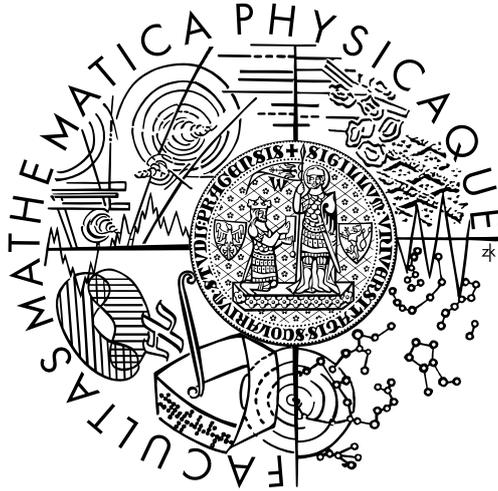


Charles University in Prague
Faculty of Mathematics and Physics

MASTER THESIS



Ondřej Souček

Thermomechanical polythermal ice-sheet model

Department of Geophysics

Supervisor: Prof. RNDr. Zdeněk Martinec, DrSc.

Study program: Physics

Here at this place I would like to thank sincerely all the people, who helped me with this work and during my studies. Most of all to my supervisor, Prof. RNDr. Zdeněk Martinec, Dr.Sc., for his care and leadership always full of enthusiasm and optimism. My thanks also go to the consultant Jan Hagedoorn, for his valuable critical notes and other support. I would also like to express my great thank to Doc. Ing. Ivan Samohýl, Dr.Sc., for his interest and valuable remarks and advices; to RNDr. Ladislav Hanyk, Ph.D., for his essential help with numerical implementations. I should not forget to thank all the members and students of the Department of geophysics for their attitude and the unique friendly atmosphere they created and last but not least my friends and family for their help and support.

Prohlašuji, že jsem svou diplomovou práci napsal samostatně a výhradně s použitím citovaných pramenů. Souhlasím se zapůjčováním práce.

V Praze dne 16.dubna 2005

Ondřej Souček

Contents

1	Introduction	1
2	Traditional formulation of glacier physics	3
2.1	Introduction	3
2.2	Cold Ice Zone	4
2.3	Temperate Ice Zone	5
3	Rational thermodynamics of mixtures	7
3.1	Introduction and basic principles	7
3.2	Kinematics of a mixture	8
3.3	Mass balance in a mixture	11
3.4	Linear momentum balance for a mixture	13
3.5	Angular momentum balance for a mixture	16
3.6	Energy balance of a mixture	19
3.7	Entropy balance in a mixture	24
3.8	Constitutive equations of a mixture	25
3.9	Mixtures of reacting and non-reacting fluids	32
3.10	Equilibrium in a mixture of fluids	34
4	Application to the water-ice mixture	39
4.1	Introduction	39
4.2	The material model	39
4.3	Equilibrium in the water-ice mixture	41
4.4	Further reductions by the entropy principle	42
4.5	Linearization with respect to the water content	46
4.5.1	Entropy inequality in terms of the barycentric velocity	50
4.5.2	The incompressibility	52
4.6	Balance equations in the water-ice mixture	61
4.6.1	Mass balance	61
4.6.2	Linear momentum balance	62
4.6.3	The angular momentum balance	63
4.6.4	The energy balance	63
4.7	Further reductions of the balance equations	63
4.7.1	Motivation	63
4.7.2	Mass balance	64

4.7.3	Linear momentum balance	64
4.7.4	Energy balance	65
5	The polythermal ice-sheet model	69
5.1	Field equations	69
5.1.1	Cold region	69
5.1.2	The temperate ice region	69
5.2	Boundary and transition conditions	70
5.2.1	Free surface	70
5.2.2	Ice-bedrock interface	76
5.2.3	Cold-temperate ice transition surface (CTS)	80
6	Numerical implementation: 2-D stationary case	85
6.1	Introduction	85
6.2	Temperate ice layer	85
6.3	Solution	90
7	Summary	95

Název práce: Termomechanický model polytermálního ledovce

Autor: Ondřej Souček

Katedra: Katedra geofyziky, MFF UK v Praze

Vedoucí diplomové práce: Prof. RNDr. Zdeněk Martinec, DrSc.

e-mail vedoucího: zdenek@gfz-potsdam.de

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

Title: Thermomechanical polythermal ice-sheet model

Author: Ondřej Souček

Department: Department of Geophysics, Charles University in Prague

Supervisor: Prof. RNDr. Zdeněk Martinec, DrSc.

Supervisor's e-mail address: zdenek@gfz-potsdam.de

Abstrakt: According to 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; it leads to the presence of 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 carefully discussed. Then a physical model for a polythermal ice sheet is set up 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 the traditional formulations are compared.

Keywords: polythermal ice sheet, rational thermodynamics of mixtures

Chapter 1

Introduction

Glaciology, as a science studying, in the broadest sense, the behaviour of ice masses under climatical and mechanical loading, has a broad interdisciplinary character. There are many fields of science relating to glaciology, as for instance, geophysics, material science, crystallography, meteorology, oceanology but also chemistry or applied mathematics. The subject of glaciology itself covers a large area of interest in time and spatial scales, including studies on ice crystal or flake growth, modelling of avalanche processes, flow of mountain glaciers and advance or retreat of large ice shelves and ice sheets during glacial cycles. The subject of this work is mostly connected with the last subject, that is modelling physical processes in ice sheets.

