{0}$:

$$0 \ \geq \ \frac{\chi_1}{T} \vec{h}_1 \cdot \vec{g} \ - \ \frac{k}{T} \vec{g}^2 \ + \ (g_1 - g_2) r_1^{(0)}. \quad (4.50)$$

Since the last two terms are independent of $\vec{h}_1$, we find

$$\chi_1 \ \equiv \ 0 \ . \quad (4.51)$$

- for $\vec{h}_2,\ \vec{u}_1$ arbitrary, $\vec{h}_1 = \vec{g} = \vec{0}$, $\mathbf{D}_1 = \mathbf{D}_2 = \mathbf{0}$:

$$0 \ \geq \ \left(\rho_1 \frac{\partial f_1}{\partial \rho_2} + \omega_2\right) \vec{h}_2 \cdot \vec{u}_1 \ + \ \left(\frac{1}{2} r_1^{(0)} - \nu\right) \vec{u}_1^2 \ + \ (g_1 - g_2) r_1^{(0)} \ . \quad (4.52)$$

The last two terms are independent of $\vec{h}_2$, thus we obtain

$$\rho_1 \frac{\partial f_1}{\partial \rho_2} \ + \ \omega_2 \ \equiv \ 0 \ . \quad (4.53)$$

- for $\vec{h}_2,\ \vec{g}$ arbitrary, $\vec{h}_1 = \vec{u}_1 = \vec{0}$, $\mathbf{D}_1 = \mathbf{D}_2 = \mathbf{0}$:

$$0 \ \geq \ \frac{\chi_2}{T} \vec{h}_2 \cdot \vec{g} \ - \ \frac{k}{T} \vec{g}^2 \ + \ (g_1 - g_2) r_1^{(0)} \ , \quad (4.54)$$

since the last two terms are independent of $\vec{h}_2$, we obtain

$$\chi_2 \ \equiv \ 0 \ . \quad (4.55)$$

Other combinations of variables need not be considered, since they do not provide any exploitable constraints. The entropy inequality (4.42) now reads

$$\begin{aligned} 0 \ \geq \ & \left\{ \rho_1 \left(\frac{\partial f_1}{\partial T} + s_1^{(0)} + s_1^{(1)} \ \mathrm{tr}\mathbf{D}_1 + s_1^{(2)} \ \mathrm{tr}\mathbf{D}_2 \right) - \frac{\lambda}{T} - \xi \right\} \vec{u}_1 \cdot \vec{g} \\ + \ & \left(\frac{1}{2} \left(r_1^{(0)} + r_1^{(1)} \ \mathrm{tr}\mathbf{D}_1 + r_1^{(2)} \ \mathrm{tr}\mathbf{D}_2 \right) - \nu \right) \vec{u}_1^2 - \ \frac{k}{T} \vec{g}^2 - \ \rho_1 (g_1 - f_1) \ \mathrm{tr}\mathbf{D}_1 \\ - \ & \rho_2 (g_2 - f_2) \ \mathrm{tr}\mathbf{D}_2 \ + \ (g_1 - g_2)(r_1^{(0)} + r_1^{(1)} \ \mathrm{tr}\mathbf{D}_1 + r_1^{(2)} \ \mathrm{tr}\mathbf{D}_2) \\ - \ & \mathbf{T}_1 : \mathbf{D}_1 \ - \ \mathbf{T}_2 : \mathbf{D}_2 \ . \end{aligned} \quad (4.56)$$

Having exploited the entropy principle, we arrived at:

$$\begin{aligned}
r_1 &= r_1^{(0)}(\rho_\gamma, T) \;+\; r_1^{(1)}(\rho_\gamma, T)\ \mathrm{tr}\mathbf{D}_1 + \; r_1^{(2)}(\rho_\gamma, T)\ \mathrm{tr}\mathbf{D}_2, && (4.57)\\
f_\alpha &= f_\alpha^{(0)}(\rho_\gamma, T)\ , && (4.58)\\
s_\alpha &= s_\alpha^{(0)}(\rho_\gamma, T) \;+\; s_\alpha^{(1)}(\rho_\gamma, T)\ \mathrm{tr}\mathbf{D}_1 + \; s_\alpha^{(2)}(\rho_\gamma, T)\ \mathrm{tr}\mathbf{D}_2, && (4.59)\\
\vec{q} &= -\, k(\rho_\gamma, T)\vec{g} \;-\; \lambda(\rho_\gamma, T)\vec{u}_1\ , && (4.60)\\
\vec{k}_1 &= -\, \xi(\rho_\gamma, T)\vec{g} \;-\; \nu(\rho_\gamma, T)\vec{u}_1 \;+\; \sum_{\psi=1}^{2} \omega_\psi(\rho_\gamma, T)\vec{h}_\psi\ , && (4.61)\\
\mathbf{T}_\alpha &= \mathbf{T}_\alpha(\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}), && (4.62)
\end{aligned}$$

4.5 Linearization with respect to the water content

In this section we make use of the fact that the water fraction (defined below) in the temperate-ice region of a glacier is only a few percent (Hutter, [4]). If we assume that the constitutive functionals are continuous and differentiable in densities ρ_1, ρ_2, and their gradients $\vec{h}_1$, $\vec{h}_2$, it is reasonable to expand the constitutive functionals into a Taylor series with respect to the water content and its gradient. This procedure, together with several additional assumptions, will provide new constraints on the constitutive model.

Let $\psi(\rho_\gamma, T)$ be any quantity occurring in the constitutive equations (4.57)–(4.61). Defining the *water mass fraction* w

$$w \;=\; \frac{\rho_1}{\rho}\ , \tag{4.63}$$

where $\rho = \rho_1 + \rho_2$ is the density of mixture, see (3.33), we can write

$$\rho_1 \;=\; w\,\rho\ , \tag{4.64}$$

$$\rho_2 \;=\; (1-w)\,\rho\ , \tag{4.65}$$

and consider a formal substitution

$$\psi(\rho_1, \rho_2, T) \;\longrightarrow\; \psi(w, \rho, T)\ .$$

Under the assumption of differentiability of the model with respect to w[1], we perform the Taylor expansion in the vicinity of $w = 0$:

$$\begin{aligned}
\psi(w, \rho, T) \;&=\; \psi(0, \rho, T) \;+\; w\, \left.\frac{\partial \psi(w, \rho, T)}{\partial w}\right|_{w=0} + O(w^2)\\
&=\; \tilde{\psi}(\rho, T) \;+\; w\hat{\psi}(\rho, T) \;+\; O(w^2),
\end{aligned} \tag{4.66}$$

where the first two terms are expressed explicitly. Since w small, at most a few percent (Hutter, [4]), we omit the higher-order terms in (4.66) and write a linearized form:

$$\psi \;= \tilde{\psi}(\rho, T) \;+\; w\hat{\psi}(\rho, T)\ . \tag{4.67}$$

---

[1] This assumption might be questionable since the presence of water may cause a discontinuity in several material parameters, but we will not consider this case here in accordance with the traditional approach in glaciology.

We will now apply the linearized form (4.67) to the bracketed terms in (4.57)–(4.61) and will only keep the terms linear with respect to $w, \vec{h}_\gamma, \vec{u}_1, \vec{g}, \mathbf{D}_\gamma$, where possible and physically meaningful leading terms elsewhere. Applying (4.67) to (4.57), we have

- r_1 :

$$\begin{aligned} r_1 &= \tilde{r}_1^{(0)}(\rho,T) + \tilde{r}_1^{(1)}(\rho,T)\ \mathrm{tr}\mathbf{D}_1 + \tilde{r}_1^{(2)}(\rho,T)\ \mathrm{tr}\mathbf{D}_2 \\ &+ w(\hat{r}_1^{(0)}(\rho,T) + \hat{r}_1^{(1)}(\rho,T)\ \mathrm{tr}\mathbf{D}_1 + \hat{r}_1^{(2)}(\rho,T)\ \mathrm{tr}\mathbf{D}_2)\ . \end{aligned} \tag{4.68}$$

We may observe two non-linear terms: $w\ \mathrm{tr}\mathbf{D}_1$ and $w\ \mathrm{tr}\mathbf{D}_2$. We want to keep such nonlinear terms in the expansions only provided they represent the leading terms for particular physical process. From this point of view, we may omit $\hat{r}_1^{(2)} w\ \mathrm{tr}\mathbf{D}_2$, as the leading term for the dependence of r_1 upon $\mathrm{tr}\mathbf{D}_2$ is the term $\tilde{r}_1^{(2)}\ \mathrm{tr}\mathbf{D}_2$ (w is small), but we keep the term with $w\ \mathrm{tr}\mathbf{D}_1$ as it will be shown to be the leading one for the dependence of r_1 upon $\mathrm{tr}\mathbf{D}_1$. Thus now we have:

$$r_1 = \tilde{r}_1^{(0)}(\rho,T) + w\hat{r}_1^{(0)}(\rho,T) + (\tilde{r}_1^{(1)}(\rho,T) + w\,\hat{r}_1^{(1)}(\rho,T))\ \mathrm{tr}\mathbf{D}_1 + \tilde{r}_1^{(2)}(\rho,T)\ \mathrm{tr}\mathbf{D}_2\ . \tag{4.69}$$

Inspecting this relation for the case when approaching the cold-ice case (i.e. here $w \to 0$), we must conclude that $\tilde{r}_1^{(1)} \equiv 0$, since no dependence on the water-component tensor $\mathbf{D}_1$ should persist. The conclusion is thus:

$$r_1 = \tilde{r}_1^{(0)}(\rho,T) + w\hat{r}_1^{(0)}(\rho,T) + w\hat{r}_1^{(1)}(\rho,T)\ \mathrm{tr}\mathbf{D}_1 + \tilde{r}_1^{(2)}(\rho,T)\ \mathrm{tr}\mathbf{D}_2\ . \tag{4.70}$$

- f_α, $\alpha = 1,2$:

$$f_\alpha = \tilde{f}_\alpha(\rho,T) + w\hat{f}_\alpha(\rho,T)\ . \tag{4.71}$$

- s_α, $\alpha = 1,2$:

$$\begin{aligned} s_\alpha &= \tilde{s}_\alpha^{(0)}(\rho,T) + \tilde{s}_\alpha^{(1)}(\rho,T)\ \mathrm{tr}\mathbf{D}_1 + \tilde{s}_\alpha^{(2)}(\rho,T)\ \mathrm{tr}\mathbf{D}_2 \\ &+ w(\hat{s}_\alpha^{(0)}(\rho,T) + \hat{s}_\alpha^{(1)}(\rho,T)\ \mathrm{tr}\mathbf{D}_1 + \hat{s}_\alpha^{(2)}(\rho,T)\ \mathrm{tr}\mathbf{D}_2)\ . \end{aligned} \tag{4.72}$$

The entropy of the mixture was defined in (3.97) as

$$\begin{aligned} s &= \frac{\rho_1}{\rho}\,s_1 + \frac{\rho_2}{\rho}\,s_2 \\ &= w\,s_1 + (1-w)\,s_2\ . \end{aligned}$$

By (4.72), we have

$$\begin{aligned} s &= \tilde{s}_2^{(0)} + \tilde{s}_2^{(1)}\ \mathrm{tr}\mathbf{D}_1 + \tilde{s}_2^{(2)}\ \mathrm{tr}\mathbf{D}_2 \\ &+ w(\tilde{s}_1^{(0)} + \tilde{s}_1^{(1)}\ \mathrm{tr}\mathbf{D}_1 + \tilde{s}_1^{(2)}\ \mathrm{tr}\mathbf{D}_2 + \hat{s}_2^{(0)} + \hat{s}_2^{(1)}\ \mathrm{tr}\mathbf{D}_1 + \hat{s}_2^{(2)}\ \mathrm{tr}\mathbf{D}_2 \\ &- \tilde{s}_2^{(0)} - \tilde{s}_2^{(1)}\ \mathrm{tr}\mathbf{D}_1 - \tilde{s}_2^{(2)}\ \mathrm{tr}\mathbf{D}_2) \\ &+ w^2(\hat{s}_1^{(0)} + \hat{s}_1^{(1)}\ \mathrm{tr}\mathbf{D}_1 + \hat{s}_1^{(2)}\ \mathrm{tr}\mathbf{D}_2 - \hat{s}_2^{(0)} - \hat{s}_2^{(1)}\ \mathrm{tr}\mathbf{D}_1 - \hat{s}_2^{(2)}\ \mathrm{tr}\mathbf{D}_2)\ . \end{aligned} \tag{4.73}$$

Making use of the result (3.122) implies

$$\frac{\partial s}{\partial \mathbf{D}_1} \equiv 0 \; , \qquad \frac{\partial s}{\partial \mathbf{D}_2} \equiv 0 \; , \tag{4.74}$$

which due to the fact that (4.73) is a polynomial in w results in the following identities:

$$\begin{aligned} \tilde{s}_2^{(1)} &\equiv 0 \; , \\ \tilde{s}_2^{(2)} &\equiv 0 \; , \\ \tilde{s}_1^{(1)} &\equiv -\hat{s}_2^{(1)} \; , \\ \hat{s}_1^{(1)} &\equiv \hat{s}_2^{(1)} \; , \\ \tilde{s}_1^{(2)} &\equiv -\hat{s}_2^{(2)} \; , \\ \hat{s}_1^{(2)} &\equiv \hat{s}_2^{(2)} \; . \end{aligned} \tag{4.75}$$

We thus arrive at the following expansions:

$$s_1 \; = \; \tilde{s}_1^{(0)} + w\hat{s}_1^{(0)} + (1-w)\tilde{s}_1^{(1)} \; \mathrm{tr}\mathbf{D}_1 + (1-w)\tilde{s}_1^{(2)} \; \mathrm{tr}\mathbf{D}_2 \; ,$$

where we decide to neglect terms w tr$\mathbf{D}_1$, w tr$\mathbf{D}_2$ being small compared with tr$\mathbf{D}_1$, tr$\mathbf{D}_2$, respectively, and write

$$s_1 \; = \; \tilde{s}_1^{(0)}(\rho,T) + w\hat{s}_1^{(0)}(\rho,T) + \tilde{s}_1^{(1)}(\rho,T) \; \mathrm{tr}\mathbf{D}_1 + \tilde{s}_1^{(2)}(\rho,T) \; \mathrm{tr}\mathbf{D}_2 \; , \tag{4.76}$$

for s_1, for s_2 the result is

$$s_2 \; = \; \tilde{s}_2^{(0)}(\rho,T) + w\hat{s}_2^{(0)}(\rho,T) - w\tilde{s}_1^{(1)}(\rho,T) \; \mathrm{tr}\mathbf{D}_1 - w\tilde{s}_1^{(2)}(\rho,T) \; \mathrm{tr}\mathbf{D}_2 \; . \tag{4.77}$$

- $\vec{q}$:
  The expansion of the coefficients k and λ in the constitutive equation (4.60) for $\vec{q}$ yields

  $$\vec{q} \; = \; -(\tilde{k}(\rho,T) + w\hat{k}(\rho,T))\vec{g} \; - \; (\tilde{\lambda}(\rho,T) \; + \; w\hat{\lambda}(\rho,T))\vec{u}_1 \; .$$

  Since the total thermal conductivity of the ice-water mixture may be sensitive to the water content, we suggest to keep the non-linear term $\hat{k}(\rho,T)\, w\vec{g}$. Moreover the last term $\hat{\lambda}(\rho,T)w\vec{u}_1$ can be identified as the Dufour effect ([16]), we thus keep it in the expansion as well. Now we realize, that for the case of the water content and its gradients of higher orders going to zero, the constitutive functional should match the situation for a cold ice, in particular the heat flux must be independent of the diffusive velocity $\vec{u}_1$. This implies that

  $$\tilde{\lambda}(\rho,T) \equiv 0 \; , \tag{4.78}$$

  and we finally arrive at an expression:

  $$\vec{q} \; = \; -(\tilde{k}(\rho,T) + w\hat{k}(\rho,T))\vec{g} \; - \; \lambda(\rho,T)w\vec{u}_1 \; , \tag{4.79}$$

  where the label ˜ at λ was dropped out.

- $\vec{k}_1$:
  To linearize $\vec{k}_1$, we must first deal with the terms $\omega_1 \vec{h}_1$ and $\omega_2 \vec{h}_2$. By (4.49), we have:

$$\omega_1 \ = \ g_1 - f_1 \ - \ \rho_1 \frac{\partial f_1}{\partial \rho_1} \ . \tag{4.80}$$

The chemical potential g_1 was defined by (3.121):

$$\begin{aligned} g_1 \quad &= \quad \frac{\partial(\rho f(\rho_\gamma, T))}{\partial \rho_1} \\ &= \quad \frac{\partial}{\partial \rho_1}(\rho_1 f_1(\rho_\gamma, T) + \rho_2 f_2(\rho_\gamma, T)) \\ &= \quad f_1(\rho_\gamma, T) + \rho_1 \frac{\partial f_1(\rho_\gamma, T)}{\partial \rho_1} + \rho_2 \frac{\partial f_2(\rho_\gamma, T)}{\partial \rho_1} \ , \end{aligned}$$

hence

$$\omega_1 \quad = \quad \rho_2 \frac{\partial f_2(\rho_\gamma, T)}{\partial \rho_1} \ .$$

However,

$$\begin{aligned} \frac{\partial f_2(\rho_\gamma, T)}{\partial \rho_1} \quad &= \quad \left.\frac{\partial}{\partial \rho_1}\right|_{\rho_2, T} (\tilde{f}_2(\rho, T) + w \, \hat{f}_2(\rho, T)) \\ &= \quad \left.\frac{\partial}{\partial \rho_1}\right|_{\rho_2, T} \left(\tilde{f}_2(\rho_1 + \rho_2, T) \ + \frac{\rho_1}{\rho_1 + \rho_2} \, \hat{f}_2(\rho_1 + \rho_2, T) \right) \\ &= \quad \frac{\partial \tilde{f}_2(\rho, T)}{\partial \rho} + \frac{\rho_2}{(\rho_1 + \rho_2)^2} \, \hat{f}_2(\rho, T) + \frac{\rho_1}{\rho_1 + \rho_2} \, \frac{\partial \hat{f}_2(\rho, T)}{\partial \rho} \\ &= \quad \frac{\partial \tilde{f}_2(\rho, T)}{\partial \rho} + \frac{(1 - w)}{\rho} \, \hat{f}_2(\rho, T) + w \, \frac{\partial \hat{f}_2(\rho, T)}{\partial \rho} \\ &= \quad \frac{\partial \tilde{f}_2(\rho, T)}{\partial \rho} + \frac{\hat{f}_2(\rho, T)}{\rho} + w \left\{ \frac{\partial \hat{f}_2(\rho, T)}{\partial \rho} - \frac{\hat{f}_2(\rho, T)}{\rho} \right\} , \end{aligned}$$

therefore ω_1 then reads

$$\begin{aligned} \omega_1 \quad &= \quad \rho \, (1 - w) \left(\frac{\partial \tilde{f}_2(\rho, T)}{\partial \rho} + \frac{\hat{f}_2(\rho, T)}{\rho} + w \left\{ \frac{\partial \hat{f}_2(\rho, T)}{\partial \rho} - \frac{\hat{f}_2(\rho, T)}{\rho} \right\} \right) \\ &= \quad \rho \, \frac{\partial \tilde{f}_2(\rho, T)}{\partial \rho} + \hat{f}_2(\rho, T) \\ &+ \quad w \left\{ \rho \, \frac{\partial \hat{f}_2(\rho, T)}{\partial \rho} - 2 \hat{f}_2(\rho, T) - \rho \, \frac{\partial \tilde{f}_2(\rho, T)}{\partial \rho} + w \, \hat{f}_2(\rho, T) \ - \ w \rho \, \frac{\partial \hat{f}_2(\rho, T)}{\partial \rho} \right\} \\ &. \end{aligned} \tag{4.81}$$

Using (4.53) we have

$$\omega_2 \quad = \quad -\rho w \, \frac{\partial f_1(\rho_\gamma, T)}{\partial \rho_2}$$

$$
\begin{aligned}
&= -\rho w \left. \frac{\partial(\tilde{f}_1(\rho,T) + w\hat{f}_1(\rho,T))}{\partial \rho_2} \right|_{\rho_1,T} \\
&= -\rho w \left. \frac{\partial}{\partial \rho_2} \right|_{\rho_1,T} \left(\tilde{f}_1(\rho_1+\rho_2,T) \; + \; \frac{\rho_1}{\rho_1+\rho_2}\, \hat{f}_1(\rho_1+\rho_2,T) \right) \\
&= -\rho w \left(\frac{\partial \tilde{f}_1(\rho,T)}{\partial \rho} \; - \; \frac{\rho_1}{(\rho_1+\rho_2)^2}\, \hat{f}_1(\rho,T) \; + \; \frac{\rho_1}{\rho_1+\rho_2}\, \frac{\partial \hat{f}_1(\rho,T)}{\partial \rho} \right) \\
&= -\rho w \left(\frac{\partial \tilde{f}_1(\rho,T)}{\partial \rho} \; - \; w\, \frac{\hat{f}_1(\rho,T)}{\rho} \; + \; w\, \frac{\partial \hat{f}_1(\rho,T)}{\partial \rho} \right) \; . \qquad (4.82)
\end{aligned}
$$

For the remaining coefficients we have the linearized expansion

$$
\begin{aligned}
\xi \; &= \tilde{\xi}(\rho,T) + w\,\hat{\xi}(\rho,T) \; , \\
\nu \; &= \tilde{\nu}(\rho,T) + w\,\hat{\nu}(\rho,T) \; .
\end{aligned}
$$

We rewrite $\vec{h}_1$, $\vec{h}_2$, according to their definition (3.83) and with the use of (4.64), (4.65), as

$$
\begin{aligned}
\vec{h}_1 \quad &= \quad \mathrm{grad}(\rho\, w) \; = \; \rho\, \mathrm{grad} w + w\, \mathrm{grad}\rho \; , && (4.83) \\
\vec{h}_2 \quad &= \quad \mathrm{grad}(\rho\,(1-w)) \; = \; -\rho\, \mathrm{grad} w + (1-w)\, \mathrm{grad}\rho \; , && (4.84)
\end{aligned}
$$

and assert that $\vec{k}_1 \to \vec{0}$ as $w \to 0$ and $\mathrm{grad} w \to \vec{0}$, since this limit (possibly also with higher-order gradients of w going to zero) corresponds to the cold-ice case, where the interaction volume force should vanish, i.e. $\vec{k}_1 = \vec{0}$. We assume the constitutive functionals to possess sufficient smoothness enabling such considerations. As a result of the limit constraint we obtain

$$
\begin{aligned}
\tilde{\xi}(\rho,T) \quad &\equiv \quad 0 \; , && (4.85) \\
\tilde{\nu}(\rho,T) \quad &\equiv \quad 0 \; . && (4.86)
\end{aligned}
$$

We neglect the following nonlinear terms: $w\, \mathrm{grad} w$, $w\, \mathrm{grad}\rho$, $O(w^2)$, in accordance with our assumption of low water content w and also small magnitude of the water-content gradient, moreover in further we will introduce an assumption of incompressibility, that's why the term $w\, \mathrm{grad}\rho$ can be omitted here as well. With these assumptions we obtain the final expression

$$
\vec{k}_1 \; = -w\xi(\rho,T)\, \vec{g} \; - \; w\nu(\rho,T)\, \vec{u}_1 \; - \; \omega(\rho,T)\, \mathrm{grad} w, \qquad (4.87)
$$

where we omitted the label $\tilde{}$ at ξ, ν, and introduced

$$
\omega \; = \; -\left(\rho^2\, \frac{\partial \tilde{f}_2(\rho,T)}{\partial \rho} + \rho \hat{f}_2(\rho,T) \right) \; . \qquad (4.88)
$$

Note that we didn't neglect nonlinear terms $w\vec{g}$ and $w\vec{u}_1$, since they are now leading terms for the dependence of $\vec{k}_1$ upon $\vec{g}$, $\vec{u}_1$, respectively.