Ice sheets are ice masses of continental size, resting on solid land. The Antarctic ice sheet with the total ice volume of $25.9 \times 10^6 \text{ km}^3$ (sea-level equivalent of 65 m) being the largest, and smaller Greenland ice sheet with $2.8 \times 10^6 \text{ km}^3$ (7m sea-water equivalent) represent the most important contemporary ice sheets, however, in the past the Earth has many times experienced periods of even more extended glaciation. For instance, during the Last Glacial Maximum 21,000 years ago, an ice sheet covered a large part of North America, another one rested on the European Alps, northern Europe and Siberia, with the total ice-sheet volume of approximately $200 \times 10^6 \text{ km}^3$.

An intense effort has been focused on modelling of time evolution of large ice sheets during glacial cycles, including various physical processes and features, starting from purely mechanical models, ending with thermo-mechanically coupled ones. This work aims at the beginning of ice-sheet modelling, that is at the stage of setting up the model equations and physical features of the model. In particular, we deal with the model formulation for the so-called temperate zone of a glacier where meltwater is present and affects material behaviour.

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

Since our aim is an alternative formulation of the temperate ice region on the base of rational thermodynamics of reacting mixtures, the basic concepts of this theory are outlined in the third chapter, including formulation of the balance laws, exploitation of the entropy principle and investigation of 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 our 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 field variables, within the framework of mixture theory.

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

Chapter 2

Traditional formulation of glacier physics

2.1 Introduction

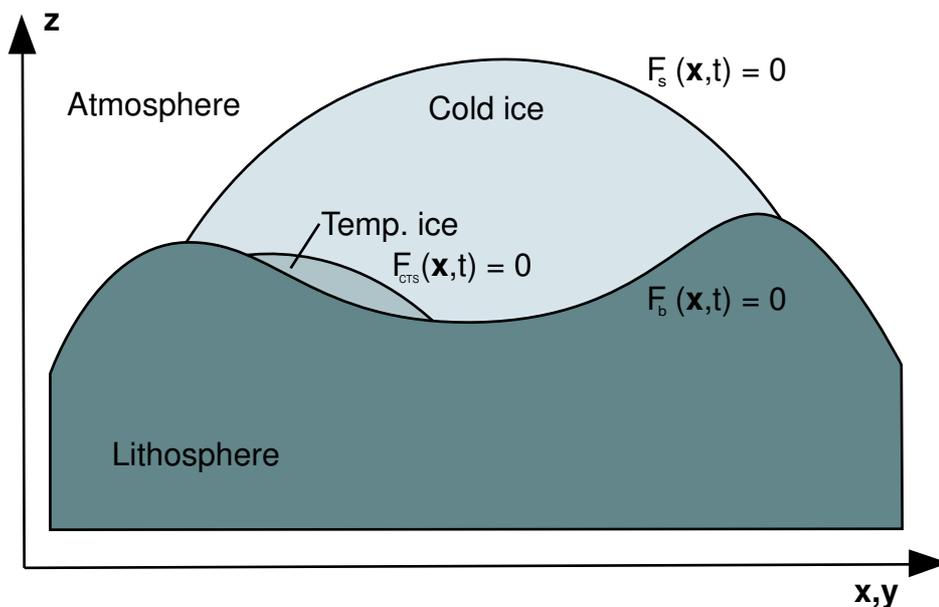


Figure 2.1: Sketch of a polythermal ice sheet.

The physical processes governing the behaviour of an ice sheet are of big complexity, but, for the purpose of large-scale modelling, we can 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 melting point and a certain amount of water is present, that 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 de-

scribing 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-variations 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*¹ (see e.g. Martinec [2]):

$$\operatorname{div} \vec{v} = 0, \quad (2.1)$$

$$\rho \dot{\vec{v}} = -\operatorname{grad} p + \operatorname{div} \overset{\circ}{\mathbf{T}} + \rho \vec{g}_F, \quad (2.2)$$

$$\rho \dot{\varepsilon} = \mathbf{T} : \mathbf{D} - \operatorname{div} \vec{q}, \quad (2.3)$$

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}_F is the gravity acceleration, ε is the internal energy,

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

the stretching tensor, and \vec{q} the heat flux.

The constitutive relations adopted to complete the system of equations are

$$\mathbf{T} = -p\mathbf{1} + \overset{\circ}{\mathbf{T}}, \quad (2.5)$$

$$\varepsilon = c_V T, \quad (2.6)$$

$$\vec{q} = -k(T) \operatorname{grad} T, \quad (2.7)$$

$$\mathbf{D} = \mathcal{A}(T) f(\sigma) \overset{\circ}{\mathbf{T}}, \quad (2.8)$$

where c_V is the specific heat at constant volume², $k(T)$ is the temperature-dependent heat conductivity of ice, σ is the effective shear stress defined as

$$\sigma = \sqrt{\frac{1}{2} \operatorname{tr}(\overset{\circ}{\mathbf{T}})^2}, \quad (2.9)$$

¹We 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.

²Hutter [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].

$\mathcal{A}(T)$ is the rate factor, $f(\sigma)$ the creep response function considered in the form

$$f(\sigma) = \sigma^{n-1} . \quad (2.10)$$

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,

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

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

2.3 Temperate Ice Zone

Due to the negative 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 is typically of a value up to 5% there, its presence affects rheological and transport properties of the surrounding ice. The traditional way of the description of temperate-ice physics is following (Greve [6]).