In the case of partial stress tensors $\mathbf{T_1}, \mathbf{T_2}$, we will write the Taylor expansion with respect to both the water content w and its gradient grad$w$, performing first the formal substitution

$$\mathbf{T}_\alpha(\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \to \mathbf{T}_\alpha(w, \mathrm{grad}w, \rho, \mathrm{grad}\rho, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \ .$$

We assume that apart from the water content, also the magnitude of the water-content gradient grad$w$ is small enough to justify neglecting the terms of quadratic and higher order in the Taylor expansion.

- $\mathbf{T}_1$:
  The expansion of the Cauchy stress tensor for the water component $\mathbf{T}_1$ then reads

$$\begin{aligned} \mathbf{T}_1 \quad &= \quad \tilde{\mathbf{T}}_1(\rho, \mathrm{grad}\rho, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \ + \ w\hat{\mathbf{T}}_1(\rho, \mathrm{grad}\rho, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \\ &+ \quad \hat{\hat{\mathbf{T}}}_1(\rho, \mathrm{grad}\rho, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g})\, \mathrm{grad}w \end{aligned} \tag{4.89}$$

  where following the notation introduced above, we denoted

$$\tilde{\mathbf{T}}_1 \quad = \quad \mathbf{T_1}\big|_{w=0,\mathrm{grad}w=\vec{0}} \ , \tag{4.90}$$

$$\hat{\mathbf{T}}_1 \quad = \quad \left.\frac{\partial \mathbf{T_1}}{\partial w}\right|_{w=0,\mathrm{grad}w=\vec{0}} \ , \tag{4.91}$$

  and here we moreover had to introduce a third-order tensor $\hat{\hat{\mathbf{T}}}_1$:

$$\hat{\hat{\mathbf{T}}}_1 \ = \ \left.\frac{\partial \mathbf{T}_1}{\partial \mathrm{grad}w}\right|_{w=0,\mathrm{grad}w=\vec{0}} \ , \tag{4.92}$$

  where (to avoid confusion) the third therm in the expansion (4.89) should be read as

$$(\hat{\hat{\mathbf{T}}}_1\, \mathrm{grad}w)_{ij} \equiv \ (\hat{\hat{\mathbf{T}}}_1)_{ijk} \frac{\partial w}{\partial x_k} \ . \tag{4.93}$$

  It is not obvious that the constitutive relation for the stress tensor is continuous or even differentiable in the water fraction and its gradient. However, following the traditional approach in glaciology, we assume such smoothness.

- $\mathbf{T}_2$:
  Analogously, we expand

$$\begin{aligned} \mathbf{T}_2 \quad &= \quad \tilde{\mathbf{T}}_2(\rho, \mathrm{grad}\rho, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \ + \ w\hat{\mathbf{T}}_2(\rho, \mathrm{grad}\rho, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \\ &+ \quad \hat{\hat{\mathbf{T}}}_2(\rho, \mathrm{grad}\rho, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g})\, \mathrm{grad}w. \end{aligned} \tag{4.94}$$

In the next step, we introduce an incompressibility condition into the constitutive model. This is done by first rewriting the entropy inequality in terms of the barycentric velocity and the diffusive velocity with respect to the barycenter.

4.5.1 Entropy inequality in terms of the barycentric velocity

Considering $r_2 = -r_1$, due to (3.32), the entropy inequality (3.77) for a two-component reacting mixture reads:

$$\begin{aligned} 0 \quad \geq \quad & \rho_1 \grave{f}_1^{1} \;+\; \rho_2 \grave{f}_2^{2} \;+\; r_1 (f_1 - f_2) \;+\; \rho_1 s_1 \grave{T}^{1} \;+\; \rho_2 s_2 \grave{T}^{2} \;+\; \frac{\vec{q}\cdot\vec{g}}{T} \\ - \quad & \mathbf{T}_1 : \mathbf{D}_1 \;-\; \mathbf{T}_2 : \mathbf{D}_2 \;+\; \vec{k}_1 \cdot \vec{u}_1 \;+\; \frac{1}{2} r_1 \vec{u}_1^{\,2} \; . \end{aligned} \tag{4.95}$$

We recall that the superscript $\grave{}^{\alpha}$ denotes the material time derivative with respect to the velocity of the α component. For the following, it is convenient to rewrite the entropy inequality in the following manner.

First we introduce the *barycentric velocity* $\vec{v}^{B}$ by (2.12)

$$\vec{v}^{B} \;=\; \frac{\rho_1}{\rho}\,\vec{v}_1 \;+\; \frac{\rho_2}{\rho}\,\vec{v}_2 \; ,$$

and the *barycentric diffusion velocities* $\vec{u}_1^{B}$, $\vec{u}_2^{B}$

$$\vec{u}_1^{B} \;=\; \vec{v}_1 - \vec{v}^{B} \; , \qquad\qquad \vec{u}_2^{B} \;=\; \vec{v}_2 - \vec{v}^{B} \; . \tag{4.96}$$

Consequently,

$$\rho_1 \vec{u}_1^{B} \;+\; \rho_2 \vec{u}_2^{B} \;=\; \vec{0} \; ,$$

and

$$\vec{u}_2^{B} \;=\; -\frac{\rho_1}{\rho_2}\,\vec{u}_1^{B} \; . \tag{4.97}$$

We now may write

$$\begin{aligned} \grave{f}_1^{1} \;&=\; \frac{\partial f_1}{\partial t} \;+\; \operatorname{grad} f_1 \cdot \vec{v}_1 \\ &=\; \frac{\partial f_1}{\partial t} \;+\; \operatorname{grad} f_1 \cdot \vec{v}^{B} \;+\; \operatorname{grad} f_1 \cdot \vec{u}_1^{B} \\ &=\; \grave{f}_1^{B} \;+\; \operatorname{grad} f_1 \cdot \vec{u}_1^{B} \; , \end{aligned} \tag{4.98}$$

where $\grave{}^{B}$ now denotes the material time derivative with respect to the barycentric velocity. Similarly, we obtain

$$\begin{aligned} \grave{f}_2^{2} \;&=\; \grave{f}_2^{B} \;+\; \operatorname{grad} f_2 \cdot \vec{u}_2^{B} \\ &=\; \grave{f}_2^{B} \;-\; \frac{\rho_1}{\rho_2} \operatorname{grad} f_2 \cdot \vec{u}_1^{B} \; , \end{aligned} \tag{4.99}$$

where we made use of (4.97). Analogously, it holds

$$\grave{T}^{1} \;=\; \grave{T}^{B} \;+\; \vec{g}\cdot\vec{u}_1^{B} \; , \tag{4.100}$$

$$\grave{T}^{2} \;=\; \grave{T}^{B} \;-\; \frac{\rho_1}{\rho_2}\,\vec{g}\cdot\vec{u}_1^{B} \; , \tag{4.101}$$

We can also write

$$\begin{aligned}
\mathbf{D}_1 &= \{\operatorname{grad}\vec{v}_1\}^{sym.} \\
&= \left\{\operatorname{grad}\vec{v}^B \;+\; \operatorname{grad}\vec{u}_1^B\right\}^{sym.} \\
&= \mathbf{D}^B \;+\; \mathbf{D}_1^B\;, \qquad (4.102)
\end{aligned}$$

with

$$\mathbf{D}^B \;=\; \{\operatorname{grad}\vec{v}^B\}^{sym.}, \qquad\qquad \mathbf{D}_1^B \;=\; \{\operatorname{grad}\vec{u}_1^B\}^{sym.}\;, \qquad (4.103)$$

and similarly

$$\begin{aligned}
\mathbf{D}_2 &= \{\operatorname{grad}\vec{v}_2\}^{sym.} \\
&= \left\{\operatorname{grad}\vec{v}^B \;+\; \operatorname{grad}\vec{u}_2^B\right\}^{sym.} \\
&= \left\{\operatorname{grad}\vec{v}^B \;-\; \frac{\rho_1}{\rho_2}\operatorname{grad}\vec{u}_1^B\right\}^{sym.} \\
&= \mathbf{D}^B \;-\; \frac{\rho_1}{\rho_2}\mathbf{D}_1^B\;. \qquad (4.104)
\end{aligned}$$

Finally

$$\begin{aligned}
\vec{u}_1 &= \vec{v}_1 \;-\; \vec{v}_2 \\
&= (\vec{v}^B + \vec{u}_1^B) \;-\; (\vec{v}^B + \vec{u}_2^B) \\
&= \left(1 + \frac{\rho_1}{\rho_2}\right)\vec{u}_1^B. \qquad (4.105)
\end{aligned}$$

We insert the expressions (4.98) – (4.105) into the entropy inequality (4.95) and arrive at the form:

$$\begin{aligned}
0 \;\geq\;& \rho_1\left\{\grave{f}_1^B \;+\; \operatorname{grad} f_1\cdot\vec{u}_1^B\right\} \;+\; \rho_2\left\{\grave{f}_2^B \;-\; \frac{\rho_1}{\rho_2}\operatorname{grad} f_2\cdot\vec{u}_1^B\right\} \;+\; r_1(f_1 - f_2) \\
+\;& \rho_1 s_1\left\{\grave{T}^B \;+\; \vec{g}\cdot\vec{u}_1^B\right\} \;+\; \rho_2 s_2\left\{\grave{T}^B \;-\; \frac{\rho_1}{\rho_2}\vec{g}\cdot\vec{u}_1^B\right\} \;+\; \frac{\vec{q}\cdot\vec{g}}{T} \\
-\;& \mathbf{T}_1 : (\mathbf{D}^B + \mathbf{D}_1^B) \;-\; \mathbf{T}_2 : (\mathbf{D}^B - \frac{\rho_1}{\rho_2}\mathbf{D}_1^B) \;+\; \left(1 + \frac{\rho_1}{\rho_2}\right)\vec{k}_1\cdot\vec{u}_1^B \\
+\;& \frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 r_1(\vec{u}_1^B)^2,
\end{aligned}$$

which, after some rearrangement of the terms, reads

$$\begin{aligned}
0 \;\geq\;& \rho_1\grave{f}_1^B \;+\; \rho_2\grave{f}_2^B \;+\; \rho_1\vec{u}_1^B\cdot\operatorname{grad}(f_1 - f_2) \;+\; r_1(f_1 - f_2) \;+\; (\rho_1 s_1 + \rho_2 s_2)\grave{T}^B \\
+\;& \rho_1(s_1 - s_2)\vec{g}\cdot\vec{u}_1^B \;+\; \frac{\vec{q}\cdot\vec{g}}{T} \;-\; (\mathbf{T}_1 + \mathbf{T}_2) : \mathbf{D}^B \;-\; \left(\mathbf{T}_1 - \frac{\rho_1}{\rho_2}\mathbf{T}_2\right) : \mathbf{D}_1^B \\
+\;& \left(1 + \frac{\rho_1}{\rho_2}\right)\vec{k}_1\cdot\vec{u}_1^B \;+\; \frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 r_1(\vec{u}_1^B)^2\;. \qquad (4.106)
\end{aligned}$$

4.5.2 The incompressibility

Let dV be an infinitesimal volume occupied by the mixture and dm_1 and dm_2 be the masses of water and ice components occupying volume elements dV_1 and dV_2, respectively. We introduce *material densities* $\tilde{\rho}_1$ and $\tilde{\rho}_2$ by

$$\tilde{\rho}_1 = \frac{dm_1}{dV_1} , \qquad \tilde{\rho}_2 = \frac{dm_2}{dV_2} , \tag{4.107}$$

and the *water volume fraction* $\tilde{w}$

$$\tilde{w} = \frac{dV_1}{dV} . \tag{4.108}$$

We assume that the ice-water mixture is *saturated*, that is

$$dV_1 + dV_2 = dV . \tag{4.109}$$

This means that the two components completely fill the space and there are no gaps, air bubbles and holes in the mixture. The densities ρ_1, ρ_2, defined in (3.25), can be expressed as

$$\begin{aligned} \rho_1 &= \frac{dm_1}{dV} \\ &= \tilde{\rho}_1 \tilde{w} , \end{aligned} \tag{4.110}$$

$$\begin{aligned} \rho_2 &= \frac{dm_2}{dV} \\ &= \tilde{\rho}_2 (1 - \tilde{w}) . \end{aligned} \tag{4.111}$$

Since both water and ice can be regarded as incompressible materials (Hutter, [4]), with the material densities $\tilde{\rho}_1$ and $\tilde{\rho}_2$ being constant, the variation of the mixture density (3.33) $\rho = \rho_1 + \rho_2$ is then estimated by

$$\begin{aligned} \delta\rho &= \delta\rho_1 + \delta\rho_2 \\ &= \tilde{\rho}_1 \, \delta\tilde{w} - \tilde{\rho}_2 \, \delta\tilde{w} \\ &= (\tilde{\rho}_1 - \tilde{\rho}_2) \, \delta\tilde{w} . \end{aligned} \tag{4.112}$$

The values $\tilde{\rho}_1$ and $\tilde{\rho}_2$ differ by approximately 10% (Hutter, [4]), the variation in the water volume fraction is of the same order as the fraction, i.e. less than 5%, thus the variation of ρ is of the order of

$$\frac{\delta\rho}{\rho} \sim 10^{-3} .$$

This motivates us to introduce an additional constraint of the form

$$\rho = \rho_1 + \rho_2 \equiv const. , \tag{4.113}$$

where the equivalence symbol in (4.113) denotes both time and spatial constancy.

The introduction of an internal constraint affects the thermo-mechanical description of a material model by additional *reaction functionals.* For example, an additional pressure $-p\mathbf{1}$ is introduced in a 1-component elastic incompressible material. In general, the constitutive functional $\mathcal{F}$ of a constrained material will be considered in the form (Gurtin & Guidugli, [5]):

$$\mathcal{F} \ = \mathcal{F}^E + \bar{\mathcal{F}} \ , \tag{4.114}$$

where $\mathcal{F}^E$ (^{E} as "extra") is the constitutive functional in the absence of the constraint and $\bar{\mathcal{F}}$ represents the reaction functional due to the constraint.

In our particular case we will consider an extension of the constitutive functions by the *reaction set* $\left\{\bar{r}_1,\ \bar{f}_\alpha,\ \bar{s}_\alpha,\ \bar{\vec{q}},\ \bar{\vec{k}}_1,\ \bar{\mathbf{T}}_\alpha\right\}$ in the form:

$$\begin{aligned}
r_1 &= r_1^E + \bar{r}_1 \ , && (4.115)\\
f_\alpha &= f_\alpha^E + \bar{f}_\alpha \ , && (4.116)\\
s_\alpha &= s_\alpha^E + \bar{s}_\alpha \ , && (4.117)\\
\vec{q} &= \vec{q}^E + \bar{\vec{q}} \ , && (4.118)\\
\vec{k}_1 &= \vec{k}_1^E + \bar{\vec{k}}_1 \ , && (4.119)\\
\mathbf{T}_\alpha &= \mathbf{T}_\alpha^E + \bar{\mathbf{T}}_\alpha \ , && (4.120)\\
\alpha &= 1,2 \ .
\end{aligned}$$

Following Gurtin & Guidugli [5], we assume that given a constraint functional $\mathcal{C}$ of the form

$$\mathcal{C}(\rho_1^t, \rho_2^t, \mathbf{F}_1^t, \mathbf{F}_2^t, T^t) = 0 \ ,$$

(where the superscript ^{t} denotes the history), the *reaction set* $\{\bar{r}_1, \bar{f}_\alpha, \bar{s}_\alpha, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_\alpha\}$ is determined by a *reaction function* $\mathcal{R}_\mathcal{C}$

$$\{\bar{r}_1, \bar{f}_\alpha, \bar{s}_\alpha, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_\alpha\} \ = \ \mathcal{R}_\mathcal{C}(\rho_1, \rho_2, \mathbf{F}_1, \mathbf{F}_2, T) \ , \tag{4.121}$$

where $\rho_1, \rho_2, \mathbf{F}_1, \mathbf{F}_2, T$ are the present values of densities, deformation gradients and temperature, respectively. The reaction set $\{\bar{r}_1, \bar{f}_\alpha, \bar{s}_\alpha, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_\alpha\}$ is, in addition, asserted to be closed to scalar multiplication (Gurtin&Guidugli [5]), thus for an arbitrary real λ, the set$\{\lambda\bar{r}_1, \lambda\bar{f}_\alpha, \lambda\bar{s}_\alpha, \lambda\bar{\vec{q}}, \lambda\bar{\vec{k}}_1, \lambda\bar{\mathbf{T}}_\alpha\}$, is also an admissible reaction.

The reaction set (4.121) will be determined using the entropy inequality (4.106). Inserting the expansion (4.115)-(4.120) of the functionals $\{r_1, f_\alpha, s_\alpha, \vec{q}, \vec{k}_1, \mathbf{T}_\alpha\}$ into the inequality (4.106) yields

$$\begin{aligned}
0 \ \geq \ \sigma^E \ &+ \ \rho_1 \grave{\bar{f}}{}_1^B \ + \ \rho_2 \grave{\bar{f}}{}_2^B \ + \ \rho_1 \vec{u}_1^B \cdot \mathrm{grad}(\bar{f}_1 - \bar{f}_2) \ + \ \bar{r}_1(f_1^E - f_2^E) \ + \ r_1^E(\bar{f}_1 - \bar{f}_2)\\
&+ \ \bar{r}_1(\bar{f}_1 - \bar{f}_2) \ + \ (\rho_1\bar{s}_1 + \rho_2\bar{s}_2)\grave{T}^B \ + \ \rho_1(\bar{s}_1 - \bar{s}_2)\vec{g} \cdot \vec{u}_1^B \ + \ \frac{\bar{\vec{q}} \cdot \vec{g}}{T}\\
&- \ (\bar{\mathbf{T}}_1 + \bar{\mathbf{T}}_2) : \mathbf{D}^B \ - \ \left(\bar{\mathbf{T}}_1 - \frac{\rho_1}{\rho_2}\bar{\mathbf{T}}_2\right) : \mathbf{D}_1^B \ + \ \left(1 + \frac{\rho_1}{\rho_2}\right)\bar{\vec{k}}_1 \cdot \vec{u}_1^B\\
&+ \ \frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 \bar{r}_1(\vec{u}_1^B)^2 \ ,
\end{aligned} \tag{4.122}$$

where for brevity we introduced quantity σ^E, which is equal to the right-hand side of (4.106) with $\{r_1, f_\alpha, s_\alpha, \vec{q}, \vec{k}_1, \mathbf{T}_\alpha\}$ replaced by $\{r_1^E, f_\alpha^E, s_\alpha^E, \vec{q}^E, \vec{k}_1^E, \mathbf{T}_\alpha^E\}$. To be able to make use of the entropy inequality (4.122), we use the balance of mass of a mixture (3.29), which now reads as

$$\grave{\rho}_1{}^1 \;+\; \grave{\rho}_2{}^2 \;+\; \rho_1 \mathrm{div}\vec{v}_1 \;+\; \rho_2 \mathrm{div}\vec{v}_2 \;=\; 0 \;,$$

and can be rewritten as

$$\frac{\partial(\rho_1+\rho_2)}{\partial t} \;+\; \mathrm{div}(\rho_1\vec{v}_1+\rho_2\vec{v}_2) \;=\; 0 \;,$$

or, in terms of the mixture density $\rho = \rho_1 + \rho_2$ and the barycentric velocity $\vec{v}^B$ (2.12),

$$\frac{\partial\rho}{\partial t} \;+\; \mathrm{div}(\rho\vec{v}^B) \;=\; 0 \;.$$

Finally, with the use of the incompressibility condition (4.113), we arrive at a constraint for $\vec{v}^B$:

$$\mathrm{div}\vec{v}^B \;=\; 0 \;, \qquad (4.123)$$

or expressed in terms of the symmetric part of the velocity gradient $\mathbf{D}^B$:

$$\mathrm{tr}\mathbf{D}^B \;=\; 0 \;. \qquad (4.124)$$

Thus, the mass balance of a mixture under the incompressibility condition (4.113) constrains $\mathbf{D}^B$ by (4.124). Since the remaining independent variables in (4.122) are not constrained by the remaining balance laws, (linear momentum, angular momentum and energy), conditions (4.113) and (4.124) represent the only additional restrictions on the admissible thermodynamic process.

In accordance with the rational-thermodynamics approach, we assert that the inequality (4.122) holds for all admissible thermodynamic processes. By a special choice of the independent variables and considering the fact that the reaction set is closed under scalar multiplications, we obtain restrictions on the reaction functionals.

Let $\grave{T}^B = 0,\ \vec{u}_1^B = \vec{g} = \vec{0},\ \mathbf{D}^B = \mathbf{D}_1^B = \mathbf{0}$ and the remaining variables be arbitrary, then the inequality (4.122) reads

$$0 \;\geq\; \sigma^E \;+\; \rho_1\grave{f}_1^B \;+\; \rho_2\grave{f}_2^B \;+\; \bar{r}_1(f_1^E - f_2^E) \;+\; r_1^E(\bar{f}_1 - \bar{f}_2) \;+\; \bar{r}_1(\bar{f}_1 - \bar{f}_2) \;. \qquad (4.125)$$

The assumption that the reaction set is closed to scalar multiplication asserts that

$$0 \;\geq\; \sigma^E \;+\; \lambda\Big(\rho_1\grave{f}_1^B \;+\; \rho_2\grave{f}_2^B \;+\; \bar{r}_1(f_1^E - f_2^E) \;+\; r_1^E(\bar{f}_1 - \bar{f}_2)\Big) \;+\; \lambda^2\left(\bar{r}_1(\bar{f}_1 - \bar{f}_2)\right) , \qquad (4.126)$$

for arbitrary real λ. Moreover, we will assume that

$$\bar{f}_1 \;=\; \bar{f}_2 \;. \qquad (4.127)$$

Note that this choice is motivated by the discussion in Gurtin & Guidugli [5] where, in a one-component material, the reaction functional for the free energy was automatically set equal to zero. Here the assumption (4.127) for a 2-component mixture is somewhat weaker. However, it is required for the following considerations and must be accepted as a postulate, otherwise no relevant information about the reaction functionals would be obtained.
The inequality (4.126) then reads

$$0 \ \geq \ \sigma^E \ + \lambda(\rho \grave{\bar{f}}_1^B + \ \bar{r}_1(f_1^E - f_2^E)) \ ,$$

and it holds for any real λ. Thus

$$0 \ \equiv \rho \grave{\bar{f}}_1^B + \ \bar{r}_1(f_1^E - f_2^E). \tag{4.128}$$

The entropy inequality (4.122) is now reduced to

$$\begin{aligned} 0 \ \geq \ \sigma^E \quad &+ \quad (\rho_1 \bar{s}_1 + \rho_2 \bar{s}_2)\grave{T}^B \ + \ \rho_1(\bar{s}_1 - \bar{s}_2)\vec{g} \cdot \vec{u}_1^B \ + \ \frac{\bar{\vec{q}} \cdot \vec{g}}{T} \ - \ (\bar{\mathbf{T}}_1 + \bar{\mathbf{T}}_2) : \mathbf{D}^B \\ &- \quad \left(\bar{\mathbf{T}}_1 - \frac{\rho_1}{\rho_2}\bar{\mathbf{T}}_2\right) : \mathbf{D}_1^B \ + \ \left(1 + \frac{\rho_1}{\rho_2}\right)\bar{\vec{k}}_1 \cdot \vec{u}_1^B \ + \ \frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 \bar{r}_1 (\vec{u}_1^B)^2 \ . \end{aligned} \tag{4.129}$$

It is convenient to rewrite (4.129) as:

$$\begin{aligned} 0 \quad \geq \quad \sigma^E \ + \ &\left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 (\vec{u}_1^B)^2, \ \rho_1 \grave{T}^B + \rho_1 \vec{g} \cdot \vec{u}_1^B, \right. \\ &\left. \rho_2 \grave{T}^B - \rho_1 \vec{g} \cdot \vec{u}_1^B, \ \frac{\vec{g}}{T}, \ \left(1 + \frac{\rho_1}{\rho_2}\right)\vec{u}_1^B, \ -\mathbf{D}^B - \mathbf{D}_1^B, \ -\mathbf{D}^B + \frac{\rho_1}{\rho_2}\mathbf{D}_1^B\right) \ , \end{aligned}$$

where the operation $\star$ has the following meaning:

$$\left(a, \vec{b}, \mathbf{c}\right) \star (d, \vec{e}, \mathbf{f}) \ = \ ad \ + \ \vec{b} \cdot \vec{e} \ + \ \mathbf{c} : \mathbf{f} \ ,$$

for a, d scalars, $\vec{b}, \vec{e}$ vectors, $\mathbf{c}, \mathbf{f}$ second-order tensors. The assumption that the reaction set is closed to scalar multiplication asserts that

$$\begin{aligned} 0 \quad \geq \quad \sigma^E \ + \ \lambda \ &\left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 (\vec{u}_1^B)^2, \ \rho_1 \grave{T}^B + \rho_1 \vec{g} \cdot \vec{u}_1^B, \right. \\ &\left. \rho_2 \grave{T}^B - \rho_1 \vec{g} \cdot \vec{u}_1^B, \ \frac{\vec{g}}{T}, \ \left(1 + \frac{\rho_1}{\rho_2}\right)\vec{u}_1^B, \ -\mathbf{D}^B - \mathbf{D}_1^B, \ -\mathbf{D}^B + \frac{\rho_1}{\rho_2}\mathbf{D}_1^B\right) \ , \end{aligned}$$

for any real λ. This immediately yields

$$\begin{aligned} 0 \quad \equiv \quad &\left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 (\vec{u}_1^B)^2, \ \rho_1 \grave{T}^B + \rho_1 \vec{g} \cdot \vec{u}_1^B, \right. \\ &\left. \rho_2 \grave{T}^B - \rho_1 \vec{g} \cdot \vec{u}_1^B, \ \frac{\vec{g}}{T}, \ \left(1 + \frac{\rho_1}{\rho_2}\right)\vec{u}_1^B, \ -\mathbf{D}^B - \mathbf{D}_1^B, \ -\mathbf{D}^B + \frac{\rho_1}{\rho_2}\mathbf{D}_1^B\right) \ . \end{aligned} \tag{4.130}$$

The reactions $\left\{\bar{r}_1,\ \bar{f}_\alpha,\ \bar{s}_\alpha,\ \bar{\vec{q}},\ \bar{\vec{k}}_1,\ \bar{\mathbf{T}}_\alpha\right\}$ are functions of $\{\rho_1, \rho_2, \mathbf{F}_1, \mathbf{F}_2, T\}$ only, see (4.121), hence, for special choices of $\vec{u}_1^B, \vec{g}, \mathbf{D}, \mathbf{D}_1^B, \grave{T}$, we obtain:

- for $\vec{u}_1^B = \vec{g} = \vec{0},\ \mathbf{D}^B = \mathbf{D}_1^B = \mathbf{0}$, and the remaining variables are arbitrary:

$$0 \quad \equiv \quad \left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(0,\ \rho_1 \grave{T}^B, \rho_2 \grave{T}^B,\ \vec{0},\ \vec{0},\ \mathbf{0},\ \mathbf{0}\right),$$

thus

$$\rho_1 \bar{s}_1 \ + \ \rho_2 \bar{s}_2 \ \equiv \ 0\ , \tag{4.131}$$

and (4.130) now reads

$$\begin{aligned} 0 \quad \equiv \quad & \left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 (\vec{u}_1^B)^2,\ \rho_1 \vec{g} \cdot \vec{u}_1^B, -\rho_1 \vec{g} \cdot \vec{u}_1^B, \right. \\ & \left. \frac{\vec{g}}{T}, \left(1 + \frac{\rho_1}{\rho_2}\right) \vec{u}_1^B,\ -\mathbf{D}^B - \mathbf{D}_1^B,\ -\mathbf{D}^B + \frac{\rho_1}{\rho_2} \mathbf{D}_1^B\right)\ , \end{aligned} \tag{4.132}$$

- for $\vec{g} = \vec{0},\ \mathbf{D}^B = \mathbf{D}_1^B = \mathbf{0}$, and the remaining variables are arbitrary:

$$0 \quad \equiv \quad \left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 (\vec{u}_1^B)^2,\ 0, 0,\ \vec{0},\ \left(1 + \frac{\rho_1}{\rho_2}\right) \vec{u}_1^B,\ \mathbf{0},\ \mathbf{0}\right)\ ,$$

thus

$$0 \ \equiv \ \vec{u}_1^B \cdot \left(\frac{1}{2}\left(1 + \frac{\rho_1}{\rho_2}\right)^2 \vec{u}_1^B \bar{r}_1 + \left(1 + \frac{\rho_1}{\rho_2}\right) \bar{\vec{k}}_1\right).$$

Since $\vec{u}_1^B$ is arbitrary and the reactions are independent of $\vec{u}_1^B$, we find:

$$\bar{r}_1 \ \equiv \ 0\ , \tag{4.133}$$

$$\bar{\vec{k}}_1 \ \equiv \ \vec{0}\ . \tag{4.134}$$

In view of (4.133), equation (4.128) yields

$$\overset{\llcorner}{f}{}_1^{B} \ \equiv \ 0\ ,$$

thus, in view of (4.127):

$$\bar{f}_1 \ \equiv \ \bar{f}_2 \ \equiv \ const.\ ,$$

and in order to keep the reaction functional closed to scalar multiplication (at each instant), it must hold

$$\bar{f}_1 \ \equiv \ \bar{f}_2 \ \equiv \ 0\ . \tag{4.135}$$

Hence, (4.132) reduces to

$$0 \quad \equiv \quad \left(\bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\rho_1 \vec{g} \cdot \vec{u}_1^B, -\rho_1 \vec{g} \cdot \vec{u}_1^B,\ \frac{\vec{g}}{T},\ -\mathbf{D}^B - \mathbf{D}_1^B,\ -\mathbf{D}^B + \frac{\rho_1}{\rho_2} \mathbf{D}_1^B\right)\ , \tag{4.136}$$

- for $\vec{g} = \vec{0}$, $\mathbf{D}^B = \mathbf{0}$, and the remaining variables are arbitrary:

$$0 \equiv \left(\bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(0,\ 0,\ \vec{0},\ -\mathbf{D}_1^B,\ \frac{\rho_1}{\rho_2}\mathbf{D}_1^B\right) ,$$

thus

$$\bar{\mathbf{T}}_1 \equiv \frac{\rho_1}{\rho_2}\bar{\mathbf{T}}_2 , \tag{4.137}$$

and (4.136) reduces to

$$0 \equiv \left(\bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\rho_1\vec{g}\cdot\vec{u}_1^B, -\rho_1\vec{g}\cdot\vec{u}_1^B,\ \frac{\vec{g}}{T},\ -\mathbf{D}^B,\ -\mathbf{D}^B\right) , \tag{4.138}$$

- for $\vec{u}_1^B = \vec{0}$, $\mathbf{D}^B = \mathbf{0}$, and the remaining variables are arbitrary:

$$0 \equiv \left(\bar{s}_1, \bar{s}_2, \bar{\vec{q}}, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(0,\ 0,\ \frac{\vec{g}}{T},\ \mathbf{0},\ \mathbf{0}\right) ,$$

thus since $\vec{g}$ is arbitrary and the reactions are independent of it,

$$\bar{\vec{q}} \equiv \vec{0} , \tag{4.139}$$

and (4.138) reduces to

$$0 \equiv \left(\bar{s}_1, \bar{s}_2, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\rho_1\vec{g}\cdot\vec{u}_1^B, -\rho_1\vec{g}\cdot\vec{u}_1^B,\ -\mathbf{D}^B,\ -\mathbf{D}^B\right) , \tag{4.140}$$

- for $\mathbf{D}^B = \mathbf{0}$, and the remaining variables are arbitrary:

$$0 \equiv \left(\bar{s}_1, \bar{s}_2, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(\rho_1\vec{g}\cdot\vec{u}_1^B, -\rho_1\vec{g}\cdot\vec{u}_1^B,\ \mathbf{0},\ \mathbf{0}\right) .$$

Therefore, since $\vec{g}$ and $\vec{u}_1^B$ are arbitrary and the reactions are independent of them, we have

$$\bar{s}_1 \equiv \bar{s}_2 , \tag{4.141}$$

which together with (4.131) immediately yields

$$\bar{s}_1 \equiv 0 , \tag{4.142}$$
$$\bar{s}_2 \equiv 0 , \tag{4.143}$$

and (4.140) reduces to

$$0 \equiv \left(\bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2\right) \star \left(-\mathbf{D}^B,\ -\mathbf{D}^B\right) , \tag{4.144}$$

or

$$(\bar{\mathbf{T}}_1 + \bar{\mathbf{T}}_2) : \mathbf{D}^B \equiv 0 . \tag{4.145}$$

The tensor $\mathbf{D}^B$ does not have arbitrary values, but according to (4.124), it must be trace-free:

$$\mathrm{tr}\mathbf{D}^B \;=\; \mathbf{D}^B : \mathbf{1} \;\equiv\; 0 \;,$$

thus (4.145) will be satisfied for any

$$\bar{\mathbf{T}}_1 \;+\; \bar{\mathbf{T}}_2 \;\equiv\; -p\mathbf{1} \;,$$

where p is an arbitrary scalar. According to (4.137) we obtain

$$\bar{\mathbf{T}}_1 \quad\equiv\quad -p\frac{\rho_1}{\rho}\mathbf{1} \;, \tag{4.146}$$

$$\bar{\mathbf{T}}_2 \quad\equiv\quad -p\frac{\rho_2}{\rho}\mathbf{1} \;. \tag{4.147}$$

In summary, we have found that the form of the reaction functionals in our 2-component mixture, for the constraint (4.113), are of the form

$$\left\{\bar{r}_1,\; \bar{f}_\alpha,\; \bar{s}_\alpha,\; \bar{\vec{q}},\; \bar{\vec{k}}_1,\; \bar{\mathbf{T}}_1,\; \bar{\mathbf{T}}_2\right\} \;=\; \left\{0,\; 0,\; 0,\; \vec{0},\; \vec{0},\; -pw\mathbf{1},\; -p(1-w)\mathbf{1}\right\} \;, \tag{4.148}$$

where p is an arbitrary scalar and w is the water mass fraction.

Making use of the incompressibility condition (4.113), we can further reduce the constitutive equations for the *extra functionals* (see (4.114)): $\{r_1^E, f_\alpha^E, s_\alpha^E, \vec{q}^E, \vec{k}_1^E, \mathbf{T}_\alpha^E\}$. In the case of $\{r_1^E, f_\alpha^E, s_\alpha^E, \vec{q}^E, \vec{k}_1^E\}$ we only omit the dependence on ρ, and gradρ since the density is now a constant. Additional information can be obtained about the extra stress functionals $\mathbf{T}_1^E$, $\mathbf{T}_2^E$.

- $\mathbf{T}_1^E$
  According to (4.89), we have (omitting the dependence on $\rho, \mathrm{grad}\rho$)

$$\begin{aligned}\mathbf{T}_1^E \quad=\quad & \tilde{\mathbf{T}}_1(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \;+\; w\hat{\mathbf{T}}_1(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \\ +\; & \hat{\hat{\mathbf{T}}}_1(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g})\,\mathrm{grad}w.\end{aligned} \tag{4.149}$$

  Since the case $w = 0,\ \mathrm{grad}w = \vec{0}$, corresponds to pure ice, where no extra "water-stress" should be exerted, we assert

$$\mathbf{T}_1^E|_{w=0,\mathrm{grad}w=\vec{0}} \;\equiv\; \mathbf{0} \;, \tag{4.150}$$

  and conclude

$$\mathbf{T}_1^E \;=\; w\hat{\mathbf{T}}_1(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \;+\; \hat{\hat{\mathbf{T}}}_1(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g})\,\mathrm{grad}w. \tag{4.151}$$

- $\mathbf{T}_2^E$
  According to (4.94), we have

$$\begin{aligned}\mathbf{T}_2^E \quad=\quad & \tilde{\mathbf{T}}_2(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \;+\; w\hat{\mathbf{T}}_2(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \\ +\; & \hat{\hat{\mathbf{T}}}_2(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g})\,\mathrm{grad}w \;.\end{aligned} \tag{4.152}$$

We split the tensor $\tilde{\mathbf{T}}_2$ into the isotropic and traceless deviatoric parts,

$$\begin{aligned} \tilde{\mathbf{T}}_2 &= -\Pi_2(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g})\mathbf{1} + \tilde{\mathring{\mathbf{T}}}_2(\mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) \ , && (4.153) \\ \Pi_2 &= -\frac{1}{3}\mathrm{tr}\tilde{\mathbf{T}}_2 \ . && (4.154) \end{aligned}$$

For $w = 0$, $\ \mathrm{grad}w = \vec{0}$, the constitutive equation for $\mathbf{T}_2$ must be reduced to that valid for pure ice (Peterson [7]), i.e. it must hold that

$$\mathring{\mathbf{T}}_2\bigg|_{w=0,\mathrm{grad}w=\vec{0}} = \mathcal{B}(T)h(\mathring{D}_{2II})\ \mathring{\mathbf{D}}_2 \ , \tag{4.155}$$

where $\mathcal{B}(T)$ is a temperature-dependent function and $\mathring{D}_{2II}$ is the second invariant of the strain deviator $\mathring{\mathbf{D}}_2$.

In view of (4.120) and (4.148), we have

$$\mathbf{T}_2 \ = \ -p(1-w)\mathbf{1} \ + \ \mathbf{T}_2^E \ . \tag{4.156}$$

Using (4.152) and (4.153), equation (4.155) implies that

$$\tilde{\mathring{\mathbf{T}}}_2 \ = \mathcal{B}(T)h(\mathring{D}_{2II})\ \mathring{\mathbf{D}}_2 \ \ . \tag{4.157}$$

At this point it is worthwhile to make the following remark. The stress – strain-rate relation in pure ice is often considered in the form (2.8):

$$\mathbf{D}_2 \ = \ \mathcal{A}(T)d(\Sigma)\ \mathring{\mathbf{T}}_2 \ , \tag{4.158}$$

where

$$\Sigma \ = \sqrt{\frac{1}{2}\mathrm{tr}(\mathring{\mathbf{T}}_2)^2}. \tag{4.159}$$

This includes the assumption of the incompressibility of pure ice, that is

$$\mathring{\mathbf{D}}_2 = \ \mathbf{D}_2 \ .$$

Hence, the relation (4.158) may also be written as

$$\mathring{\mathbf{D}}_2 = \ \mathcal{A}(T)d(\Sigma)\ \mathring{\mathbf{T}}_2 \ \ . \tag{4.160}$$

We now intend to express the inverse relation, i.e. to express $\mathring{\mathbf{T}}_2$ as a function of $\mathring{\mathbf{D}}_2$ and its invariants. The double-dot product of (4.160) is

$$\mathring{\mathbf{D}}_2{\cdot\cdot}\mathring{\mathbf{D}}_2 = \ (\mathcal{A}(T)d(\Sigma))^2\ \mathring{\mathbf{T}}_2{\cdot\cdot}\mathring{\mathbf{T}}_2 \ \ . \tag{4.161}$$

Using the definition of the second invariant of a second-order tensor $\mathbf{Y}$ (see e.g. Maršík [8]):

$$Y_{II} \ = \ -\frac{1}{2}\left(\mathrm{tr}\mathbf{Y^2} - (\mathrm{tr}\mathbf{Y})^2\right) \ ,$$

and considering (4.159), we obtain

$$\overset{\circ}{D}_{2II} \;=\; -(\mathcal{A}(T)\,d(\Sigma))^2\Sigma^2 \ .$$

Provided that the function $d(\Sigma)$ is invertible[2], we may express Σ by means of $\overset{\circ}{D}_{2II}$ and T. As a result, we have

$$\overset{\circ}{\mathbf{T}}_2 = \ \mathcal{B}(T)h(\overset{\circ}{D}_{2II})\ \overset{\circ}{\mathbf{D}}_2 \ \ . \tag{4.162}$$

The expression (4.157) will only be used in theoretical treatment since $\mathbf{T}$ is chosen to be the dependent variable. However, in numerical implementation (Chapter 6), we will apply the inverse relation.
Using (4.157), we can write (4.152) as

$$\begin{aligned}\mathbf{T}^E_2 \ &= \ -\Pi_2(\mathbf{D}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g})\mathbf{1} + \mathcal{B}(T)h(\overset{\circ}{D}_{2II})\ \overset{\circ}{\mathbf{D}}_2 \\ &+ \ w\hat{\mathbf{T}}_2(\mathbf{D}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g}) \ + \hat{\hat{\mathbf{T}}}_2(\mathbf{D}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g})\,\mathrm{grad}w \ .\end{aligned}$$

To summarize, after applying the partial linearization, the entropy principle, and the incompressibility constraint, and requiring that the model of the ice-water mixture reduces to the model of pure ice in the limit $w \to 0$, $\mathrm{grad}w \to \vec{0}$, we arrived at the following general form of the constitutive equations of the ice-water mixture:

$$r_1 \ = \ \tilde{r}_1^{(0)}(T) + w\hat{r}_1^{(0)}(T) + w\hat{r}_1^{(1)}(T)\ \mathrm{tr}\mathbf{D}_1 + \tilde{r}_1^{(2)}(T)\ \mathrm{tr}\mathbf{D}_2 \ , \tag{4.163}$$

$$f_\alpha \ = \ \tilde{f}_\alpha(T) + w\hat{f}_\alpha(T) \ , \tag{4.164}$$

$$s_1 \ = \ \tilde{s}_1^{(0)}(T) + w\hat{s}_1^{(0)}(T) + \tilde{s}_1^{(1)}(T)\ \mathrm{tr}\mathbf{D}_1 + \tilde{s}_1^{(2)}(T)\ \mathrm{tr}\mathbf{D}_2 \ , \tag{4.165}$$

$$s_2 \ = \ \tilde{s}_2^{(0)}(T) + w\hat{s}_2^{(0)}(T) - w\tilde{s}_1^{(1)}(T)\ \mathrm{tr}\mathbf{D}_1 - w\tilde{s}_1^{(2)}(T)\ \mathrm{tr}\mathbf{D}_2 \ , \tag{4.166}$$

$$\vec{q} \ = \ -(\tilde{k}(T) + w\hat{k}(T))\vec{g} \ - \ \lambda(T)w\vec{u}_1 \ , \tag{4.167}$$

$$\vec{k}_1 \ = \ -w\xi(T)\vec{g} \ - \ w\nu(T)\vec{u}_1 \ - \ \omega(T)\,\mathrm{grad}\,w \ , \tag{4.168}$$

$$\mathbf{T}_1 \ = \ -pw\,\mathbf{1} \ + \ w\hat{\mathbf{T}}_1(\mathbf{D}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g}) \ + \ \hat{\hat{\mathbf{T}}}_1(\mathbf{D}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g})\,\mathrm{grad}w \ , \tag{4.169}$$

$$\begin{aligned}\mathbf{T}_2 \ &= \ -p(1-w)\,\mathbf{1} \ - \ \Pi_2(\mathbf{D}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g})\mathbf{1} + \mathcal{B}(T)h(\overset{\circ}{D}_{2II})\ \overset{\circ}{\mathbf{D}}_2 \\ &+ \ w\hat{\mathbf{T}}_2(\vec{\mathbf{D}}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g}) \ + \hat{\hat{\mathbf{T}}}_2(\vec{\mathbf{D}}_\gamma,\boldsymbol{\Omega}_1,\vec{u}_1,T,\vec{g})\,\mathrm{grad}w \ ,\end{aligned} \tag{4.170}$$

$$\alpha,\gamma = 1,2 \ .$$

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[2] The usual form of the function $f(\Sigma)$ is according to the Glen's flow law (see e.g. Paterson [7]) $f(\Sigma) = \Sigma^{n-1}$, $n = 3$.