Several features of the mixture concept are introduced. The temperate ice is 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

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

where ρ is the mixture density

$$\rho = \rho_1 + \rho_2 , \quad (2.13)$$

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

$$w = \frac{\rho_1}{\rho} . \quad (2.14)$$

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

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

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

$$\operatorname{div} \vec{v}^B = 0 , \quad (2.16)$$

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

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

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

which is equivalent to

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

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

$$\mathbf{T} = -p\mathbf{1} + \overset{\circ}{\mathbf{T}}, \quad (2.20)$$

$$\mathbf{D}^B = \mathcal{A}(T, w) f(\sigma) \overset{\circ}{\mathbf{T}}, \quad (2.21)$$

$$\vec{j} = -\nu \operatorname{grad} w, \quad (2.22)$$

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

where

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

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

$$f(\sigma) = \sigma^{n-1}, \quad (2.25)$$

with

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

\vec{v} 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 the constitutive equations are still a subject of discussion and several new modifications of the theory appeared recently (Greve [6]). In the following chapters, we will attempt to formulate a thermo-mechanical temperate-ice model, strictly by means of rational thermodynamics of mixtures, which would involve the transport processes connected with water diffusion. We will adopt a fully-mixture concept, hoping that a consistent formulation can be carried out, without an 'ad hoc' stress – strain-rate relation expressed in terms of the barycentric velocity. We also hope that all derivations will show the simplifications implicitly involved in the above equations and may serve as a starting point for 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. 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 enabled by the spatial scale intended for the large-scale glacier modelling being in question here.

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

Chapter 3

Rational thermodynamics of mixtures

3.1 Introduction and basic principles

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 principle 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 components are first introduced as independent primitive quantities, the properties of the mixture are then derived. The second point gives a general idea how to formulate balance laws for components of a mixture and the third principle constrains the mixture balance laws. They must be consistent with balance laws for a 1-component material in the following sense. 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}_α , a set of particles $\{X_\alpha\}$. We express the configuration of this body by a mapping $\vec{\kappa}_\alpha$ (see e.g. Martinec [2]):

$$\left. \begin{aligned} \vec{\kappa}_\alpha : \quad \mathcal{B}_\alpha &\rightarrow \mathbb{E}^3 \\ X_\alpha &\rightarrow \vec{X}_\alpha = \vec{\kappa}_\alpha(X_\alpha) \end{aligned} \right\} \alpha = 1, \dots, n ,$$

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

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

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

where \vec{x}_α is the α -particle position in the present configuration. The reference, frame to which the vector \vec{X}_α is related, and the present frame, to which \vec{x}_α corresponds, need not coincide. But we will assume that reference frames of all components coincide and that present frames of all components coincide. The **mixture** is now defined as an intersection of 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 present at the same position $\vec{x}_\alpha = \vec{x}$, $\alpha = 1, \dots, n$.

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

- *deformation gradient:*

$$\mathbf{F}_{\kappa\alpha} = \text{Grad}_{\kappa\alpha} \vec{\chi}_{\kappa\alpha}(\vec{X}_\alpha, t) = \frac{\partial \vec{\chi}_{\kappa\alpha}(\vec{X}_\alpha, t)}{\partial \vec{X}_\alpha} , \quad (\mathbf{F}_{\kappa\alpha})^{iJ} = \frac{\partial \chi_{\kappa\alpha}^i(\vec{X}_\alpha, t)}{\partial X_\alpha^J} , \quad (3.1)$$

- *second deformation gradient:*

$$\mathbf{G}_{\kappa\alpha} = \text{Grad}_{\kappa\alpha} \mathbf{F}_{\kappa\alpha} = \frac{\partial \mathbf{F}_{\kappa\alpha}(\vec{X}_\alpha, t)}{\partial \vec{X}_\alpha} , \quad (\mathbf{G}_{\kappa\alpha})^{iJK} = \frac{\partial^2 \chi_{\kappa\alpha}^i(\vec{X}_\alpha, t)}{\partial X_\alpha^J \partial X_\alpha^K} , \quad (3.2)$$

- *jacobian:*

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

- *Cauchy polar decomposition of deformation gradient:*¹

$$\begin{aligned} \mathbf{F}_{\kappa\alpha} &= \mathbf{R}_{\kappa\alpha} \mathbf{U}_{\kappa\alpha} = \mathbf{V}_{\kappa\alpha} \mathbf{R}_{\kappa\alpha} , \\ (\mathbf{F}_{\kappa\alpha})^{iJ} &= (\mathbf{R}_{\kappa\alpha})^{iK} (\mathbf{U}_{\kappa\alpha})^{KJ} = (\mathbf{V}_{\kappa\alpha})^{ik} (\mathbf{R}_{\kappa\alpha})^{kJ} , \end{aligned} \quad (3.3)$$

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

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

¹We are using the Einstein summation convention.

- *right and left Cauchy-Green tensors:*

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

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

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

$$\frac{\partial \psi_\alpha}{\partial \vec{x}} = \text{grad } \psi_\alpha. \quad (3.6)$$

The second equation has the following meaning:

- for ψ_α being a scalar quantity:

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

- for ψ_α being a vector:

$$(\text{grad } \vec{\psi}_\alpha)^{ij} = \frac{\partial (\vec{\psi}_\alpha)^i}{\partial x^j}, \quad (3.8)$$

- for ψ_α being a second-order tensor:

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

and likewise for higher-order tensors.