4.6 Balance equations in the water-ice mixture

In this section, we will investigate the balance laws in the ice-water mixture using the constitutive equations (4.163)-(4.170).

4.6.1 Mass balance

The ice component
From the general mass-balance law (3.28) for mixture components we obtain

$$\frac{\partial \rho_2}{\partial t} \;+\; \mathrm{grad}\,\rho_2 \cdot \vec{v}_2 \;+\; \rho_2\,\mathrm{div}\,\vec{v}_2 \;=\; r_2 \;.$$

Since

$$r_2 \;=\; -r_1 \;,$$

as follows from (3.32), we can write with the use of (4.65)

$$\frac{\partial\{\rho(1-w)\}}{\partial t} \;+\; \mathrm{grad}\,\{\rho(1-w)\}\cdot\vec{v}_2 \;+\; \rho(1-w)\,\mathrm{div}\,\vec{v}_2 \;=\; -r_1 \;.$$

Assuming ρ constant, we further have

$$\frac{\partial w}{\partial t} \;+\; \mathrm{grad}\,w\cdot\vec{v}_2 \;-\; (1-w)\,\mathrm{div}\,\vec{v}_2 \;=\; \frac{r_1}{\rho} \;. \tag{4.171}$$

The water component
The mass balance for the water component reads

$$\frac{\partial \rho_1}{\partial t} \;+\; \mathrm{grad}\,\rho_1 \cdot \vec{v}_1 \;+\; \rho_1\,\mathrm{div}\,\vec{v}_1 \;=\; r_1 \;,$$

or by (4.64)

$$\frac{\partial(\rho w)}{\partial t} \;+\; \mathrm{grad}\,(\rho w)\cdot\vec{v}_1 \;+\; \rho w\,\mathrm{div}\,\vec{v}_1 \;=\; r_1 \;,$$

and assuming additionally ρ to be constant, we have

$$\frac{\partial w}{\partial t} \;+\; \mathrm{grad}\,w\cdot\vec{v}_1 \;+\; w\,\mathrm{div}\,\vec{v}_1 \;=\; \frac{r_1}{\rho} \;. \tag{4.172}$$

Since the independent field variables are the ice velocity $\vec{v}_2$ and the diffusion velocity $\vec{u}_1 = \vec{v}_1 - \vec{v}_2$, equation (4.172) is further rearranged by (4.171):

$$\mathrm{grad}\,w\cdot(\vec{v}_1-\vec{v}_2) \;+\; \mathrm{div}\,\vec{v}_2 \;+\; w\,\mathrm{div}\,(\vec{v}_1-\vec{v}_2) \;=\; 0 \;,$$

or

$$\mathrm{grad}\,w\cdot\vec{u}_1 \;+\; \mathrm{div}\,\vec{v}_2 \;+\; w\,\mathrm{div}\,\vec{u}_1 \;=\; 0 \;. \tag{4.173}$$

4.6.2 Linear-momentum balance

The ice component
With the use of the general linear momentum balance for a mixture component (3.41), we arrive at

$$\rho_2 \frac{D_2\,\vec{v}_2}{Dt} \;=\; \operatorname{div}\mathbf{T}_2 \;+\; \rho_2 \vec{b}_2 \;+\; \vec{k}_2 \;.$$

The only volume force $\vec{b}$ present in our problem is gravity, thus $\vec{b}_1 = \vec{b}_2 = \vec{g}_a$. Using

$$\vec{k}_2 \;=\; -\vec{k}_1 - r_1 \vec{u}_1 \;,$$

following from (3.45), and using (4.168), we obtain

$$\rho(1-w)\frac{D_2\,\vec{v}_2}{Dt} \;=\; \operatorname{div}\mathbf{T}_2 + \;\rho(1-w)\vec{g}_a \;+\; w\xi\vec{g} \;+\; w\nu\vec{u}_1 + \;\omega\,\operatorname{grad} w \;-\; r_1\vec{u}_1 \;. \tag{4.174}$$

The water component
Similarly, for the water component:

$$\rho_1 \frac{D_1\,\vec{v}_1}{Dt} \;=\; \operatorname{div}\mathbf{T}_1 \;+\; \rho_1 \vec{b}_1 \;+\; \vec{k}_1 \;,$$

or, if we express $\vec{b}_1$ and $\vec{k}_1$ from (4.168), we obtain

$$\rho w \frac{D_1\,\vec{v}_1}{Dt} \;=\; \operatorname{div}\mathbf{T}_1 \;+\; \rho w \vec{g}_a \;-\; w\xi\vec{g} \;-\; w\nu\vec{u}_1 \;-\; \omega\,\operatorname{grad} w \;. \tag{4.175}$$

Note that neither here, nor in the previous case of ice momentum balance, do we expand all the terms (e.g. stress tensors) according to their constitutive equations. This is done for the sake of brevity, because several further reductions of the system of balance equations will be done in the next section.

4.6.3 The angular-momentum balance

The angular- momentum balance (3.49) implies the symmetry of the constitutive functionals for $\mathbf{T}_1$ and $\mathbf{T}_2$:

$$\mathbf{T}_1 \;=\; \mathbf{T}_1^T \;, \qquad\qquad \mathbf{T}_2 \;=\; \mathbf{T}_2^T \;,$$

which, in view of (4.169) and (4.170) leads to

$$\hat{\mathbf{T}}_1 \;=\; \hat{\mathbf{T}}_1^T, \qquad \text{and} \qquad \hat{\mathbf{T}}_2 \;=\; \hat{\mathbf{T}}_2^T, \tag{4.176}$$

$$(\hat{\hat{\mathbf{T}}}_1)_{ijk} \;=\; (\hat{\hat{\mathbf{T}}}_1)_{jik} \qquad \text{and} \qquad (\hat{\hat{\mathbf{T}}}_2)_{ijk} \;=\; (\hat{\hat{\mathbf{T}}}_2)_{jik} \;. \tag{4.177}$$

4.6.4 The energy balance

As discussed before, we are dealing only with the energy balance of the mixture as a whole. This, according to (3.66), has the form

$$\begin{aligned}\rho_1\frac{D_1\varepsilon_1}{Dt} + \rho_2\frac{D_2\varepsilon_2}{Dt} &= \mathbf{T}_1 : \mathbf{D_1} + \mathbf{T}_2 : \mathbf{D}_2 - \operatorname{div}\vec{q} - r_1\varepsilon_1 - r_2\varepsilon_2 \\ &- \vec{v}_1\cdot\vec{k}_1 - \vec{v}_2\cdot\vec{k}_2 - \frac{1}{2}r_1\vec{v}_1^2 - \frac{1}{2}r_2\vec{v}_2 ,\end{aligned}$$

where we do not consider any internal heating Q. By (3.69), it holds that

$$\vec{v}_1\cdot\vec{k}_1 + \vec{v}_2\cdot\vec{k}_2 + \frac{1}{2}r_1\vec{v}_1^2 + \frac{1}{2}r_2\vec{v}_2 = \vec{u}_1\cdot\vec{k}_1 + \frac{1}{2}r_1\vec{u}_1^2 .$$

By (3.32), it follows

$$r_2 = -r_1 .$$

Hence, using the constitutive equations for $\vec{q}$, see (4.167), and $\vec{k}_1$, see (4.168), we arrive at

$$\begin{aligned}\rho w\,\frac{D_1\varepsilon_1}{Dt} + \rho(1-w)\,\frac{D_2\varepsilon_2}{Dt} &= \mathbf{T}_1 : \mathbf{D_1} + \mathbf{T}_2 : \mathbf{D}_2 + \operatorname{div}\left((\tilde{k}+w\hat{k})\vec{g} + \lambda w\vec{u}_1\right) \\ &- r_1\left(\varepsilon_1-\varepsilon_2\right) + \vec{u}_1\cdot\left(w\xi\,\vec{g} + w\nu\,\vec{u}_1 + \omega\operatorname{grad}w\right) - \frac{1}{2}r_1\vec{u}_1^2 .\end{aligned} \tag{4.178}$$

4.7 Further reductions of the balance equations

4.7.1 Motivation

Our aim is to obtain a set of equations describing the most important physical features of the temperate-ice zone and to solve them numerically for a simple geometry (2D) to study the role of the particular processes involved. For this purpose, we now introduce several additional simplifications.

4.7.2 Mass balance

We will neglect the term $w\operatorname{div}\vec{v}_2$ in the mass balance of the component ice (4.171), since it is small compared to $\operatorname{div}\vec{v}_2$, and therefore write

$$\frac{\partial w}{\partial t} + \operatorname{grad}w\cdot\vec{v}_2 - \operatorname{div}\vec{v}_2 = \frac{r_1}{\rho} . \tag{4.179}$$

The mass balance of water (4.173) will be kept unchanged

$$\operatorname{grad}w\cdot\vec{u}_1 + \operatorname{div}\vec{v}_2 + w\operatorname{div}\vec{u}_1 = 0 . \tag{4.180}$$

4.7.3 Linear-momentum balance

We start with the linear-momentum balance for the water component (4.175):

$$\rho w \frac{D_1 \vec{v}_1}{Dt} \;=\; \operatorname{div} \mathbf{T}_1 \;+\; \rho w \vec{g}_a \;-\; w\xi \vec{g} \;-\; w\nu \vec{u}_1 \;-\; \omega \operatorname{grad} w \;.$$

In the first approximation, we omit the inertia term on the left-hand side and the term $\operatorname{div}(w\, \hat{\mathbf{T}}_1 + \hat{\hat{\mathbf{T}}}_1 \operatorname{grad} w)$ occurring in the expansion

$$\operatorname{div}\mathbf{T}_1 \;=\; \operatorname{div}(-pw\, \mathbf{1} \;+\; w\, \hat{\mathbf{T}}_1 + \hat{\hat{\mathbf{T}}}_1 \operatorname{grad} w) \;,$$

thus keeping only the partial reaction pressure pw from the partial stress tensor $\mathbf{T_1}$, assuming its role to be minor thanks to the assumed low water concentration. Hence, we arrive at

$$w\nu \vec{u}_1 \;=\; -\operatorname{grad}(pw) \;-\; w\xi \vec{g} \;-\; \omega \operatorname{grad} w \;+\; \rho w \vec{g}_a \tag{4.181}$$

which may be interpreted as the equation for the diffusive water velocity $\vec{u}_1$.
The linear-momentum balance for the ice component (4.174) reads,

$$\rho(1-w) \frac{D_2 \vec{v}_2}{Dt} \;=\; \operatorname{div}\mathbf{T}_2 + \;\rho(1-w)\vec{g}_a \;+\; w\xi\vec{g} \;+\; w\nu\vec{u}_1 + \;\omega \operatorname{grad} w \;-\; r_1 \vec{u}_1 . \tag{4.182}$$

We again neglect the inertia term on the left-hand side and also the term $r_1 \vec{u}_1$, corresponding to the linear-momentum change induced by the mass exchange between the components. We further expand $\mathbf{T}_2$, according to (4.170):

$$\mathbf{T}_2 \;=\; -p(1-w)\mathbf{1} \;-\; \Pi_2 \mathbf{1} \;+\; \mathcal{B}(T) h(\overset{\circ}{D}_{2II})\, \overset{\circ}{\mathbf{D}}_2 \;+ w\hat{\mathbf{T}}_2 \;+\; \hat{\hat{\mathbf{T}}}_2 \operatorname{grad} w.$$

Since the constitutive functional for the thermodynamic pressure Π_2 is not known, and the ice-water mixture compressibility is assumed to be low, we neglect this term. In the first approximation we also neglect $\hat{\hat{\mathbf{T}}}_2 \operatorname{grad} w$, and following (Larson, [9]), specify the functional $\hat{\mathbf{T}}_2$ by substituting

$$\mathcal{B}(T) h(\overset{\circ}{D}_{2II})\, \overset{\circ}{\mathbf{D}}_2 \;+ w\hat{\mathbf{T}}_2 \;\longrightarrow\; \mathcal{B}(T,w) h(\overset{\circ}{D}_{2II})\, \overset{\circ}{\mathbf{D}}_2 \;,$$

where $\mathcal{B}$ is assumed to be linear in w. Hence, (4.182) becomes

$$\begin{aligned} \vec{0} \;&=\; \operatorname{grad}(pw) \;+\; w\xi\vec{g} \;+\; w\nu\vec{u}_1 \;+\; \omega \operatorname{grad} w \;-\; \rho w \vec{g}_a \\ &-\; \operatorname{grad} p \;+\; \operatorname{div}(\mathcal{B}(T,w) h(\overset{\circ}{D}_{2II})\, \overset{\circ}{\mathbf{D}}_2) \;+\; \rho \vec{g}_a \;, \end{aligned}$$

which, due to (4.181), is further simplified to become

$$\vec{0} \;=\; -\operatorname{grad} p \;+\; \operatorname{div}(\mathcal{B}(T,w) h(\overset{\circ}{D}_{2II})\, \overset{\circ}{\mathbf{D}}_2) \;+\; \rho \vec{g}_a \;. \tag{4.183}$$

4.7.4 Energy balance

Let us recall the constitutive equations for free energy and entropy. By (4.164) and (4.165), (4.166), we have

$$\begin{aligned} f_\alpha &= \tilde{f}_\alpha(T) \ + \ w\hat{f}_\alpha(T) \ , \\ s_1 &= \tilde{s}_1^{(0)}(T) + w\hat{s}_1^{(0)}(T) + \tilde{s}_1^{(1)}(T) \ \mathrm{tr}\mathbf{D}_1 + \tilde{s}_1^{(2)}(T) \ \mathrm{tr}\mathbf{D}_2 \ , \\ s_2 &= \tilde{s}_2^{(0)}(T) + w\hat{s}_2^{(0)}(T) - w\tilde{s}_1^{(1)}(T) \ \mathrm{tr}\mathbf{D}_1 - w\tilde{s}_1^{(2)}(T) \ \mathrm{tr}\mathbf{D}_2 \ . \end{aligned}$$

For the following derivations, it will be necessary to omit the terms $\hat{f}_\alpha$, $\hat{s}_\alpha^{(0)}$, $\tilde{s}_1^{(1)}$, $\tilde{s}_1^{(2)}$, i.e. to keep s_α, f_α dependent only upon the absolute temperature. This can only be justified in view of the approach commonly applied in glaciology, however by means of rational thermodynamics we were not able to reduce the constitutive functionals in such a manner. An argument for this step might be the lack of experimental evidence for the presence of the discussed terms, and hence an absence of any constraints on the possible shape of the omitted functions. Thus henceforth, we will consider

$$f_\alpha \ = \ f_\alpha(T) \ , \tag{4.184}$$

$$s_\alpha \ = \ s_\alpha(T) \ , \tag{4.185}$$

where we have omitted the ˜ label.

On the left-hand side of equation (4.178), we neglect the terms $\rho w \,\grave{\varepsilon}_1^1$, $\rho w \,\grave{\varepsilon}_2^2$, since these are small compared to $\rho \,\grave{\varepsilon}_2^2$. On the right-hand side of (4.178), we expand

$$\begin{aligned} \mathbf{T}_1 : \mathbf{D}_1 + \mathbf{T}_2 : \mathbf{D}_2 \quad &= \quad -pw\mathbf{1} : \mathbf{D}_1 \ + \ \Big(-p(1-w)\mathbf{1} + \mathcal{B}(T,w)h(\overset{\circ}{D}_{2II}) \ \overset{\circ}{\mathbf{D}}_2\Big) : \mathbf{D}_2 \\ &= \quad -pw \,\mathrm{div}\vec{u}_1 \ - \ p\,\mathrm{div}\vec{v}_2 \ + \ \mathcal{B}(T,w)h(\overset{\circ}{D}_{2II}) \ \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 \ , \end{aligned}$$

where we repeated the simplifications of the stress-tensors introduced above, and made use of

$$\overset{\circ}{\mathbf{D}}_2 : \mathbf{D}_2 \ = \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 \ ,$$

that follows from the fact that the deviator $\overset{\circ}{\mathbf{D}}_2$ is traceless. In the energy balance, we also neglect the term corresponding to the kinetic-energy changes $\frac{1}{2} r_1 \vec{u}_1^2$. Inspecting (4.181) we write

$$\vec{u}_1 \cdot (w\xi\vec{g} + w\nu\vec{u}_1 + \omega \,\mathrm{grad}w) \ = \ \vec{u}_1 \cdot (-\mathrm{grad}(pw) + \rho w\vec{g}_a) \ .$$

The equation (4.178) therefore becomes

$$\begin{aligned} \rho\frac{D_2\varepsilon_2}{Dt} \ = \ &- \ pw \,\mathrm{div}\vec{u}_1 \ - \ p\,\mathrm{div}\vec{v}_2 \ + \ \mathcal{B}(T,w)h(\overset{\circ}{D}_{2II}) \ \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 \ + \mathrm{div}((\tilde{k} + w\hat{k})\vec{g} + \lambda w\vec{u}_1) \\ &- \ r_1(\varepsilon_1 - \varepsilon_2) \ + \ \vec{u}_1 \cdot (-\mathrm{grad}(pw) + \rho w\vec{g}_a) \ , \end{aligned} \tag{4.186}$$

which we rewrite as

$$\begin{aligned} \rho\frac{D_2\varepsilon_2}{Dt} \ = \ &- \ p(\mathrm{div}(w\vec{u}_1) + \mathrm{div}\vec{v}_2) \ + \ w\vec{u}_1 \cdot (-\mathrm{grad}p + \rho\vec{g}_\alpha) + \ \mathcal{B}(T,w)h(\overset{\circ}{D}_{2II}) \ \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 \\ &+ \ \ \mathrm{div}((\tilde{k} + w\hat{k})\vec{g} + \lambda w\vec{u}_1) \ - \ r_1(\varepsilon_1 - \varepsilon_2) \ , \end{aligned} \tag{4.187}$$

and inspecting (4.180) we see that the first bracket at the right-hand side is zero, thus finally

$$\begin{aligned} \rho \frac{D_2 \varepsilon_2}{Dt} &= w\vec{u}_1 \cdot (-\mathrm{grad} p + \rho \vec{g}_\alpha) + \mathcal{B}(T,w) h(\overset{\circ}{D}_{2II})\, \overset{\circ}{\mathbf{D}}_2 {\cdot}{:} \overset{\circ}{\mathbf{D}}_2 \\ &+ \mathrm{div}((\tilde{k} + w\hat{k})\vec{g} + \lambda w \vec{u}_1) \;-\; r_1(\varepsilon_1 - \varepsilon_2) \;. \end{aligned} \tag{4.188}$$

Ice in the temperate zone is, by definition, at the melting temperature T_M. Despite the fact that the ice-water mixture is treated as an incompressible material, we assume that the melting temperature can be determined by the Clausius-Clapeyron relation,

$$T_M \;=\; T_M(p). \tag{4.189}$$

By (4.189), we implicitly assume that the mixture is close to the thermodynamic equilibrium, since relation (4.189) follows from the equilibrium analysis, namely from equality of chemical potentials. Strictly speaking, relation (4.189) is correct only in compressible fluids (see Hutter [4]), the term $-p\mathbf{1}$ then denotes the total equilibrium stress. Adopting such a relation in our particular case, with the incompressibility involved, can only be justified by assuming the incompressible model to be an approximation of a material model with very low compressibility. Such an interpretation may justify the Clausius-Clapeyron relation, however, in (4.189) we moreover replaced the total equilibrium stress by only $-p\mathbf{1}$, where p is the reaction pressure. We are not able to quantitatively estimate the error introduced by such an assumption but, following (Hutter [4]), we expect it to be negligible.

As expressed by (3.76), it holds

$$\varepsilon_\alpha \;=\; f_\alpha \;+\; T\, s_\alpha \;,$$

thus, with the assumptions (4.184) and (4.185), we obtain

$$\varepsilon_\alpha \;=\; \varepsilon_\alpha(T) \;. \tag{4.190}$$

Therefore, we may write

$$\frac{D_2 \varepsilon_2}{Dt} \;=\; c_\rho \frac{D_2 T_M(p)}{Dt} \;, \tag{4.191}$$

where we introduced

$$c_\rho \;=\; \left. \frac{d\varepsilon_2}{dT} \right|_{T=T_M} \;. \tag{4.192}$$

The energy balance (4.188) can now be rewritten as a definition relationship for the water production term r_1:

$$\begin{aligned} r_1(\varepsilon_1 - \varepsilon_2) &= \mathcal{B}(T,w) h(\overset{\circ}{D}_{2II})\, \overset{\circ}{\mathbf{D}}_2 {\cdot}{:} \overset{\circ}{\mathbf{D}}_2 \;+ \mathrm{div}((\tilde{k} + w\hat{k})\vec{g} + \lambda w \vec{u}_1) \;-\; \rho c_\rho \frac{D_2 T_M(p)}{Dt} \\ &+ w\vec{u}_1 \cdot (-\mathrm{grad} p + \rho \vec{g}_\alpha) \;. \end{aligned} \tag{4.193}$$

This form of the energy balance is already satisfactory. However, following the common approach in glaciology, we intend to rewrite the difference $\varepsilon_1 - \varepsilon_2$ in terms of the latent heat. To do this, we consider a system that contains ice mass m of volume V_2, that melts to the same mass of water with volume V_1. We denote the internal energy and entropy of the ice mass by U_2, S_2, and of the water mass by U_1, S_1, respectively. We assume that the ice temperature before melting and the water temperature are equal, and if we assume that the process of melting was quasi-static, i.e. the ice-water system remained in thermodynamic equilibrium, and reversible (which is true), the first law of thermodynamics (Kvasnica [12]) states that

$$[U] \;=\; T[S] - W \;,$$

where

$$[U] \;=\; U_1 - U_2 \;, \qquad\qquad [S] \;=\; S_1 - S_2 \;,$$

and W is the mechanical work performed by the system during the process of melting. If the system is in thermodynamic equilibrium, then the equilibrium stress reduces to pressure and we may arrive at

$$[U] \;=\; T[S] - p[V] \;,$$

or dividing this equation by the mass m

$$[\varepsilon] \;=\; T[s] - p\left[\frac{1}{\tilde{\rho}}\right] \;, \tag{4.194}$$

where ε is the internal energy density (related to mass), and

$$T[s] \;=\; L \;, \tag{4.195}$$

where L is the *specific latent heat of melting of ice* and $\tilde{\rho}$ denotes the "material" density.