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

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

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

where the superscript in the first term and the subscript at D in the second term denote the differentiation at fixed \vec{X}_α .

Using $\vec{X}_\alpha = \vec{\chi}_{\kappa\alpha}^{-1}(\vec{x}, t)$ and $\vec{x} = \vec{\chi}_{\kappa\gamma}(\vec{X}_\gamma, t)$, it analogously holds:

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

- *referential gradient:*

$$\text{Grad } \psi_\alpha = \frac{\partial \psi_\alpha(\vec{X}_\alpha, t)}{\partial \vec{X}_\alpha}, \quad (3.12)$$

- α -component velocity:

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

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

$$\dot{\psi}^\alpha = \frac{\partial \psi}{\partial t} + \text{grad} \psi \cdot \vec{v}_\alpha, \quad \dot{\psi}^\alpha = \frac{\partial \psi}{\partial t} + v_\alpha^i \frac{\partial \psi}{\partial x^i}, \quad (3.14)$$

- spatial velocity gradient:

$$\mathbf{L}_\alpha = \text{grad } \vec{v}_\alpha, \quad (\mathbf{L}_\alpha)^{ij} = \frac{\partial v_\alpha^i}{\partial x^j}, \quad (3.15)$$

and its symmetric and antisymmetric parts:

- velocity of deformation:

$$\mathbf{D}_\alpha \equiv \mathbf{L}_\alpha^{\text{sym.}} = \frac{1}{2}(\mathbf{L}_\alpha + \mathbf{L}_\alpha^T), \quad (3.16)$$

- spin:

$$\mathbf{W}_\alpha \equiv \mathbf{L}_\alpha^{\text{antis.}} = \frac{1}{2}(\mathbf{L}_\alpha - \mathbf{L}_\alpha^T). \quad (3.17)$$

It will be also convenient to introduce the following quantities:

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

$$\vec{u}_\alpha^{(k)} = \vec{v}_\alpha - \vec{v}_k, \quad \alpha = 1, \dots, n, \quad (3.18)$$

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

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

- spin relative to the k -th component $\Omega_\alpha^{(k)}$, $k \in (1, \dots, n)$:

$$\Omega_\alpha^{(k)} = \mathbf{W}_\alpha - \mathbf{W}_k, \quad \alpha = 1, \dots, n, \quad (3.20)$$

in particular we also define spin relative to the n -th component Ω_α ,

$$\Omega_\alpha = \Omega_\alpha^{(n)}. \quad (3.21)$$

We will often use the **Reynold's transport theorem**:

Following Martinec [2], we can derive the modified Reynold's transport theorem for a mixture. Consider a material volume v intersected by a discontinuity surface $\sigma(t)$ across which a field variable ψ_α , $\alpha \in (1, \dots, n)$, undergoes a finite jump. Let the points of $\sigma(t)$

move with velocity \vec{v} . Denoting the parts of the body separated by the surface v^+ and v^- , we can derive

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

or, equivalently,

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

where the square brackets denote the jump across the singular surface $\sigma(t)$, i.e. for an arbitrary field quantity φ , $[\varphi]_-^+ = \varphi^+ - \varphi^-$.

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]):

$$\int_{v \setminus \sigma(t)} \operatorname{div} \psi_\alpha \, dv = \int_{s^+ \cup s^-} \psi_\alpha \cdot \vec{n} \, da - \int_{\sigma(t)} [\psi_\alpha]_-^+ \cdot \vec{n} \, da, \quad (3.24)$$

where s^+ and s^- are the parts of the bounding surface separated by the discontinuity surface $\sigma(t)$.

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:

$$\rho_\alpha = \rho_\alpha(\vec{x}, t) \geq 0, \quad \alpha = 1, \dots, n,$$

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

$$m_\alpha(v) = \int_v \rho_\alpha \, dv, \quad (3.25)$$

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

$$r_\alpha = r_\alpha(\vec{x}, t), \quad \vec{x} \in v(t), \quad \alpha = 1, \dots, n,$$

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

$$r_\alpha^S = r_\alpha^S(\vec{x}, t), \quad \vec{x} \in \sigma(t), \quad \alpha = 1, \dots, n,$$

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

$$\delta m_\alpha(v) = \int_v r_\alpha dv + \int_{\sigma(t)} r_\alpha^S da.$$

We distinguish

- reacting components:

$$r_\varphi \neq 0 \quad \text{or} \quad r_\varphi^S \neq 0, \quad \varphi = 1, \dots, m,$$

- non-reacting components:

$$r_\omega \equiv 0 \quad \text{and} \quad r_\omega^S \equiv 0, \quad \omega = m + 1, \dots, n.$$

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

$$\frac{D_\alpha}{Dt} \int_v \rho_\alpha dv = \int_v r_\alpha dv + \int_{\sigma(t)} r_\alpha^S da, \quad \alpha = 1, \dots, n, \quad (3.26)$$

and the mass balance of a mixture:

$$\sum_{\alpha=1}^n \left(\frac{D_\alpha}{Dt} \int_v \rho_\alpha dv \right) = 0, \quad (3.27)$$

using (3.23), we obtain

$$\frac{D_\alpha}{Dt} \int_v \rho_\alpha dv = \int_{v \setminus \sigma(t)} (\dot{\rho}_\alpha^\alpha + \rho_\alpha \operatorname{div} \vec{v}_\alpha) dv + \int_{\sigma(t)} [\rho_\alpha(\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} da,$$

which, with the use of (3.26), yields

$$\int_{v \setminus \sigma(t)} (\dot{\rho}_\alpha^\alpha + \rho_\alpha \operatorname{div} \vec{v}_\alpha - r_\alpha) dv + \int_{\sigma(t)} ([\rho_\alpha(\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} - r_\alpha^S) da = 0.$$