Thus, under the simplifying assumptions (quasi-static melting, equilibrium pressure equal to the reaction stress), we may write (4.196) as follows

$$\begin{aligned} r_1 \;&=\; \frac{1}{(L - p\Delta)}\Big\{\mathcal{B}(T,w)h(\overset{\circ}{D}_{2II})\;\overset{\circ}{\mathbf{D}}_2 \!:\! \overset{\circ}{\mathbf{D}}_2 \;+\, \mathrm{div}((\tilde{k} + w\hat{k})\vec{g} + \lambda w \vec{u}_1) \\ &-\; \rho c_\rho \frac{D_2 T_M(p)}{Dt} \;+\; w\vec{u}_1 \cdot (-\mathrm{grad}p + \rho \vec{g}_\alpha)\Big\} \,. \end{aligned} \tag{4.196}$$

where we introduced

$$\Delta \;=\; \frac{1}{\tilde{\rho}_1} \;-\; \frac{1}{\tilde{\rho}_2} \;. \tag{4.197}$$

Chapter 5

The polythermal ice-sheet model

The aim of this chapter is to summarize the knowledge obtained so far, and after introducing the appropriate boundary and transition conditions set up the description of a typical polythermal ice-sheet configuration as depicted in Fig. 2.1.

5.1 Field equations

5.1.1 The cold-ice zone

For the cold-ice zone we adopt the traditional formulation as summarized in the first chapter. *The mass balance*, *the linear momentum balance* and *the internal-energy balance* read as

$$\begin{aligned} \operatorname{div} \vec{v} &= 0 \,, && (5.1)\\ \rho \dot{\vec{v}} &= -\operatorname{grad} \mathrm{p} \;+\; \operatorname{div} \overset{\circ}{\mathbf{T}} \;+\; \rho\, \vec{\mathrm{g}}_{\mathrm{a}} \,, && (5.2)\\ \rho \dot{\varepsilon} &= \mathbf{T} \cdot \mathbf{D} \;-\; \operatorname{div} \vec{q} \,, && (5.3) \end{aligned}$$

with the constitutive relations

$$\begin{aligned} \mathbf{T} &= -p\mathbf{1} + \overset{\circ}{\mathbf{T}} \,, && (5.4)\\ \varepsilon &= c_V T \,, && (5.5)\\ \vec{q} &= -k(T) \operatorname{grad} T \,, && (5.6)\\ \mathbf{D} &= \mathcal{A}(T)\, d(\Sigma)\, \overset{\circ}{\mathbf{T}} \,. && (5.7) \end{aligned}$$

5.1.2 The temperate-ice zone

In the previous chapter, we arrived at the set of equations for the temperate ice-zone behaviour in the view of the mixture theory. Namely, the two *mass-balance laws* (4.179), (4.180):

$$\begin{aligned} \frac{\partial w}{\partial t} \;+\; \operatorname{grad} w \cdot \vec{v}_2 \;-\; \operatorname{div} \vec{v}_2 &= \frac{r_1}{\rho} \,, && (5.8)\\ \operatorname{grad} w \cdot \vec{u}_1 \;+\; \operatorname{div} \vec{v}_2 \;+\; w \operatorname{div} \vec{u}_1 &= 0 \,, && (5.9) \end{aligned}$$

the two *linear-momentum balance laws*, (4.181) and (4.183):

$$\begin{aligned} w\nu\vec{u}_1 &= -\mathrm{grad}(pw) \;-\; w\xi\vec{g} \;-\; \omega\,\mathrm{grad}\,w \;+\; \rho w\vec{g}_a && (5.10)\\ \vec{0} &= -\mathrm{grad}p \;+\; \mathrm{div}\left(\mathcal{B}(T,w)h(\overset{\circ}{D}_{2II})\,\overset{\circ}{\mathbf{D}}_2\right) \;+\; \rho\vec{g}_a\;, && (5.11)\end{aligned}$$

and *the energy balance* (4.197):

$$\begin{aligned} r_1 \;=\; & \frac{1}{(L-p\Delta)}\Big\{\mathcal{B}(T,w)h(\overset{\circ}{D}_{2II})\,\overset{\circ}{\mathbf{D}}_2\cdot\overset{\circ}{\mathbf{D}}_2 \;+\mathrm{div}((\tilde{k}+w\hat{k})\vec{g}+\lambda w\vec{u}_1)\\ - \;& \rho c_\rho\frac{D_2T_M(p)}{Dt} \;+\; w\vec{u}_1\cdot(-\mathrm{grad}p+\rho\vec{g}_\alpha)\Big\}\,. && (5.12)\end{aligned}$$

5.2 Boundary and transition conditions

So far we have tacitly assumed that the investigated quantities are continuous, mostly also differentiable. However, in reality, e.g. inside glaciers, even in the "smoothing" continuous description, we can identify singular surfaces at which the constitutive functionals or material parameters can undergo a finite jump. In this section, we will investigate the general conditions for such jumps as a consequence of the balance laws. We will also rearrange them to a form applicable in numerical computations. To complete the description, we must add the appropriate boundary conditions, both on the free surface (ice-air boundary) and at the base (ice-bedrock boundary). In all cases, we will use a similar approach. The boundary will be considered as a singular surface, at which all components of the mixture are present on both sides, but the density of some components may tend to zero. This unusual approach will enable the unification of the transition and boundary conditions within the theoretical framework of Chapter 3 and provide the description of the physical processes at the mixture boundaries.

Note on notation: in the following sections we will use superscripts + and − to distinguish the field variables at the opposite sides of a singular surface. The reader should not confuse it with the notation of equilibrium values of the field variables, as introduced in section 3.10.

5.2.1 Free surface

The *free surface* is a cold or temperate-ice – air boundary. At this interface accumulation of ice due to snowfalls may occur as well as ice melting or refreezing of water. Due to these processes, a free surface is generally not material and therefore *kinematic conditions* must be introduced to determine its evolution.

Let us assume that the points of the free surface at time t in the present configuration are given by an implicit equation

$$F_S(\vec{x},t) \;=\; 0 \qquad (5.13)$$

for a certain function F_S. Let

$$\mathcal{S}_t \;=\; \{\vec{x}\in E^3 : F_S(\vec{x},t)=0\}$$

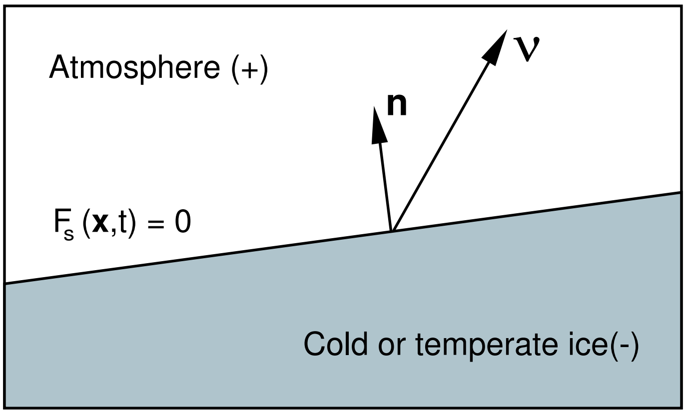

Figure 5.1: Free-surface geometry.

be the free surface at time t. Let us assume that there exists a one-parametric one-to-one mapping

$$\chi_S : \mathcal{S}_0 \times E \longrightarrow \mathcal{S}_t \ ,$$

where for any $\vec{x} \in \mathcal{S}_t$ there exists $\vec{x}_0 \in \mathcal{S}_0$ such that

$$\vec{x} \ = \ \chi_S(\vec{x}_0, t) \ .$$

We can then define the *surface velocity* $\vec{\nu}$ (the mapping is assumed to be sufficiently smooth) by

$$\vec{\nu} \ = \ \left.\frac{\partial \chi_S(\vec{x}_0, t)}{\partial t}\right|_{\vec{x}_0} \ . \tag{5.14}$$

The time derivative at constant $\vec{x}_0$ of the implicit equation (5.13) then yields

$$\frac{\partial F_S}{\partial t} \ + \ \vec{\nu} \cdot \mathrm{grad} F_S \ = \ 0 \ , \tag{5.15}$$

which is the evolution equation for the free surface. It might be convenient to rewrite this equation as

$$\frac{\partial F_S}{\partial t} \ + \ \vec{v}_2^{\,-} \cdot \mathrm{grad} F_S \ = \ (\vec{v}_2^{\,-} - \vec{\nu}) \cdot \mathrm{grad} F_S \ , \tag{5.16}$$

where $\vec{v}_2^{\,-}$ is the ice velocity on the negative side of the surface, the orientation being determined by the unit vector $\vec{n}$:

$$\vec{n}(\vec{x}, t) \ = \frac{\mathrm{grad} F_S(\vec{x}, t)}{\|\mathrm{grad} F_S(\vec{x}, t)\|} \ , \qquad \qquad \vec{x} \in \mathcal{S}_t \ , \tag{5.17}$$

which points, by definition, from the negative to positive side of $\mathcal{S}_t$. With the use of $\vec{n}$, equation (5.16) can be also written as

$$\frac{\partial F_S}{\partial t} \ + \ \vec{v}_2^{\,-} \cdot \mathrm{grad} F_S \ = \ (\vec{v}_2^{\,-} - \vec{\nu}) \cdot \vec{n} \, \|\mathrm{grad} F_S\| \ . \tag{5.18}$$

The evolution equation (5.15) represents a *kinematic* constraint for the free surface. In addition, the analysis of the balance laws yields a set of *dynamic constraints* as listed below.

Mass-jump conditions
The free surface will be considered as a singular surface in the water-ice-air mixture ($\alpha = 1, 2, 3$, respectively). We assume that air at the negative side (Fig. 5.1) of the free surface (in the glacier) is highly diluted, and its density is sufficiently small that it does not affect the behaviour of the ice-water mixture. To express that, we will here and henceforth adopt the following notation

$$\rho_3^- \to 0 \ . \tag{5.19}$$

By this assumption, we can apply the mixture theory (see Chapter 3) to a 3-component mixture, formulate the boundary conditions at the free surface as the interface conditions at a singular surface in the mixture. The densities ρ_1^+ and ρ_2^+, of water and ice, respectively, in the atmosphere are usually assumed to be small[1], but cannot be put equal to zero since it would contradict the accumulation or ablation process on the free surface.

The above formulation is applied to the temperate ice–air boundary. The cold ice–air boundary will be represented by a singular surface at which $\rho_1^- \to 0$, that is water is not present inside the glacier.

The general form of the mass-jump conditions at a singular surface, following from the mass balance of a n-component mixture (3.28), (3.32) reads as

$$[\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \ = \ r_\alpha^s \ , \qquad \sum_{\alpha=1}^{3} r_\alpha^s \ = \ 0 \ . \tag{5.20}$$

At the free surface, we further assume that there is no surface air production,

$$r_3^s \equiv 0 \ . \tag{5.21}$$

Eq. (5.20) then implies that

$$r_1^s \ = \ -r_2^s \ , \tag{5.22}$$

where the surface production terms r_1^s and r_2^s represent the mass exchange between the ice and water component, i.e. melting or refreezing of ice at the free surface.

The ice component
The jump condition (5.20) for the ice component ($\alpha = 2$) reads

$$[\rho_2(\vec{v}_2 - \vec{\nu})]_-^+ \cdot \vec{n} \ = \ r_2^s \ . \tag{5.23}$$

The term $\rho_2^+(\vec{v}_2 - \vec{\nu})^+ \cdot \vec{n}$, means the mass influx or outflow of ice through the free surface from the glacier to the atmosphere (per unit time and unit surface). We usually do not have information about ρ_2^+ and $\vec{v}_2^+$ separately, but their product can be measured by a so-called *free-surface ice accumulation-ablation function* (positive for accumulation):

$$a_{2\perp}^s \ = \ -\rho_2^+(\vec{v}_2^+ - \vec{\nu}) \cdot \vec{n} \ . \tag{5.24}$$

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[1] Except the case of an ice layer overlain by a water layer, which is not explicitly considered here, however extension of the description to such a situation is straightforward.

With (5.24), equation (5.23) becomes

$$\rho_2^-(\vec{v}_2^- - \vec{\nu}) \cdot \vec{n} \;=\; -(a_{2\perp}^s + r_2^s) \;, \tag{5.25}$$

or expressed in terms of the water content w and ice-water mixture density ρ, we have

$$(1 - w^-)(\vec{v}_2^- - \vec{\nu}) \cdot \vec{n} \;=\; -\frac{a_{2\perp}^s + r_2^s}{\rho} \;. \tag{5.26}$$

The water component
The jump condition (5.20) for water ($\alpha = 1$) reads:

$$[\rho_1(\vec{v}_1 - \vec{\nu})]_-^+ \cdot \vec{n} \;=\; r_1^s. \tag{5.27}$$

The process of snow and water accumulation and ablation is very complex and of course seasonally dependent. We look for the formulation of the boundary conditions in a time-averaged sense (say over a one-year period of the accumulation-ablation cycle), and replace the time dependent accumulation, ablation and surface production terms by their average values. In analogy with the previous case of the ice component, we introduce another climatological input quantity, an average *liquid-precipitation rate* $\mathcal{P}^s$ corresponding to the mass of water fallen at the glacier surface during rainfalls over the year.

There is a problem with an interpretation of the term $\rho_1^+(\vec{v}_1^+ - \vec{\nu}) \cdot \vec{n}$. Although an analogous term for the ice component was identified as the snow accumulation-ablation function, a climatological quantity, describing the time-averaged snowfall rate, the considered term for the water component is somewhat more difficult to relate to the liquid-precipitation rate. The difference is that whereas all the fallen snow is assumed either to stay at the given location, or to melt partially, water may also flow away along the glacier surface in the surface water system (streams, rivers,...). Therefore only a fraction of the total liquid-precipitation rate affects the water-mass balance of an ice sheet.

To handle this, we suggest the water inflow rate to be related to the precipitation and melting rate as follows:

$$\rho_1^-(\vec{v}_1^- - \vec{\nu}) \cdot \vec{n} \;=\; -\gamma(r_1^s + \mathcal{P}^s) \;, \qquad \text{where } \gamma \in \langle 0, 1\rangle \;. \tag{5.28}$$

Thus we assume that the inflow of water to the glacier volume is a γ-fraction of the total liquid precipitation plus the γ-fraction of the water surface production rate (surface ice-melting rate). The remaining water is assumed to be driven away in the surface water system, not entering the glacier volume.

Equation (5.28) can be equivalently rewritten as

$$\rho w^-(\vec{v}_2^- - \vec{\nu}) \cdot \vec{n} \;+\; \rho w^- \vec{u}_1^- \cdot \vec{n} \;=\; -\gamma(r_1^s + \mathcal{P}^s) \;, \tag{5.29}$$

which, with the use of (5.26) and (5.22) reads

$$\rho w^- u_1^- \cdot \vec{n} \;=\; \frac{w^-}{1 - w^-}(a_{2\perp}^s + r_2^s) \;+\; \gamma(r_2^s - \mathcal{P}^s). \tag{5.30}$$

The air component
Considering jump condition (5.20) and assuming that there is no air-mass flux through the free surface into the glacier, in accordance with (5.19), that is

$$\rho_3^-(\vec{v}_3^- - \vec{\nu})\cdot\vec{n} \;=\; 0\;, \tag{5.31}$$

we obtain

$$\rho_3^+(\vec{v}_3^+ - \vec{\nu})\cdot\vec{n} \;=\; 0\;. \tag{5.32}$$

As mentioned above, the mass-jump condition for the case of a *cold-ice–air boundary* is only a special case of the condition on a temperate-ice – air boundary. We additionally assume that $\rho_1^- \to 0$, i.e. $w^- \to 0$, no water is present in the glacier volume. Then the mass balance for *the ice component* (5.26) reads

$$(\vec{v}_2^- - \vec{\nu})\cdot\vec{n} \;=\; -\frac{a_\perp^s + r_2^s}{\rho}\;, \tag{5.33}$$

mass balance for *the water component* (5.27) need not be considered since no water is present at the negative side of the free surface (in the glacier volume), formally (5.27) states that $\rho_1^+(\vec{v}_1^+ - \vec{\nu})\cdot\vec{n} \;=\; r_1^s$, being equivalent to an assumption that all meltwater flows away from the glacier volume, moreover $\gamma = 0$, as can be seen from (5.30) considering $w^- = 0$. For *the air component*, (5.31) and (5.32) remain unaltered.

Linear-momentum-jump conditions
The general form of these conditions follows from (3.41) and (3.45):

$$[\mathbf{T}_\alpha - \rho_\alpha\vec{v}_\alpha\otimes(\vec{v}_\alpha - \vec{\nu})]_-^+\cdot\vec{n} = -\vec{f}_\alpha^{\,s}\;, \qquad\qquad \sum_{\alpha=1}^{3}\vec{f}_\alpha^{\,s} \;=\; \vec{0}\;. \tag{5.34}$$

Due to the simplifications we have introduced for the stress constitutive equations, it is sufficient to use only the linear-momentum jump condition for the mixture as a whole:

$$\sum_{\alpha=1}^{3}[\mathbf{T}_\alpha - \rho_\alpha\vec{v}_\alpha\otimes(\vec{v}_\alpha - \vec{\nu})]_-^+\cdot\vec{n} = \vec{0}\;.$$

Since the accumulation velocities at the free surface are small, we neglect the terms $[\rho_\alpha\vec{v}_\alpha\otimes(\vec{v}_\alpha - \vec{\nu})]_-^+\cdot\vec{n}$, corresponding to the linear-momentum jumps across the free surface. We arrive at

$$[\mathbf{T}_1 \;+\; \mathbf{T}_2 \;+\; \mathbf{T}_3]_-^+\cdot\vec{n} \;=\; 0\;, \tag{5.35}$$

Additionally, we will assume

$$\mathbf{T}_3^- \;=\; \mathbf{0}\;, \tag{5.36}$$

since air is not considered to be present in the glacier. Likewise, for a *cold-ice – air boundary*, we assume

$$\mathbf{T}_1^- \;=\; \mathbf{0}\;. \tag{5.37}$$

Energy-jump condition
At all singular surfaces, the free surface, the glacier bed and the cold-temperate ice-transition surface (CTS), the temperature will be considered continuous,

$$[T]_-^+ = 0 \ . \tag{5.38}$$

The energy-jump condition for a mixture (3.66) is

$$\left[\sum_{\alpha=1}^{n} \left\{ \rho_\alpha (\varepsilon_\alpha + \frac{1}{2}\ \vec{v}_\alpha{}^2)(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha \right\} + \vec{q} \right]_-^+ \cdot \vec{n} \ = \ 0.$$

For our case, i.e. $n = 3$:

$$\begin{aligned} 0 \ &= \ \Big[\rho_1 \left(\varepsilon_1 + \frac{1}{2}\vec{v}_1^2 \right) (\vec{v}_1 - \vec{\nu}) \ + \ \rho_2 \left(\varepsilon_2 + \frac{1}{2}\vec{v}_2^2 \right) (\vec{v}_2 - \vec{\nu}) \ + \ \rho_3 \left(\varepsilon_3 + \frac{1}{2}\vec{v}_3^2 \right) (\vec{v}_3 - \vec{\nu}) \\ &- \ \vec{v}_1 \cdot \mathbf{T}_1 \ - \ \vec{v}_2 \cdot \mathbf{T}_2 \ - \ \vec{v}_3 \cdot \mathbf{T}_3 \ + \ \vec{q} \Big]_-^+ \cdot \vec{n}. \end{aligned} \tag{5.39}$$

Since the accumulation velocities at the free surface are small, we neglect $\frac{1}{2}(\rho_1 \vec{v}_1^2)^\pm$, $\frac{1}{2}(\rho_2 \vec{v}_2^2)^\pm$, $\frac{1}{2}(\rho_3 \vec{v}_3^2)^\pm$, that describe the jump in kinetic energies. Moreover, ε_1 and ε_2 are functions of temperature only (see (4.190)) and temperature is continuous across the surface, which implies continuity of ε_1, ε_2 across the free surface, and (5.39) reads:

$$\begin{aligned} 0 \ &= \ \varepsilon_1 \left[\rho_1 (\vec{v}_1 - \vec{\nu}) \right]_-^+ \cdot \vec{n} + \ \varepsilon_2 \left[\rho_2 (\vec{v}_2 - \vec{\nu}) \right]_-^+ \cdot \vec{n} \ + \ \left[\varepsilon_3 \rho_3 (\vec{v}_3 - \vec{\nu}) \right]_-^+ \cdot \vec{n} \\ &- \ \left[\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + \vec{v}_3 \cdot \mathbf{T}_3 \right]_-^+ \cdot \vec{n} \ + \ [\vec{q}]_-^+ \cdot \vec{n} \ . \end{aligned}$$

Using (5.22), (5.23), (5.27), (5.31) and (5.32), we find:

$$0 \ = \ r_2^s (\varepsilon_2 - \varepsilon_1) \ - \ \left[\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + \vec{v}_3 \cdot \mathbf{T}_3 \right]_-^+ \cdot \vec{n} \ + \ [\vec{q}]_-^+ \cdot \vec{n} \ . \tag{5.40}$$

The terms $\vec{v}_\alpha^\pm \cdot \mathbf{T}_\alpha^\pm \cdot \vec{n}$ represent the mechanical work of the rest of the mixture on the α component at the singular surface (from the (+) or (−) side). In view of this interpretation, we can put

$$\vec{v}_3^- \cdot \mathbf{T}_3^- \cdot \vec{n} \ = \ 0 \ , \tag{5.41}$$

keeping in mind the assumption that air is not present at the negative side of the surface, that is in the glacier.

In the special case of a *cold-ice – air surface*, in addition to the above conditions, it holds that $\vec{v}_1^- \cdot \mathbf{T}_1^- \cdot \vec{n} \ = \ 0$.