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

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

Using (3.23) in (3.27), we arrive at

$$\int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n (\dot{\rho}_\alpha^\alpha + \rho_\alpha \operatorname{div} \vec{v}_\alpha) dv + \int_{\sigma(t)} \sum_{\alpha=1}^n [\rho_\alpha(\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} da = 0.$$

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

$$\boxed{\begin{aligned} \sum_{\alpha=1}^n (\dot{\rho}_\alpha^\alpha + \rho_\alpha \operatorname{div} \vec{v}_\alpha) &= 0 & \text{in} & \quad v \setminus \sigma(t) , \\ \sum_{\alpha=1}^n [\rho_\alpha(\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} &= 0 & \text{at} & \quad \sigma(t) . \end{aligned}} \quad (3.29)$$

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

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

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

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

$$\boxed{\begin{aligned} \sum_{\alpha=1}^n r_\alpha &= 0 & \text{in} & \quad v \setminus \sigma(t) , \\ \sum_{\alpha=1}^n r_\alpha^S &= 0 & \text{at} & \quad \sigma(t) . \end{aligned}} \quad (3.32)$$

It is convenient to introduce:

- *mass density of a mixture* ρ :

$$\rho = \sum_{\alpha=1}^n \rho_\alpha , \quad (3.33)$$

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

$$w_\alpha = \frac{\rho_\alpha}{\rho} , \quad \alpha = 1, \dots, n , \quad (3.34)$$

consequently

$$\sum_{\alpha=1}^n w_\alpha = 1 . \quad (3.35)$$

3.4 Linear momentum balance for a mixture

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

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

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

$$\begin{aligned} \frac{D_\alpha}{Dt} \int_v \rho_\alpha \vec{v}_\alpha dv &= \int_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} da + \int_v \rho_\alpha \vec{b}_\alpha dv + \int_v \vec{k}_\alpha dv \\ &+ \int_v r_\alpha \vec{v}_\alpha dv + \int_{\sigma(t)} \vec{f}_\alpha^S da, \\ \alpha &= 1, \dots, n, \end{aligned} \quad (3.36)$$

where

- $\int_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} da$
expresses all surface forces exerted on the particular α -component at the surface ∂v . These are:

- *inner surface forces*
which appear at the part of the surface ∂v , which is inside the mixture volume. They represent surface forces exerted by the rest of mixture from the outer side of such a surface segment.
- *outer surface forces*,
exterior surface forces, exerted from the outer side on the part of the surface ∂v , which is at the same time a part of the mixture boundary.
- *interaction surface forces*
representing the surface forces exerted by all the other mixture components on the surface ∂v from the inner side of the volume v .

- $\int_v \rho_\alpha \vec{b}_\alpha dv$
expresses the volume forces (e.g. gravity).

- $\int_v \vec{k}_\alpha dv$
expresses the interaction volume forces – volume interaction with the rest of the mixture.

The *interaction* and *inner surface forces* together with *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.

- $\int_v r_\alpha \vec{v}_\alpha dv$
is the linear momentum induced by composition changes, e.g. for a two-component ice-water mixture, both components are considered as continua moving with different velocities, freezing of certain water amount or melting of ice, described by density changes, therefore, results in appropriate linear momentum changes.

- $\int_{\sigma(t)} \vec{f}_\alpha^S da$

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

$$\begin{aligned}
& \frac{D_\alpha}{Dt} \int_v \rho_\alpha \varphi_\alpha dv \\
&= \int_{v \setminus \sigma(t)} \left(\frac{D_\alpha(\rho_\alpha \varphi_\alpha)}{Dt} + \rho_\alpha \varphi_\alpha \operatorname{div} \vec{v}_\alpha \right) dv + \int_{\sigma(t)} [\rho_\alpha \varphi_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} da \\
&= \int_{v \setminus \sigma(t)} \{ \varphi_\alpha (\dot{\rho}_\alpha^\alpha + \rho_\alpha \operatorname{div} \vec{v}_\alpha) + \rho_\alpha \dot{\varphi}_\alpha^\alpha \} dv + \int_{\sigma(t)} [\rho_\alpha \varphi_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} da \\
&= \int_{v \setminus \sigma(t)} \varphi_\alpha r_\alpha dv + \int_{v \setminus \sigma(t)} \rho_\alpha \dot{\varphi}_\alpha^\alpha dv + \int_{\sigma(t)} [\rho_\alpha \varphi_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} da .
\end{aligned} \tag{3.37}$$

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

$$\frac{D_\alpha}{Dt} \int_v \rho_\alpha \vec{v}_\alpha dv = \int_{v \setminus \sigma(t)} \vec{v}_\alpha r_\alpha dv + \int_{v \setminus \sigma(t)} \rho_\alpha \dot{\vec{v}}_\alpha^\alpha dv + \int_{\sigma(t)} [\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} da .$$