Entropy-jump condition
The general condition (3.74) at the singular surface is

$$0 \ \leq \ \left[\ \sum_{\alpha=1}^{3} \rho_\alpha s_\alpha (\vec{v}_\alpha - \vec{\nu}) + \frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n} \ ,$$

which at the free surface for $n = 3$ holds

$$0 \;\leq\; \left[\rho_1 s_1 (\vec{v}_1 - \vec{\nu}) \;+\; \rho_2 s_2 (\vec{v}_2 - \vec{\nu}) \;+\; \rho_3 s_3 (\vec{v}_3 - \vec{\nu}) \;+\; \frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n} \; . \tag{5.42}$$

Since s_1 and s_2 are continuous across the free surface, being functions of T only (see (4.185)), we obtain:

$$0 \;\leq\; s_1 \left[\rho_1 (\vec{v}_1 - \vec{\nu}) \right]_-^+ \cdot \vec{n} \;+\; s_2 \left[\rho_2 (\vec{v}_2 - \vec{\nu}) \right]_-^+ \cdot \vec{n} \;+\; \left[s_3 \rho_3 (\vec{v}_3 - \vec{\nu}) \right]_-^+ \cdot \vec{n} \;+\; \left[\frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n} \; .$$

Using (5.22), (5.23), (5.27), (5.31) and (5.32), we finally have

$$0 \;\leq\; r_2^s T (s_2 - s_1) \;+\; [\vec{q}]_-^+ \cdot \vec{n} \; . \tag{5.43}$$

5.2.2 Ice-bedrock interface

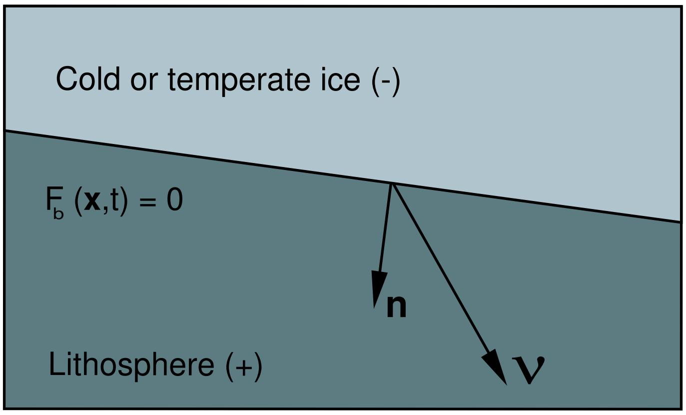

Figure 5.2: Ice-bedrock boundary.

The situation at the ice-bedrock interface is analogous to the situation at the free surface. The interface lies between cold or temperate ice ((−) side of the interface), and the bedrock ((+) side of the interface). The mixture approach is adopted again for a three-component water-ice-bedrock mixture ($\alpha = 1, 2, 3$, respectively). We consider the limits

$$\rho_2^+ \to 0, \;\; \rho_3^- \to 0 \; , \tag{5.44}$$

i.e. ice does not penetrate into the bedrock and vice versa. Similar assumptions need not be made for ρ_1^+, since we generally assume the bedrock to be permeable for water. The above formulation describes the boundary with temperate ice at one side, the case with cold ice can be obtained by considering $\rho_1^- \to 0$.

The kinematic equation for the ice-bedrock surface evolution is assumed to be defined by a given function $F_B(\vec{x}, t)$. We also assume that the surface velocity $\vec{\nu}$ is again well defined.

The dynamic constraints are derived from the balance equations as follows.

Mass-jump condition
The mass jump conditions (3.28) and (3.32) are:

$$[\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]^+_- \cdot \vec{n} \ = \ r^b_\alpha \ , \qquad \sum_{\alpha=1}^{3} r^b_\alpha \ = \ 0 \ . \tag{5.45}$$

We assume that bedrock material is not produced at the ice-bedrock interface, that is

$$r^b_3 \equiv \ 0 \ . \tag{5.46}$$

Thus, (5.45) yields

$$r^b_1 \ = \ -r^b_2 \ , \tag{5.47}$$

where the surface-production terms r^b_1 and r^b_2, describe the mass exchange between ice and water, caused by the melting of ice or the refreezing of water at the ice-bedrock interface.

Ice component
The general mass-jump condition (5.45) for $\alpha = 2$ reads

$$[\rho_2(\vec{v}_2 - \vec{\nu})]^+_- \cdot \vec{n} \ = \ r^b_2 \ . \tag{5.48}$$

As stated before, we consider the bedrock to be impermeable to ice, thus

$$\rho^+_2(\vec{v}^+_2 - \vec{\nu}) \cdot \vec{n} \ = \ 0 \ . \tag{5.49}$$

Hence it holds

$$\rho^-_2(\vec{v}^-_2 - \vec{\nu}) \cdot \vec{n} \ = \ -r^b_2 \ , \tag{5.50}$$

or,

$$\rho(1 - w^-)(\vec{v}^-_2 - \vec{\nu}) \cdot \vec{n} \ = \ -r^b_2 \ . \tag{5.51}$$

Water component
The jump condition (5.45) for the water component ($\alpha = 1$) reads

$$[\rho_1(\vec{v}_1 - \vec{\nu})]^+_- \cdot \vec{n} \ = \ r^b_1 \tag{5.52}$$

We define the function

$$o^b_{1\perp} \ = \ \rho^+_1(\vec{v}^+_1 - \vec{\nu}) \cdot \vec{n} \ , \tag{5.53}$$

that describes the outflow (inflow) of water from the glacier to the bedrock. Inspecting (5.47), eq. (5.52) becomes

$$\rho^-_1(\vec{v}^-_1 - \vec{\nu}) \cdot \vec{n} \ = \ o^b_{1\perp} + r^b_2 \ , \tag{5.54}$$

or, equivalently,

$$\rho w^-(\vec{v}^-_2 - \vec{\nu}) \cdot \vec{n} \ + \ \rho w^- \vec{u}^-_1 \cdot \vec{n} \ = \ o^b_{1\perp} + r^b_2 \ . \tag{5.55}$$

Using (5.51), we obtain

$$\begin{aligned} -r_2^b \frac{w^-}{1-w^-} \; + \; \rho w^- \vec{u}_1^- \cdot \vec{n} &= o_{1\perp}^b + r_2^b \;, \\ \rho w^- \vec{u}_1^- \cdot \vec{n} &= o_{1\perp}^b + \frac{r_2^b}{1-w^-} \;. \end{aligned} \tag{5.56}$$

Bedrock-material component

The mass-jump condition (5.45) for the bedrock-material component ($\alpha = 3$) reads

$$[\rho_3(\vec{v}_3 - \vec{\nu})]_-^+ \cdot \vec{n} \; = \; 0 \;. \tag{5.57}$$

Since bedrock material does not penetrate to the glacier, it holds

$$\rho_3^-(\vec{v}_3^- - \vec{\nu}) \cdot \vec{n} \; = \; 0 \;, \tag{5.58}$$

and thus (5.57) yields

$$\rho_3^+(\vec{v}_3^+ - \vec{\nu}) \cdot \vec{n} \; = \; 0 \;. \tag{5.59}$$

Here again we summarize the above results for the special case of *the cold-ice – bedrock boundary*, where, in addition, $\rho_1^- \to 0$. The mass balance for *the ice component* (5.50) reduces to

$$\rho(\vec{v}_2^- - \vec{\nu}) \cdot \vec{n} \; = \; -r_2^b \;. \tag{5.60}$$

The mass balance (5.56) for *the water component* simplifies to

$$o_{1\perp}^b \; = \; -r_2^b \;. \tag{5.61}$$

The mass balance (5.59) for the bedrock-material component remains unaltered.

Sliding law

At the ice-bedrock interface, we also prescribe a relation between *the ice-sliding velocity* $\vec{v}_{2sl}$, and *the basal shear stress* $\vec{t}_{2\|}^{\,-}$. The sliding velocity is defined as the tangential velocity of ice relative to the bedrock:

$$\vec{v}_{2sl} \; = \; \vec{v}_{2\|}^{\,-} - \vec{v}_{3\|}^{\,+} \;, \tag{5.62}$$

where

$$\vec{v}_{\alpha\|}^{\,\pm} \; = \; \vec{v}_\alpha^{\,\pm} - \vec{n}(\vec{v}_\alpha^{\,\pm} \cdot \vec{n}) \;.$$

The basal shear stress is defined as

$$\vec{t}_{2\|}^{\,-} \; = \; \mathbf{T}_2^- \cdot \vec{n} \; - \; \vec{n}(\vec{n} \cdot \mathbf{T}_2^- \cdot \vec{n}) \;.$$

The sliding law therefore has the form

$$\vec{v}_{2sl} \; = \; -C(\vec{n} \cdot \mathbf{T}_2^- \cdot \vec{n}, \ldots)\vec{t}_{2\|}^{\,-} \;. \tag{5.63}$$

The form of function $C()$ is a subject of discussion and experiments, since various different types of sliding mechanisms may occur. The most simple approximation considers the sliding function to be constant for the temperate-ice – bedrock boundary, and zero for the cold-ice – bedrock boundary with temperature below melting point (see Greve [6]).

Linear-momentum-jump conditions
The situation is analogous to the free surface, hence we will only discuss it briefly. The linear-momentum jump conditions (3.41) and (3.45) read:

$$[\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]^+_- \cdot \vec{n} = -\vec{f}^{\,b}_\alpha \,, \qquad \sum_{\alpha=1}^{3} \vec{f}^{\,b}_\alpha = \vec{0}\,. \tag{5.64}$$

We will again make use of only the linear-momentum jump condition for the mixture as a whole:

$$\sum_{\alpha=1}^{3} [\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]^+_- \cdot \vec{n} = \vec{0}\,. \tag{5.65}$$

We neglect the terms with $[\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]^+_- \cdot \vec{n}$, that correspond to the linear-momentum jumps across the boundary since they are assumed to be small:

$$[\mathbf{T}_1 + \mathbf{T}_2 + \mathbf{T}_3]^+_- \cdot \vec{n} = 0\,.$$

In view of the density limits (5.44):

$$\mathbf{T}_2^+ = \mathbf{T}_3^- = \mathbf{0}\,, \tag{5.66}$$

the linear-momentum jump condition finally reads:

$$(\mathbf{T}_3^+ + \mathbf{T}_1^+) \cdot \vec{n} = (\mathbf{T}_1^- + \mathbf{T}_2^-) \cdot \vec{n}\,. \tag{5.67}$$

For the cold-ice – bedrock boundary, no water is present in the glacier volume, thus $\mathbf{T}_\mathbf{1}^- = \mathbf{0}$.

Energy-jump condition
Analogously to the free surface, temperature is considered to be continuous across the ice-bedrock interface:

$$[T]^+_- = 0\,. \tag{5.68}$$

The general energy-jump condition for the mixture (3.66) is

$$0 = \left[\sum_{\alpha=1}^{n} \left\{\rho_\alpha (\varepsilon_\alpha + \frac{1}{2}\,\vec{v}_\alpha^{\,2})(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha\right\} + \vec{q}\,\right]^+_- \cdot \vec{n}\,,$$

and for a 3-component mixture:

$$\begin{aligned} 0 \;=\; & \Big[\rho_1 \left(\varepsilon_1 + \frac{1}{2}\vec{v}_1^{\,2}\right)(\vec{v}_1 - \vec{\nu}) + \rho_2 \left(\varepsilon_2 + \frac{1}{2}\vec{v}_2^{\,2}\right)(\vec{v}_2 - \vec{\nu}) + \rho_3 \left(\varepsilon_3 + \frac{1}{2}\vec{v}_3^{\,2}\right)(\vec{v}_3 - \vec{\nu}) \\ & - \vec{v}_1 \cdot \mathbf{T}_1 - \vec{v}_2 \cdot \mathbf{T}_2 - \vec{v}_3 \cdot \mathbf{T}_3 + \vec{q}\,\Big]^+_- \cdot \vec{n}. \end{aligned}$$

We omit the terms $\frac{1}{2}(\rho_1\vec{v}_1^2)^{\pm}$, $\frac{1}{2}(\rho_2\vec{v}_2^2)^{\pm}$ and $\frac{1}{2}(\rho_3\vec{v}_3^2)^{\pm}$, that describe jumps in the kinetic energies, and since ε_1 and ε_2 are continuous, being functions of temperature only, we obtain

$$\begin{aligned} 0 \;&=\; \varepsilon_1\,[\rho_1(\vec{v}_1-\vec{\nu})]_-^+\cdot\vec{n} +\; \varepsilon_2\,[\rho_2(\vec{v}_2-\vec{\nu})]_-^+\cdot\vec{n} \;+\; [\varepsilon_3\rho_3(\vec{v}_3-\vec{\nu})]_-^+\cdot\vec{n} \\ &-\; [\vec{v}_1\cdot\mathbf{T}_1+\vec{v}_2\cdot\mathbf{T}_2+\vec{v}_3\cdot\mathbf{T}_3]_-^+\cdot\vec{n} \;+\; [\vec{q}]_-^+\cdot\vec{n}\;. \end{aligned}$$

Using (5.47), (5.48), (5.52), (5.58) and (5.59):

$$0 \;=\; r_2^b(\varepsilon_2-\varepsilon_1) \;-\; [\vec{v}_1\cdot\mathbf{T}_1+\vec{v}_2\cdot\mathbf{T}_2+\vec{v}_3\cdot\mathbf{T}_3]_-^+\cdot\vec{n} \;+\; [\vec{q}]_-^+\cdot\vec{n}\;. \tag{5.69}$$

The terms $\vec{v}_\alpha^{\pm}\cdot\mathbf{T}_\alpha^{\pm}\cdot\vec{n}$ represent the mechanical work at the singular surface exerted at the α component. Hence, we may assume that

$$\vec{v}_2^{+}\cdot\mathbf{T}_2^{+}\cdot\vec{n} \;=\; \vec{v}_3^{-}\cdot\mathbf{T}_3^{-}\cdot\vec{n} \;=\; 0\;,$$

in accordance with the assumption that ice at the positive side and the bedrock-material at the negative side of the ice-bedrock interface are highly diluted. As a result, we have

$$0 \;=\; r_2^b(\varepsilon_2-\varepsilon_1) \;+\; \vec{v}_1^{-}\cdot\mathbf{T}_1^{-}\cdot\vec{n} + \vec{v}_2^{-}\cdot\mathbf{T}_2^{-}\cdot\vec{n} - \vec{v}_3^{+}\cdot\mathbf{T}_3^{+}\cdot\vec{n} \;-\vec{v}_1^{+}\cdot\mathbf{T}_1^{+}\cdot\vec{n} \;+\; [\vec{q}]_-^+\cdot\vec{n}\;. \tag{5.70}$$

The special case of a cold-ice–bedrock interface follows the same procedure, but since no water is present in the glacier volume, we put $\vec{v}_1^{-}\cdot\mathbf{T}_1^{-}\cdot\vec{n} \;=\; 0$.

Entropy-jump condition

From (3.74), we have

$$0 \;\le\; \left[\,\sum_{\alpha=1}^{3}\rho_\alpha s_\alpha(\vec{v}_\alpha-\vec{\nu})+\frac{\vec{q}}{T}\right]_-^+\cdot\vec{n}\;,$$

thus, for a 3-component mixture

$$0 \;\le\; \left[\rho_1 s_1(\vec{v}_1-\vec{\nu}) \;+\; \rho_2 s_2(\vec{v}_2-\vec{\nu}) \;+\; \rho_3 s_3(\vec{v}_3-\vec{\nu}) \;+\; \frac{\vec{q}}{T}\right]_-^+\cdot\vec{n}\;. \tag{5.71}$$

Since T is continuous, so are s_1, and s_2, being functions of T only (see (4.185)). Thus it holds

$$0 \;\le\; s_1\,[\rho_1(\vec{v}_1-\vec{\nu})]_-^+\cdot\vec{n} \;+\; s_2\,[\rho_2(\vec{v}_2-\vec{\nu})]_-^+\cdot\vec{n} \;+\; [s_3\rho_3(\vec{v}_3-\vec{\nu})]_-^+\cdot\vec{n} \;+\; \left[\frac{\vec{q}}{T}\right]_-^+\cdot\vec{n}\;,$$

and finally, using (5.47), (5.48), (5.52), (5.58) and (5.59), we find

$$0 \;\le\; r_2^b T(s_2-s_1) \;+\; [\vec{q}]_-^+\cdot\vec{n}\;. \tag{5.72}$$

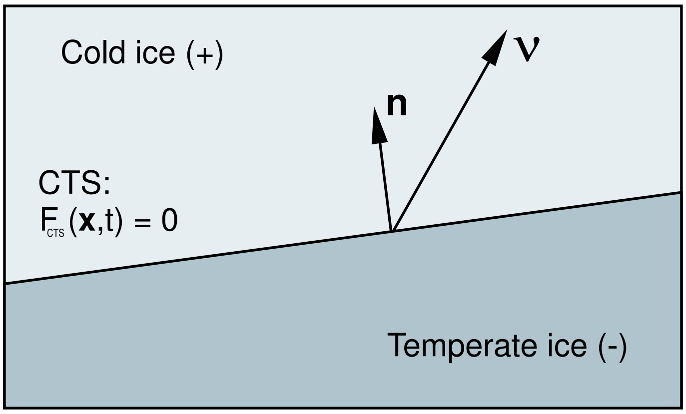

Figure 5.3: Cold-temperate ice transition surface geometry.

5.2.3 Cold-temperate ice transition surface (CTS)

The cold-temperate ice transition surface (CTS) is a surface between the cold (sign (+)) and temperate (sign (−)) region of an ice sheet, where the melting of ice and refreezing of meltwater may occur. In view of the mixture theory approach, the CTS is described as a singular surface in the water-ice mixture ($\alpha = 1, 2$, respectively), at which the water fraction tends to zero at the positive (cold) side:

$$\rho_1^+ \to 0 \ . \tag{5.73}$$

The kinematic conditions for the CTS are of the same form as for the free surface. Provided that the CTS is given by an implicit equation $F_{CTS}(\vec{x}, t) \ = \ 0$ and the surface velocity $\vec{\nu}$ is defined, the evolution equation for the CTS is

$$\frac{\partial F_{CTS}}{\partial t} \ + \ \vec{v}_2^+ \cdot \mathrm{grad} F_{CTS} \ = \ (\vec{v}_2^+ - \vec{\nu}) \cdot \vec{n} \, \|\mathrm{grad} F_{CTS}\| \ , \tag{5.74}$$

where

$$\vec{n}(\vec{x}, t) \ = \frac{\mathrm{grad} F_{CTS}(\vec{x}, t)}{\|\mathrm{grad} F_{CTS}(\vec{x}, t)\|} \ , \qquad \vec{x} \in \mathrm{CTS} \ , \tag{5.75}$$

and $\vec{v}_2^+$ is the material velocity of the ice component at the positive (temperate) side of the CTS.

The dynamic conditions again follow from the general jump conditions in mixtures.

Mass-jump conditions

The mass-jump conditions (3.28) and (3.32) read as

$$[\rho_\alpha(\vec{v}_\alpha - \vec{\nu})]_-^+ \cdot \vec{n} \ = \ r_\alpha^{cts} \ , \qquad \sum_{\alpha=1}^{2} r_\alpha^{cts} \ = \ 0 \ , \tag{5.76}$$

hence

$$r_1^{cts} \ = \ -r_2^{cts} \ . \tag{5.77}$$

The surface production terms r_1^{cts},r_2^{cts}, describe the mass exchange between the ice and water component, i.e. the melting of ice or refreezing of water at the CTS.