Substituting this into (3.36) yields

$$\begin{aligned}
\int_{v \setminus \sigma(t)} \rho_\alpha \dot{\vec{v}}_\alpha^\alpha dv + \int_{\sigma(t)} [\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} da &= \int_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} da + \int_{v \setminus \sigma(t)} \rho_\alpha \vec{b}_\alpha dv \\
&+ \int_{v \setminus \sigma(t)} \vec{k}_\alpha dv + \int_{\sigma(t)} \vec{f}_\alpha^S da .
\end{aligned}$$

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

$$\begin{aligned}
\vec{0} &= \int_{v \setminus \sigma(t)} (\rho_\alpha \dot{\vec{v}}_\alpha^\alpha - \operatorname{div} \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha - \vec{k}_\alpha) dv \\
&- \int_{\sigma(t)} ([\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} + \vec{f}_\alpha^S) da .
\end{aligned} \tag{3.38}$$

Since the volume v was chosen arbitrarily, we conclude that

$$\boxed{
\begin{aligned}
\rho_\alpha \dot{\vec{v}}_\alpha^\alpha &= \operatorname{div} \mathbf{T}_\alpha + \rho_\alpha \vec{b}_\alpha + \vec{k}_\alpha && \text{in } v \setminus \sigma(t) , \\
\vec{0} &= [\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} + \vec{f}_\alpha^S && \text{at } \sigma(t) .
\end{aligned}
} \tag{3.39}$$

The balance of linear momentum of a mixture is postulated as

$$\sum_{\alpha=1}^n \frac{D_\alpha}{Dt} \int_v \rho_\alpha \vec{v}_\alpha \, dv = \sum_{\alpha=1}^n \int_{\partial v} \mathbf{T}_\alpha \cdot \vec{n} \, da + \sum_{\alpha=1}^n \int_{v \setminus \sigma(t)} \rho_\alpha \vec{b}_\alpha \, dv . \quad (3.40)$$

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

$$\begin{aligned} \vec{0} &= \int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n \left(\rho_\alpha \dot{\vec{v}}_\alpha^\alpha + r_\alpha \vec{v}_\alpha - \operatorname{div} \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha \right) \, dv + \\ &+ \int_{\sigma(t)} \left[\sum_{\alpha=1}^n \left\{ \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v}) - \mathbf{T}_\alpha \right\} \right]_+^+ \cdot \vec{n} \, da . \end{aligned} \quad (3.41)$$

Since the material volume v was arbitrary, we conclude that

$$\boxed{\begin{aligned} \vec{0} &= \sum_{\alpha=1}^n \left(\rho_\alpha \dot{\vec{v}}_\alpha^\alpha + r_\alpha \vec{v}_\alpha - \operatorname{div} \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha \right) && \text{in } v \setminus \sigma(t) , \\ \vec{0} &= \left[\sum_{\alpha=1}^n \left\{ \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v}) - \mathbf{T}_\alpha \right\} \right]_+^+ \cdot \vec{n} && \text{at } \sigma(t) . \end{aligned}} \quad (3.42)$$

Summing up the balance laws and boundary conditions (3.39) over all components yields

$$\begin{aligned} \sum_{\alpha=1}^n \left(\rho_\alpha \dot{\vec{v}}_\alpha^\alpha - \operatorname{div} \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha - \vec{k}_\alpha \right) &= \vec{0} && \text{in } v \setminus \sigma(t) , \\ \sum_{\alpha=1}^n \left([\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_+^+ \cdot \vec{n} + \vec{f}_\alpha^S \right) &= \vec{0} && \text{at } \sigma(t) , \end{aligned}$$

which with the use of (3.42) implies

$$\boxed{\begin{aligned} \sum_{\alpha=1}^n (\vec{k}_\alpha + r_\alpha \vec{v}_\alpha) &= \vec{0} && \text{in } v \setminus \sigma(t) . \\ \sum_{\alpha=1}^n \vec{f}_\alpha^S &= \vec{0} && \text{at } \sigma(t) . \end{aligned}} \quad (3.43)$$

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 place \vec{y}_0 is defined as a second-order tensor

$$\mathbf{l}_\alpha(v) = \int_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{v}_\alpha \, dv , \quad \alpha = 1, \dots, n ,$$

where \vec{y}_0 is assumed to be a constant vector and the operator \wedge is defined by²

$$\vec{a} \wedge \vec{b} = \vec{a} \otimes \vec{b} - \vec{b} \otimes \vec{a} , \quad (\vec{a} \wedge \vec{b})^{ij} = (a^i b^j - a^j b^i) , \quad (3.44)$$

² \otimes denotes the tensor (dyadic) product

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

$$\begin{aligned} \frac{D_\alpha}{Dt} \int_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{v}_\alpha \, dv &= \int_{\partial v} (\vec{x} - \vec{y}_0) \wedge \mathbf{T}_\alpha \cdot \vec{n} \, da + \int_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{b}_\alpha \, dv \\ &+ \int_v (\vec{x} - \vec{y}_0) \wedge (\vec{k}_\alpha + r_\alpha \vec{v}_\alpha) \, dv + \int_{\sigma(t)} (\vec{x} - \vec{y}_0) \wedge \vec{f}_\alpha^S \, da , \\ \alpha &= 1, \dots, n . \end{aligned} \quad (3.45)$$

By (3.37) we have

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

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 theorem³ (3.24) on the first surface integral in (3.45), we have

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

Equation (3.45) can be written as follows:

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

³We 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 (3.39), we can see that the second and the third integral vanish, so we conclude that

$$\int_{v \setminus \sigma(t)} (\mathbf{T}_\alpha - \mathbf{T}_\alpha^T) dv = \mathbf{0} . \quad (3.46)$$

Since the material volume v was chosen arbitrarily, we obtain

$$\boxed{\mathbf{T}_\alpha = \mathbf{T}_\alpha^T \quad \text{in} \quad v \setminus \sigma(t) .} \quad (3.47)$$

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

$$\sum_{\alpha=1}^n \frac{D_\alpha}{Dt} \int_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{v}_\alpha dv = \sum_{\alpha=1}^n \int_{\partial v} (\vec{x} - \vec{y}_0) \wedge \mathbf{T}_\alpha \cdot \vec{n} da + \sum_{\alpha=1}^n \int_v (\vec{x} - \vec{y}_0) \wedge \rho_\alpha \vec{b}_\alpha dv . \quad (3.48)$$

Applying (3.37), we derive

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

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

$$\begin{aligned} \sum_{\alpha=1}^n \int_{\partial v} (\vec{x} - \vec{y}_0) \wedge \mathbf{T}_\alpha \cdot \vec{n} da &= \int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n (\mathbf{T}_\alpha^T - \mathbf{T}_\alpha) dv + \int_{v \setminus \sigma(t)} (\vec{x} - \vec{y}_0) \wedge \operatorname{div} \left(\sum_{\alpha=1}^n \mathbf{T}_\alpha \right) dv + \\ &+ \int_{\sigma(t)} \left[(\vec{x} - \vec{y}_0) \wedge \sum_{\alpha=1}^n \mathbf{T}_\alpha \right]_{-}^{+} \cdot \vec{n} da . \end{aligned} \quad (3.49)$$

After substituting this into (3.48) and rearranging the terms, we arrive at

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

where we have used the continuity of $(\vec{x} - \vec{y}_0)$ across the singular surface $\sigma(t)$. In view of (3.42), we finally obtain the angular momentum balance for a mixture

$$\int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n (\mathbf{T}_\alpha - \mathbf{T}_\alpha^T) dv = \mathbf{0} , \quad (3.50)$$

but this is a trivial result of the angular momentum balance for components (3.47).

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}_α
- *internal heating* Q_α
- *volume interaction energy* e_α
- *surface energy production* e_α^S

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

$$\begin{aligned} \frac{D_\alpha}{Dt} \int_v \rho_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) dv &= \int_{\partial v} \vec{v}_\alpha \cdot \mathbf{T}_\alpha \cdot \vec{n} da + \int_v \rho_\alpha \vec{b}_\alpha \cdot \vec{v}_\alpha dv + \int_v \vec{k}_\alpha \cdot \vec{v}_\alpha dv \\ &- \int_{\partial v} \vec{q}_\alpha \cdot \vec{n} da + \int_v Q_\alpha dv + \int_v r_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) dv \\ &+ \int_v e_\alpha dv + \int_{\sigma(t)} e_\alpha^S da, \quad \alpha = 1, \dots, n. \end{aligned} \quad (3.51)$$

The terms additionally appeared in (3.51) compared to the energy balance of a one-component material (see e.g. Samohýl [1]) are

- $\int_{v \setminus \sigma(t)} \vec{k}_\alpha \cdot \vec{v}_\alpha dv$
is the power produced by the interaction volume force \vec{k}_α ,
- $\int_{v \setminus \sigma(t)} e_\alpha dv$
is the volume interaction power,
- $\int_{\sigma(t)} e_\alpha^S da$
is the energy production at the singular surface $\sigma(t)$,
- $\int_{v \setminus \sigma(t)} r_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) dv$
is the rate of energy change due to compositional changes.

In handling of (3.51), 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 (3.51):

$$\begin{aligned} \frac{D_\alpha}{Dt} \int_v \rho_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) dv &= \int_{v \setminus \sigma(t)} \rho_\alpha \left(\dot{\varepsilon}_\alpha^\alpha + \vec{v}_\alpha \cdot \dot{\vec{v}}_\alpha^\alpha \right) dv + \int_{v \setminus \sigma(t)} r_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) dv + \\ &+ \int_{\sigma(t)} \left[\rho_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) (\vec{v}_\alpha - \vec{v}) \right]_+^- \cdot \vec{n} da. \end{aligned} \quad (3.52)$$

We now use the Gauss theorem (3.24) and express the surface integral as⁴

$$\begin{aligned}
\int_{\partial v} \vec{v}_\alpha \cdot \mathbf{T}_\alpha \cdot \vec{n} \, da &= \int_{\partial v} v_\alpha^i T_\alpha^{ij} n^j \, da = \int_{v \setminus \sigma(t)} \frac{\partial}{\partial x^j} (v_\alpha^i T_\alpha^{ij}) \, dv + \int_{\sigma(t)} [v_\alpha^i T_\alpha^{ij}]_-^+ n^j \, da \\
&= \int_{v \setminus \sigma(t)} \frac{\partial v_\alpha^i}{\partial x^j} T_\alpha^{ij} \, dv + \int_{v \setminus \sigma(t)} v_\alpha^i \frac{\partial T_\alpha^{ij}}{\partial x^j} \, dv + \int_{\sigma(t)} [v_\alpha^i T_\alpha^{ij}]_-^+ n^j \, da \\
&= \int_{v \setminus \sigma(t)} \mathbf{L}_\alpha : \mathbf{T}_\alpha \, dv + \int_{v \setminus \sigma(t)} \vec{v}_\alpha \cdot \operatorname{div} \mathbf{T}_\alpha \, dv + \int_{\sigma(t)} [\vec{v}_\alpha \cdot \mathbf{T}_\alpha]_-^+ \cdot \vec{n} \, da ,
\end{aligned} \tag{3.53}$$