The ice component
The jump condition (5.76) for the ice component ($\alpha = 2$) implies

$$[\rho_2(\vec{v}_2 - \vec{\nu})]^+_- \cdot \vec{n} \;=\; r_2^{cts} \; . \tag{5.78}$$

We will assume that the ice velocity remains continuous across the CTS, i.e. $\vec{v}_2^+ = \vec{v}_2^-$, a usual assumption in glaciology ([6]), since the CTS can be primarily viewed as a thermal, not a mechanical boundary. Considering $\rho_2^+ = \rho$ (no water present in the cold-ice zone and the difference between the mixture density and the density of pure ice is negligible, see discussion in section 4.5.2), equation (5.78) can be written as

$$(\rho - \rho_2^-)(\vec{v}_2 - \vec{\nu}) \cdot \vec{n} \;=\; r_2^{cts} \; , \tag{5.79}$$

or in terms of the water content w as

$$w^-(\vec{v}_2 - \vec{\nu}) \cdot \vec{n} \;=\; \frac{r_2^{cts}}{\rho} \; . \tag{5.80}$$

The water component
The jump condition (5.76) for the water component ($\alpha = 1$) reads

$$[\rho_1(\vec{v}_1 - \vec{\nu})]^+_- \cdot \vec{n} \;=\; r_1^{cts}. \tag{5.81}$$

We have

$$\rho_1^+(\vec{v}_1^+ - \vec{\nu}) \cdot \vec{n} \;=\; 0 \; ,$$

since there is no meltwater in the cold-ice zone. By this and (5.77), we conclude that

$$\rho_1^-(\vec{v}_1^- - \vec{\nu}) \cdot \vec{n} \;=\; r_2^{cts} \; , \tag{5.82}$$

or,

$$\rho w^-(\vec{v}_2^- - \vec{\nu}) \cdot \vec{n} \;+\; \rho w^- \vec{u}_1^- \cdot \vec{n} \;=\; r_2^{cts},$$

which, in view of (5.80), may be written as

$$\rho w^- \vec{u}_1^- \cdot \vec{n} \;=\; 0 \; . \tag{5.83}$$

Linear-momentum-jump conditions

The linear-momentum-jump condition at the CTS follows from (3.41) and (3.45):

$$[\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]^+_- \cdot \vec{n} = \; -\vec{f}_\alpha^{cts} \; , \qquad \sum_{\alpha=1}^{2} \vec{f}_\alpha^{cts} \;=\; \vec{0} \; . \tag{5.84}$$

We again use only the linear-momentum-jump condition for the mixture as a whole:

$$\sum_{\alpha=1}^{2} [\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]^+_- \cdot \vec{n} = \; \vec{0} \; . \tag{5.85}$$

Neglecting the terms $[\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{\nu})]^+_- \cdot \vec{n}$, corresponding to the linear momentum jumps across the CTS, which are considered to be small, we arrive at

$$[\mathbf{T}_1 \ + \ \mathbf{T}_2]^+_- \cdot \vec{n} \ = \ 0 \ . \tag{5.86}$$

According to (5.73), we assume:

$$\mathbf{T}_1^+ \ = \ \mathbf{0} \ .$$

Hence, we obtain

$$\mathbf{T}_2^+ \cdot \vec{n} = \ (\mathbf{T}_1^- + \mathbf{T}_2^-) \cdot \vec{n} \ . \tag{5.87}$$

Energy-jump condition
Temperature is considered to be continuous across the CTS:

$$[T]^+_- \ = \ 0 \ . \tag{5.88}$$

The general energy-jump condition (3.66) for the mixture reads:

$$0 \ = \ \sum_{\alpha=1}^{n} \Big[\rho_\alpha(\varepsilon_\alpha + \frac{1}{2}\ \vec{v}_\alpha^{\ 2})(\vec{v}_\alpha - \vec{\nu}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha + \vec{q}_\alpha\Big]^+_- \cdot \vec{n} \ .$$

In our particular case $n = 2$:

$$\begin{aligned} 0 \quad &= \quad \Big[\rho_1 \left(\varepsilon_1 + \frac{1}{2}\vec{v}_1^2\right)(\vec{v}_1 - \vec{\nu}) \ + \ \rho_2 \left(\varepsilon_2 + \frac{1}{2}\vec{v}_2^2\right)(\vec{v}_2 - \vec{\nu}) \\ &- \quad \vec{v}_1 \cdot \mathbf{T}_1 \ - \ \vec{v}_2 \cdot \mathbf{T}_2 \ + \ \vec{q}\Big]^+_- \cdot \vec{n}. \end{aligned}$$

We omit $\frac{1}{2}(\rho_1\vec{v}_1^2)^\pm$ and $\frac{1}{2}(\rho_2\vec{v}_2^2)^\pm$, that describe the jump in kinetic energies, since they are small. Moreover, since ε_1 and ε_2 are continuous across the CTS, being functions of temperature only, we have

$$\begin{aligned} 0 \quad &= \quad \varepsilon_1 \, [\rho_1(\vec{v}_1 - \vec{\nu})]^+_- \cdot \vec{n} + \ \varepsilon_2 \, [\rho_2(\vec{v}_2 - \vec{\nu})]^+_- \cdot \vec{n} \\ &- \quad [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + \ \vec{q}]^+_- \cdot \vec{n} \ . \end{aligned}$$

Using (5.77), (5.78) and (5.81):

$$0 \ = \ r_2^{cts}(\varepsilon_2 - \varepsilon_1) \ - \ [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2]^+_- \cdot \vec{n} \ + \ [\vec{q}]^+_- \cdot \vec{n} \ . \tag{5.89}$$

The terms $\vec{v}_\alpha^\pm \cdot \mathbf{T}_\alpha^\pm \cdot \vec{n}$ represent the mechanical work at the singular surface (from (+) or (−) side) provided by the rest of the mixture and exerted at the α component. In view of this interpretation, we conclude that

$$\vec{v}_1^+ \cdot \mathbf{T}_1^+ \cdot \vec{n} = \ 0 \ ,$$

in accordance with the assumption that the water at the positive side is highly diluted. As a result, concerning also the assumebd continuity of the ice velocity, we obtain

$$0 \ = \ r_2^{cts}(\varepsilon_2 - \varepsilon_1) \ + \ \vec{v}_1^- \cdot \mathbf{T}_1^- \cdot \vec{n} \ + \vec{v}_2 \cdot (\mathbf{T}_2^- - \mathbf{T}_2^+) \cdot \vec{n} + \ [\vec{q}]^+_- \cdot \vec{n} \ . \tag{5.90}$$

We may further make use of the linear-momentum jump condition (5.87) and obtain

$$0 \;=\; r_2^{cts}(\varepsilon_2 - \varepsilon_1) \;+\; \vec{u}_1^- \cdot \mathbf{T}_1^- \cdot \vec{n} \;+\; [\vec{q}]_-^+ \cdot \vec{n} \;. \qquad (5.91)$$

Entropy-jump condition

The general entropy-jump condition (3.74) reads:

$$0 \;\leq\; \left[\, \sum_{\alpha=1}^{2} \rho_\alpha s_\alpha (\vec{v}_\alpha - \vec{\nu}) + \frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n} \;,$$

i.e. for a 2-component mixture:

$$0 \;\leq\; \left[\rho_1 s_1(\vec{v}_1 - \vec{\nu}) \;+\; \rho_2 s_2(\vec{v}_2 - \vec{\nu}) \;+\; \frac{\vec{q}}{T}\right]_-^+ \cdot \vec{n} \;. \qquad (5.92)$$

Temperature T is continuous across the CTS, which implies the continuity of s_1 and s_2, since they are functions of T only (according to (4.185)). Then

$$0 \;\leq\; s_1 \left[\rho_1(\vec{v}_1 - \vec{\nu})\right]_-^+ \cdot \vec{n} \;+\; s_2 \left[\rho_2(\vec{v}_2 - \vec{\nu})\right]_-^+ \cdot \vec{n} \;+\; \left[\frac{\vec{q}}{T}\right]_-^+ \cdot \vec{n} \;,$$

and finally, using (5.77), (5.78) and (5.81), we find

$$0 \;\leq\; r_2^{cts}\, T(s_2 - s_1) \;+\; [\vec{q}]_-^+ \cdot \vec{n} \;. \qquad (5.93)$$

Chapter 6

Numerical implementation: 2-D stationary case

6.1 Introduction

In the previous chapter we finalized the theoretical description of an ice sheet. The original aim of this chapter was the numerical implementation of the theory for an ice slab of uniform thickness under stationary conditions, and an elementary study of the differences in physical behaviour in the present and the traditional formulation. However, several numerical problems emerged that we weren't able to manage. In particular, the main problems were to determine the position of the CTS interface. The nonlinearity of the field equations and the uncertainty of several material parameters and boundary conditions considered, made the resulting problem numerically ill-conditioned. We therefore confine ourselves to numerically solve the temperate-zone equations only. This limited solution, however, demonstrates physical features and properties of the present formulation in comparison with the traditional approach.

6.2 Temperate ice layer

We will consider a two-dimensional inclined temperate-ice layer of uniform thickness. The following assumptions are made:

- Constant inclination angle γ of the slab, with uniformity in the x-direction:

$$\frac{\partial}{\partial x}(\cdot) \;=\; 0\;. \tag{6.1}$$

- Steady-state configuration:

$$\frac{\partial}{\partial t}(\cdot) \;=\; 0\;. \tag{6.2}$$

- Neglect of the pressure dependence of the melting point of ice,

$$T_M \;\equiv\; 0^{\circ}\mathrm{C}\;. \tag{6.3}$$

- Parameter values:

$$\begin{aligned}\rho &= 910 \text{ kg m}^{-3},\ k = 2.1\text{Wm}^{-1}\text{K}^{-1}, c_V = 2009\text{J kg}^{-1}\text{K}^{-1}, L = 335\text{kJ kg}^{-1},\\ g_a &= 9.81 \text{ m s}^{-2}.\end{aligned}$$

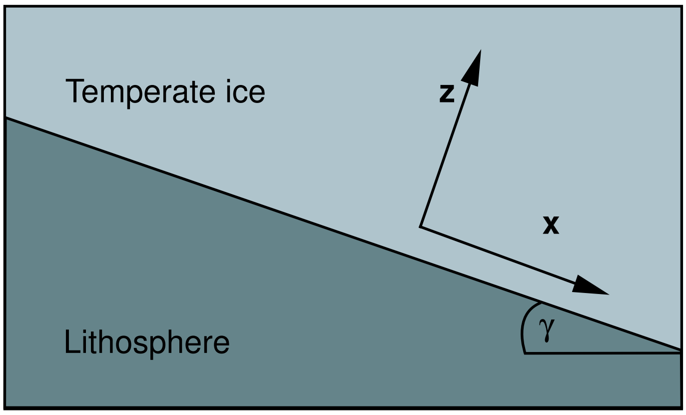

Figure 6.1: The coordinate system of the inclined temperate-ice layer.

In the coordinate system shown in Fig. 6.1, all field variables are functions of the z-variable only.

The traditional formulation

Under the assumptions (6.1)-(6.3), the field equations for the temperate-ice zone, listed in Chapter 2, reduce to:

Mass balance for the mixture (see (2.16))

$$\frac{dv_z^B}{dz} = 0\ . \tag{6.4}$$

Linear-momentum balance for the mixture

By omitting the inertia term $\rho\dot{\vec{v}}^B$ (Greve, [6]), (2.17) reads:

$$-\frac{dp}{dz} + \frac{d(\overset{\circ}{\mathbf{T}})_{zz}}{dz} - \rho g_a \cos\gamma = 0\ , \tag{6.5}$$

$$\frac{d(\overset{\circ}{\mathbf{T}})_{xz}}{dz} + \rho g_a \sin\gamma = 0\ . \tag{6.6}$$

Mass balance for the water component (see (2.19))

$$\rho\frac{dw}{dz}v_z^B = -\frac{dj_z}{dz} + M\ . \tag{6.7}$$

Stress-strain rate relation (see (2.21):

Using (6.4) and (6.1), we obtain

$$(\overset{\circ}{\mathbf{T}})_{xx} = 0\ , \tag{6.8}$$

$$(\overset{\circ}{\mathbf{T}})_{zz} = 0\ , \tag{6.9}$$

$$\frac{dv_x^B}{dz} = 2\mathcal{A}(T,w)d(\Sigma)(\overset{\circ}{\mathbf{T}})_{xz}, \tag{6.10}$$

where the temperature T_M is assumed to equal zero, see (6.3), and for the function $d(\Sigma)$ we adopt *Glen's flow law* with $n = 3$:

$$d(\Sigma) \; = \; \Sigma^2 \; . \tag{6.11}$$

The Σ variable was defined (see (2.26)) as

$$\Sigma \; = \sqrt{\frac{1}{2}\mathrm{tr}\{(\overset{\circ}{\mathbf{T}})^2\}} \; , \tag{6.12}$$

and now yields

$$\Sigma^2 \; = (\overset{\circ}{\mathbf{T}})^2_{xz} \; . \tag{6.13}$$

The dependence of $\mathcal{A}(w)$ on w is restricted to a linear function (see Lliboutry&Duval [11])

$$\mathcal{A}(w) \; = \; \mathrm{A}(1+\alpha w) \; , \tag{6.14}$$

with (Greve [6])

$$A \; = \; 5.3 \cdot 10^{-24}\mathrm{s}^{-1} \; \mathrm{Pa}^{-3}, \qquad \alpha = 184 \; . \tag{6.15}$$

Thus, the stress-strain rate relation (6.10) can be rewritten as

$$\frac{dv_x^B}{dz} \; = \; 2A(1+\alpha w)((\overset{\circ}{\mathbf{T}})_{xz})^3. \tag{6.16}$$

Constitutive equation for the diffusive water flux $\vec{j}$ (see (2.22)):

$$j_z \; = \; -\tilde{\nu}\frac{dw}{dz} \; , \tag{6.17}$$

and constitutive relation for water mass-production term M (see (2.23)):

$$\begin{aligned} M \; &= \; 2\frac{\mathcal{A}(w)d(\Sigma)\Sigma^2}{L} \\ &= \; 2\frac{\mathrm{A}(1+\alpha w)(\overset{\circ}{\mathbf{T}})^4_{xz}}{L} \; . \end{aligned} \tag{6.18}$$

The present formulation:
We rewrite the field equations, listed at the beginning of Chapter 5;
Mass balance for the ice component (see (5.8)):

$$\frac{dw}{dz}v_{2z} \; - \; \frac{dv_{2z}}{dz} \; = \; \frac{r_1}{\rho} \; . \tag{6.19}$$

Mass balance for the water component (see (5.9)):

$$\frac{dw}{dz}u_{1z} \; + \; \frac{dv_{2z}}{dz} \; + \; w\frac{du_{1z}}{dz} \; = \; 0 \; . \tag{6.20}$$

Linear-momentum balance for the water component (see (5.10)):

$$\begin{aligned} w\nu u_{1x} &= w\rho g_a \sin\gamma \ , && (6.21)\\ w\nu u_{1z} &= -\frac{d(pw)}{dz} - w\rho g_a \cos\gamma - \omega\frac{dw}{dz} \ . && (6.22) \end{aligned}$$

Linear-momentum balance for the ice component
For the numerical implementation, we consider $\overset{\circ}{\mathbf{T}}_2$ instead of $\overset{\circ}{\mathbf{D}}_2$ as an independent variable in the stress-strain rate relation. The linear-momentum balance for the ice component (5.11) is then written as

$$\begin{aligned} \frac{d(\overset{\circ}{\mathbf{T}}_2)_{xz}}{dz} + \rho g_a \sin\gamma &= 0 \ , && (6.23)\\ -\frac{dp}{dz} + \frac{d(\overset{\circ}{\mathbf{T}}_2)_{zz}}{dz} - \rho g_a \cos\gamma &= 0 \ . && (6.24) \end{aligned}$$

The *stress – strain-rate relation* adopted for the numerical implementation is of the form discussed in Chapter 4 (see (4.160)):

$$\overset{\circ}{\mathbf{D}}_2 = \mathcal{A}(w) d(\Sigma)\, \overset{\circ}{\mathbf{T}}_2 \ , \qquad (6.25)$$

that is, inverse to the relation considered in theoretical investigations. We will also use the linear dependence of $\mathcal{A}(w)$ on w (6.14) and apply Glen's flow law (6.11). For the purpose of the modelling, we need to specify the values of parameters A and α. Due to the lack of reliable estimates, we use the same values as in the traditional formulation. Consequently, the stress – strain-rate relations coincide formally in both approaches, but whilst in the traditional formulation, the relation for the strain deviator is related to the barycentric velocity, in the present formulation the strain deviator is related to the velocity of ice.

Since in our 2-D case,

$$\mathbf{D_2} = \begin{pmatrix} 0 & \frac{1}{2}\frac{dv_{2x}}{dz} \\ \frac{1}{2}\frac{dv_{2x}}{dz} & \frac{dv_{2z}}{dz} \end{pmatrix} , \qquad (6.26)$$

and the deviator of a second-order tensor in two dimensions in defined as

$$\overset{\circ}{\mathbf{D}}_2 = \mathbf{D_2} - \frac{1}{2}\mathrm{tr}(\mathbf{D}_2)\mathbf{1} \ , \qquad (6.27)$$

the relation (6.25) reads

$$\frac{1}{2}\begin{pmatrix} -\frac{dv_{2z}}{dz} & \frac{dv_{2x}}{dz} \\ \frac{dv_{2x}}{dz} & \frac{dv_{2z}}{dz} \end{pmatrix} = \mathcal{A}(w) d(\Sigma) \begin{pmatrix} \overset{\circ}{T}_{2xx} & \overset{\circ}{T}_{2xz} \\ \overset{\circ}{T}_{2xz} & \overset{\circ}{T}_{2zz} \end{pmatrix} . \qquad (6.28)$$

In view of (4.159), we have

$$\begin{aligned} 2\Sigma^2 &= \mathrm{tr}\{(\overset{\circ}{\mathbf{T}}_2)^2\} \\ &= (\overset{\circ}{\mathbf{T}}_2)^2_{xx} \ + \ (\overset{\circ}{\mathbf{T}}_2)^2_{zz} \ + \ 2(\overset{\circ}{\mathbf{T}}_2)^2_{xz} \\ &= 2\left((\overset{\circ}{\mathbf{T}}_2)^2_{zz} \ + \ (\overset{\circ}{\mathbf{T}}_2)^2_{xz}\right) \ . \end{aligned} \tag{6.29}$$

In addition, using the Glen's flow law (6.11) and (6.14), eq. (6.28) implies:

$$\frac{dv_{2z}}{dz} = 2A(1+\alpha w)\left((\overset{\circ}{\mathbf{T}}_2)^2_{zz} + (\overset{\circ}{\mathbf{T}}_2)^2_{xz}\right)(\overset{\circ}{\mathbf{T}}_2)_{zz} \ , \tag{6.30}$$

$$\frac{dv_{2x}}{dz} = 2A(1+\alpha w)\left((\overset{\circ}{\mathbf{T}}_2)^2_{zz} + (\overset{\circ}{\mathbf{T}}_2)^2_{xz}\right)(\overset{\circ}{\mathbf{T}}_2)_{xz} \ . \tag{6.31}$$

Finally, the balance of energy (see (4.197)):

$$\begin{aligned} (L - p\Delta)r_1 &= 2A(1+\alpha w)\left((\overset{\circ}{\mathbf{T}}_2)^2_{zz} + (\overset{\circ}{\mathbf{T}}_2)^2_{xz}\right)^2 + \lambda\frac{d(wu_{1z})}{dz} - wu_{1z}\frac{dp}{dz} \\ &+ w\rho g_a(u_{1x}\sin\gamma - u_{1z}\cos\gamma) \ . \end{aligned} \tag{6.32}$$

Moreover, we assign $\lambda = 0$, i.e. we neglect the Dufour effect (Mortimer [16]).

6.3 Examples

The equations from the preceding section were solved numerically by a program `t_ice.f90` written in Fortran 90. We made use of the IMSL routine DDASPG (see Press [15]), which provides the solution of a set of first-order ordinary differential equations, expressed in the implicit form

$$\vec{f}(\vec{y}(z)', \vec{y}(z), z) \ = \ \vec{0} \ .$$

We are solving an initial-value problem, the ice-bedrock boundary as the initial point. The thickness of the ice sheet is $H = 200$m, and we are inspecting only a part of the temperate - ice layer at the bottom of a thickness 10m. The exact position of the CTS would have to be calculated as a part of the solution, this task is however beyond our scope at the moment since we want to focus only on the way temperate-ice movement is affected by varying the diffusion parameters. In the first place we search for the threshold values of the diffusivities above which significant affection in the ice-velocity profiles can be observed. This could provide a chance to estimate the relative importance of water diffusion as soon as realistic estimates of the diffusivities are available from experiments. The initial values for the model are:

$$\begin{aligned} w(0) &= 0.05 \ , \\ p(0) &= H\rho g_a \ [\mathrm{Pa}] \ , \\ \overset{\circ}{T}_{xz}(0) &= 0.07 \cdot H\rho g_a \ [\mathrm{Pa}] \ , \end{aligned}$$

$$\begin{aligned}
\overset{\circ}{T}_{zz}(0) &= 0\ [\mathrm{Pa}]\ ,\\
u_{1z}(0) &= 0\ [\mathrm{ma}^{-1}]\ ,\\
v_{2x}(0) &= 5\ [\mathrm{m\,a}^{-1}]\ ,\\
v_{2z}(0) &= -0.2\ [\mathrm{m\,a}^{-1}]\ ,\\
j_z(0) &= 0\ [\mathrm{kg\,m}^{-2}\,\mathrm{a}^{-1}]\ .
\end{aligned}$$

We introduce the parameters

$$a = \frac{1}{\nu}\ , \qquad b = \frac{\omega}{\nu}\ , \qquad c = \tilde{\nu}\ , \tag{6.33}$$

where the first two are the diffusion parameters of the present formulation and c is the diffusivity considered in the traditional model.

The physical dimensions are

$$[a] = \mathrm{kg}^{-1}\,\mathrm{m}^3\,\mathrm{s}, \qquad [b] = \mathrm{m}^2\,\mathrm{s}^{-1}, \qquad [c] = \mathrm{kg\,m}^{-1}\mathrm{s}^{-1}\ .$$

- A)
  In the first example, we demonstrate that the traditional and new formulation coincide when the water transport is neglected. This is not surprising, we have systematically aimed during our derivations at the traditional model with an intent to derive it from basic physical principles. The results are depicted in Figure 6.2.

- B)
  In the next example, we inspect the role of the diffusion parameter c in the traditional formulation. After several tests we found that the bottom value where sensitivity to the diffusion of water emerges is about $c = 10^{-7}$. We therefore chose the range $c = 10^{-9}$ – 10^{-5}, to show the changes in the velocity profiles v_{2x}, and in the water content w, and z-component of the diffusive flux j_z (the x-component is identically zero due to our assumptions of uniformness in the x-direction). The remaining quantities, i.e. the stress field components and z-component of the ice velocity v_{2z} are not affected.

	c
B1:	10^{-9}
B2:	10^{-8}
B3:	10^{-7}
B4:	10^{-6}
B5:	10^{-5}

We display only first 8m of the temperate-ice layer, because the CTS position has lowered due to the diffusion and with increasing z-distance we would obtain negative, i.e. non-physical water-content.

- C)
  Finally, in the last example presented here, we deal with the diffusion parameters a and b from our derived formulation. We found that the threshold values of the diffusion parameters a and b, above which ice-velocity profiles are significantly affected are 10^{-15}, and 10^{-10}, respectively. We therefore display the computed results for the following range of parameter values:

	a	b
C1:	10^{-15}	10^{-10}
C2:	10^{-15}	10^{-9}
C3:	10^{-15}	10^{-8}
C4:	10^{-14}	10^{-10}
C5:	10^{-14}	10^{-9}
C6:	10^{-14}	10^{-8}
C7:	10^{-13}	10^{-10}
C8:	10^{-13}	10^{-9}
C9:	10^{-13}	10^{-8}

  The results are shown in Figure 6.4. We may see, that apart from the pressure p and $\overset{\circ}{\mathbf{T}}_{xz}$, all the remaining computed quantities show considerable variations. Again we display only first 8m of the temperate-ice layer, from the same reasons as in B).

To conclude, this elementary numerical example demonstrates that above certain threshold values of diffusion parameters in both the traditional and the new formulation, the ice-velocity profiles are affected by a water-transport in the ice matrix, as a result of the assumed water-content dependence of temperate-ice rheology. The threshold values are approximately 10^{-15}, 10^{-10}, 10^{-7}, for a, b, and c, respectively.

The differences between the formulations are difficult to quantify, however, we may observe, after inspecting the model equations, that for our easy model situation there is a connection between b and c parameters. They both correspond to diffusion driven by water-content gradient and it should hold $c \sim \rho b$. The analogy is valid with the limitation that we describe the water flux relative to the ice matrix while the traditional formulation describe the movement relative to the barycenter.

On the other hand the diffusion parameter a is a feature of our formulation and is connected with both the gravity-driven diffusion and with the diffusion caused by change in water partial pressure. The partial pressure in our formulation results from the assumption of incompressibility of the mixture and is somehow a formal quantity without clear physical interpretation. More appropriate and intuitively more correct should be an analogous term with a gradient of real water-pressure, but a correct derivation must be performed first.

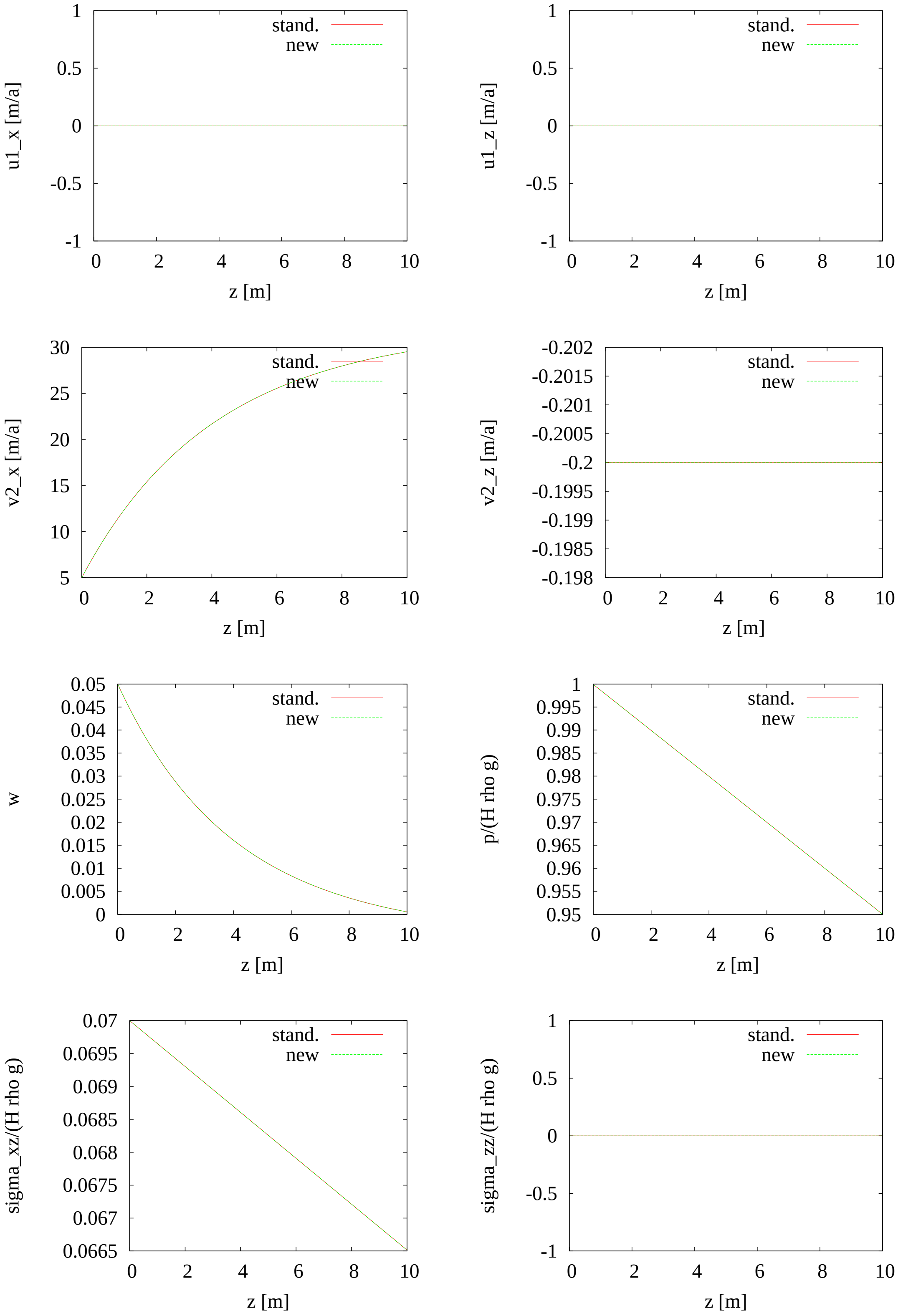

Figure 6.2: The solutions of the initial-value problem in the temperate-ice zone for the standard, traditional approach ('stand.'), and the present formulation ('new'), for the case a = b = c = 0, i.e. no water diffusion is allowed into the ice. We denoted $\overset{\circ}{T}_{xz}$ by "sigma_xz" and $\overset{\circ}{T}_{zz}$ by "sigma_zz". Both solutions coincide.

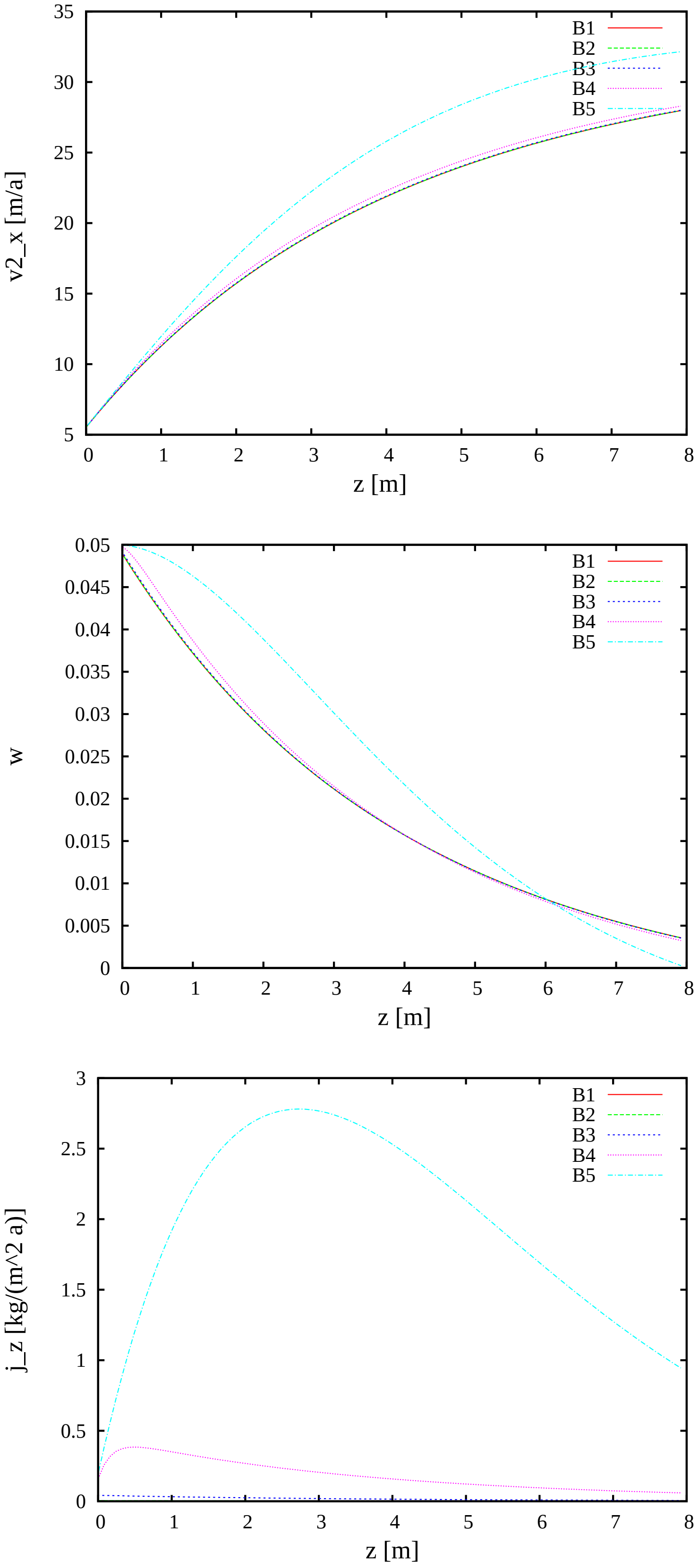

Figure 6.3: The solutions of the initial-value problem in the temperate-ice zone for the traditional approach, the values of the diffusive parameter c is: B1: $c = 10^{-9}$, B2: $c = 10^{-8}$, B3: $c = 10^{-7}$, B4: $c = 10^{-6}$, B5: $c = 10^{-5}$, respectively. We may observe that in this range the diffusive parameter c substantially affects the resultant velocity profile.

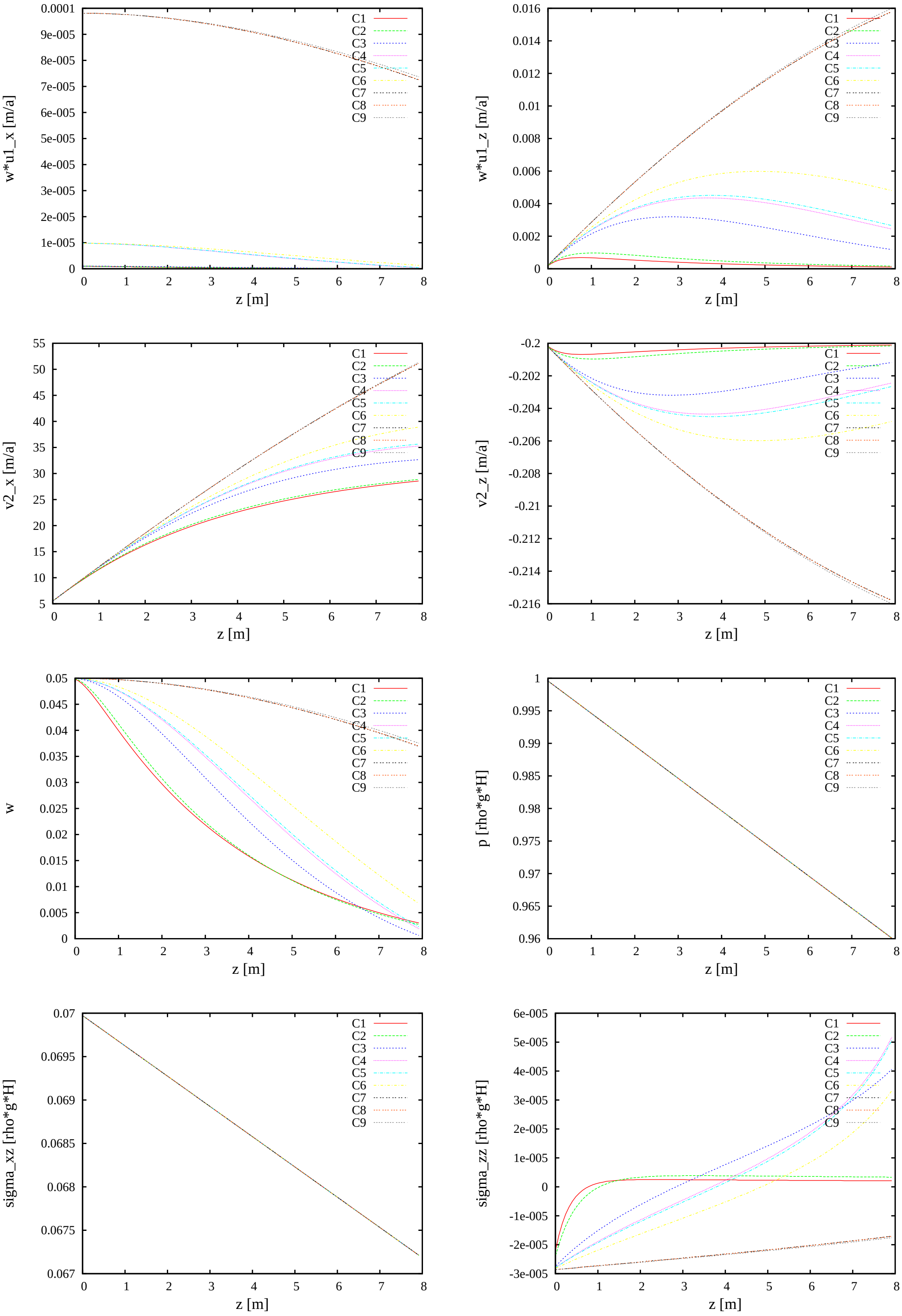

Figure 6.4: The solutions of the initial-value problem in the temperate-ice zone for our new formulation, the values of diffusion parameters as follows: C1: $a = 10^{-15}, b = 10^{-10}$, C2: $a = 10^{-15}, b = 10^{-9}$, C3: $a = 10^{-15}, b = 10^{-8}$, C4: $a = 10^{-14}, b = 10^{-10}$, C5: $a = 10^{-14}, b = 10^{-9}$, C6: $a = 10^{-14}, b = 10^{-8}$, C7: $a = 10^{-13}, b = 10^{-10}$, C8: $a = 10^{-13}, b = 10^{-9}$, C9: $a = 10^{-13}, b = 10^{-8}$. We denoted $\overset{\circ}{T}_{xz}$ by "sigma_xz" and $\overset{\circ}{T}_{zz}$ by "sigma_zz".

Chapter 7

Summary

We have dealt with the formulation of a physical model of a polythermal ice sheet. For the temperate-ice zone, we applied the mixture approach based on the rational thermodynamics of reacting mixtures. We derived the balance laws for reacting mixtures containing discontinuity surfaces, while including surface-production terms at each surface. We applied the general results of the mixture theory to a 2-component ice-water mixture and set up the constitutive equations for this material model.

The model was further simplified by means of rational thermodynamics, firstly by inspecting the entropy principle, then by partial linearization of the material model with respect to the equilibrium state.

In accordance with the observed conditions in real glaciers, an incompressibility constraint was introduced and the form of the reaction functionals was derived. The constitutive model was then applied to the balance laws and the resulting field equations were reduced to a form convenient for numerical implementation.

The polythermal ice-sheet model was completed by setting up the boundary conditions at the free surface and at the ice-bedrock boundary, and by interface conditions at the cold-temperate ice transition surface. The formulation of the boundary and transition conditions was unified on the basis of the mixture-theory framework.

The field equations were solved numerically for a simple 2-D case of an inclined temperate-ice layer of uniform thickness under steady-state conditions and the role of the diffusion parameters was studied. The computed water-content profiles differ significantly for a certain range of the diffusion parameters, threshold values of the parameters were found. The stress – strain-rate relation is assumed to be sensitive to the water content, which implies considerable variability in the velocity profiles. There is a lack of knowledge about the real values of the diffusive parameters, which makes it difficult to quantify the difference between the full-mixture formulation, presented here, and the traditional approach. Nevertheless, both formulations coincide if the diffusion of water is neglected.

Appendix A

Notation

$\mathcal{B}_\alpha$	...	abstract body, α-component of a mixture
X_α	...	mixture particle
$\vec{X}_\alpha$	...	reference configuration of α - mixture particle
$\vec{\kappa}_\alpha$	...	reference mapping
$\vec{\chi}_\alpha$	...	motion mapping
$\vec{x}$	...	position of the mixture particle in the present configuration
$\mathbf{F}_{\kappa\alpha}$	...	deformation gradient (α-component of a mixture)
$\mathbf{G}_{\kappa\alpha}$	...	second deformation gradient
$J_{\kappa\alpha}$	...	Jacobian
$\mathbf{R}_{\kappa\alpha}$	...	orthogonal part of the Cauchy polar decomposition of $\mathbf{F}_{\kappa\alpha}$
$\mathbf{U}_{\kappa\alpha}$	...	right stretch tensor
$\mathbf{V}_{\kappa\alpha}$	...	left stretch tensor
${}^{\backprime\alpha} = \frac{D_\alpha}{Dt}$	...	material time derivative with respect to the α-component
$\mathbf{C}_{\kappa\alpha}$	...	right Cauchy-Green tensor
$\mathbf{B}_{\kappa\alpha}$	...	left Cauchy-Green tensor
$\vec{v}_\alpha$	...	velocity of the α component
$\vec{v}$	...	velocity of ice in the traditional formulation
$\vec{v}^B$	...	barycentric velocity
$\mathbf{L}_\alpha$	...	velocity gradient
$\mathbf{D}_\alpha$	...	strain-rate tensor – the symmetric part of $\mathbf{L}_\alpha$
$\mathbf{D}$	...	ice strain-rate tensor in the traditional formulation
$\mathbf{W}_\alpha$	...	spin – the antisymmetric part of $\mathbf{L}_\alpha$
$\vec{u}_\alpha^{(k)}$	...	diffusion velocity of the α-component relative to the k-th component
$\vec{u}_\alpha$	...	$\vec{u}_\alpha^{(k)}$ for $k = n$, i.e. relative to the last n-th component
$\Omega_\alpha^{(k)}$	...	spin of the α-component relative to the k-th component
Ω_α	...	$\Omega_\alpha^{(k)}$ for $k = n$, i.e. relative to the last n-th component
v	...	material volume
$\sigma(t)$	...	discontinuity surface
$\vec{\nu}$	...	velocity of the discontinuity surface
$\vec{n}$	...	normal vector
ρ_α	...	mass density of the α-component
$\tilde{\rho}_\alpha$	...	'material' density of the α-component

r_α ... volume rate of mass change of the α-component
r_α^S ... surface rate of mass change of the α-component
w_α ... mass fraction of the α-component
w ... mass fraction of water
$\mathbf{T}_\alpha$ ... partial Cauchy stress tensor
$\mathbf{T}$ ... Cauchy stress tensor in the traditional formulation
$\vec{b}_\alpha$ ... volume force acting at the α-component
$\vec{k}_\alpha$ ... interaction volume force
$\vec{f}_\alpha^S$ ... linear-momentum surface production
ε_α ... partial internal-energy density
ε ... internal-energy density in the traditional formulation
$\vec{q}_\alpha$ ... partial-heat flux
Q_α ... partial-internal heating
e_α ... partial-volume interaction energy
e_α^S ... partial-surface energy production
$\vec{q}$ ... total heat flux
Q ... total internal heating
s_α ... partial entropy density
T ... absolute temperature
T_M ... melting temperature
f_α ... partial free-energy density
$\vec{h}_\gamma$ ... density gradient
$\vec{g}$ ... temperature gradient
$\vec{g}_a$ ... gravity acceleration
f ... specific free energy of a mixture
s ... specific entropy of a mixture
g_α ... partial chemical potential
$\vec{p}_\alpha$ ... $\vec{p}_\alpha = \frac{\partial(\rho f)}{\partial \vec{h}_\alpha}$
$\vec{u}_\alpha^B$ ... diffusion velocity of the α-component relative to the barycenter
$\mathbf{D}^B$ ... strain-rate tensor related to the barycentric velocity $\mathbf{D}^B = \{\mathrm{grad}\vec{v}^B\}^{sym.}$
$\mathbf{D}_\alpha^B$ ... $\mathbf{D}_\alpha^B = \{\mathrm{grad}\vec{u}_\alpha^B\}^{sym.}$
$\tilde{k}, \hat{k}, \lambda$ ... expansion coefficients: $\vec{q} = -(\tilde{k} + w\hat{k})\vec{g} - \lambda w \vec{u}_1$
ξ, ν, ω ... expansion coefficients: $\vec{k}_1 = -w\xi\vec{g} - w\nu\vec{u}_1 - \rho\omega \mathrm{grad} w$
$\tilde{\nu}$ ... diffusivity (traditional formulation)
p ... constraint pressure
Π_α ... partial thermodynamic pressure
L ... specific latent heat of melting of ice
F_S ... free-surface implicit function (glacier-air interface)
F_B ... glacier base implicit function (glacier-bedrock interface)
F_{CTS} ... CTS implicit function (cold-temperate ice interface)
r_α^s ... mass-production term at the free surface
r_α^b ... mass-production term at the ice-bedrock interface
r_α^{cts} ... mass-production term at the CTS

$\mathcal{P}^s$ ... free-surface liquid-precipitation function
$a^{s}_{2\perp}$ ... free-surface ice accumulation-ablation function
$o^{b}_{1\perp}$ ... water outflow function at the ice-bedrock interface
$a_{2\perp}^{cts}$ ... ice accumulation-ablation function at the CTS
c_V ... specific heat of ice at constant volume
M ... water mass-production in the traditional formulation
$\vec{j}$ ... diffusion water flux in the traditional formulation
Σ ... effective shear stress
$\circ$ ... deviatoric part of a second-order tensor
$\overset{\circ}{D}_{2II}$ ... second invariant of the ice strain-rate tensor deviator
$d(\Sigma)$ ... creep response function
$h(\overset{\circ}{D}_{2II})$ ... creep response function
$\mathcal{A}$ ... rate factor
$\mathcal{B}$ ... rate factor

Bibliography

[1] Samohýl I. (1982): Racionální termodynamika chemicky reagujících směsí, Academia, Praha

[2] Martinec Z. (2002): Continuum mechanics (Lecture notes), http://geo.mff.cuni.cz/teaching_cz.htm

[3] Passman S.L., Nunziato J.W. & Walsh E.K. (1984): A theory of multiphase mixtures. *In C. Truesdell (ed.), Rational Thermodynamics*, 286-325, Springer–Verlag, Berlin, Heidelberg, New York

[4] Hutter K. (1983): Theoretical glaciology; material science of ice and the mechanics of glaciers and ice sheets, D. Reidel Publishing Company, Dordrecht, Holland

[5] Gurtin M. E., Podio-Guidugli P. (1973): The thermodynamics of constrained materials, *Archive for Rational Mechanics and Analysis* **51**, 192-208

[6] Greve, R. (2000): Large-scale glaciation on Earth and on Mars. Habilitation thesis, Fachbereich Mechanik, Technische Universität Darmstadt

[7] Paterson W. S. B. (1981): The Physics of Glaciers, Pergamon Press, Oxford

[8] Maršík F. (1999): Termodynamika kontinua, Academia, Praha

[9] Fowler A. C., Larson D. A. (1978): On the flow of polythermal glaciers, I. Model and preliminary analysis, *Proc. Royal Soc. London* **A363**, 217–171

[10] van der Veen C.J. (1999): Fundamentals of glacier dynamics, A.A. Balkema, Rotterdam, Netherlands

[11] Lliboutry L., Duval P. (1985): Various isotropic and anisotropic ices found in glaciers and polar ice caps and their corresponding rheologies, *Ann. Geophys.* **3** (2), 207–224

[12] Kvasnica J. (1965): Termodynamika, SNTL, Praha

[13] Zweck, C., Huybrechts P. (2004): Northern hemisphere ice sheet modeling of the last glacial cycle and glaciological sensitivity, *Journal of Geophysical Research Atmospheres (in print)*

[14] Truesdell C.A. (1969): Rational Thermodynamics, A Course of Lectures on Selected Topics, McGraw-Hill, New York

[15] Press W.H. et al. (1992): Numerical Recepies in FORTRAN: The Art of Scientific Computing, Second edition, Cambridge University Press

[16] Mortimer R.G., Eyring H. (1980): Elementary transition state theory of the Soret and Dufour Effects, *Proc. Natl. Acad. Sci. USA Vol. 77, No. 4, pp.* **1728-1731**