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

$$\mathbf{A} : \mathbf{B} \equiv A^{ij} B^{ij} . \tag{3.54}$$

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

$$\int_{\partial v} \vec{q}_\alpha \cdot \vec{n} \, da = \int_{v \setminus \sigma(t)} \operatorname{div} \vec{q}_\alpha \, dv + \int_{\sigma(t)} [q_\alpha]_-^+ \cdot \vec{n} \, da . \tag{3.55}$$

Substituting (3.52), (3.53) and (3.55) into (3.51) yields

$$\begin{aligned}
0 &= \int_{v \setminus \sigma(t)} \left\{ \rho_\alpha \dot{\varepsilon}_\alpha^\alpha - \mathbf{T}_\alpha : \mathbf{L}_\alpha + \operatorname{div} \vec{q}_\alpha - Q_\alpha - e_\alpha + \vec{v}_\alpha \cdot (\rho_\alpha \dot{\vec{v}}_\alpha^\alpha - \operatorname{div} \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha - \vec{k}_\alpha) \right\} \, dv \\
&+ \int_{\sigma(t)} \left(\left[\rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) (\vec{v}_\alpha - \vec{v}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha + \vec{q}_\alpha \right]_-^+ \cdot \vec{n} - e_\alpha^S \right) \, da .
\end{aligned}$$

With the help of the linear momentum balance of the α -component (3.39), this equation further reduces to

$$\begin{aligned}
0 &= \int_{v \setminus \sigma(t)} \left\{ \rho_\alpha \dot{\varepsilon}_\alpha^\alpha - \mathbf{T}_\alpha : \mathbf{L}_\alpha + \operatorname{div} \vec{q}_\alpha - Q_\alpha - e_\alpha \right\} \, dv \\
&+ \int_{\sigma(t)} \left(\left[\rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) (\vec{v}_\alpha - \vec{v}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha + \vec{q}_\alpha \right]_-^+ \cdot \vec{n} - e_\alpha^S \right) \, da .
\end{aligned}$$

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

$\rho_\alpha \dot{\varepsilon}_\alpha^\alpha$	$=$	$\mathbf{T}_\alpha : \mathbf{D}_\alpha - \operatorname{div} \vec{q}_\alpha + Q_\alpha + e_\alpha$	in	$v \setminus \sigma(t)$,
e_α^S	$=$	$\left[\rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) (\vec{v}_\alpha - \vec{v}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha + \vec{q}_\alpha \right]_-^+ \cdot \vec{n}$	at	$\sigma(t)$,

(3.56)

⁴To make the derivation transparent, we use the componental description.

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

$$\mathbf{T}_\alpha : \mathbf{L}_\alpha = \mathbf{T}_\alpha : (\mathbf{L}_\alpha^{sym.} + \mathbf{L}_\alpha^{antis.}) = \mathbf{T}_\alpha : \mathbf{L}_\alpha^{sym.} = \mathbf{T}_\alpha : \mathbf{D}_\alpha . \quad (3.57)$$

Now we postulate the energy balance of a mixture

$$\begin{aligned} \sum_{\alpha=1}^n \frac{D_\alpha}{Dt} \int_v \rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) dv &= \sum_{\alpha=1}^n \int_{\partial v} \vec{v}_\alpha \cdot \mathbf{T}_\alpha \cdot \vec{n} da + \sum_{\alpha=1}^n \int_v \vec{v}_\alpha \cdot \rho_\alpha \vec{b}_\alpha dv - \\ &- \int_{\partial v} \vec{q} \cdot \vec{n} da + \int_v Q dv , \end{aligned} \quad (3.58)$$

where we have defined

- total heat flux \vec{q}

$$\vec{q} = \sum_{\alpha=1}^n \vec{q}_\alpha , \quad (3.59)$$

- total internal heating Q

$$Q = \sum_{\alpha=1}^n Q_\alpha . \quad (3.60)$$

Similarly to (3.52), the left-hand side of (3.58) reads

$$\begin{aligned} \sum_{\alpha=1}^n \frac{D_\alpha}{Dt} \int_v \rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) dv &= \int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n \rho_\alpha (\dot{\varepsilon}_\alpha^\alpha + \vec{v}_\alpha \cdot \dot{\vec{v}}_\alpha^\alpha) dv + \\ + \int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n r_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) dv &+ \int_{\sigma(t)} \sum_{\alpha=1}^n \left[\rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) (\vec{v}_\alpha - \vec{v}) \right]_-^+ \cdot \vec{n} da . \end{aligned} \quad (3.61)$$

With the help of (3.53) and (3.57), the surface integral on the right-hand side of (3.58) is

$$\begin{aligned} \sum_{\alpha=1}^n \int_{\partial v} \vec{v}_\alpha \cdot \mathbf{T}_\alpha \cdot \vec{n} da &= \int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n (\mathbf{D}_\alpha : \mathbf{T}_\alpha) dv + \int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n (\vec{v}_\alpha \cdot \text{div } \mathbf{T}_\alpha) dv + \\ &+ \int_{\sigma(t)} \sum_{\alpha=1}^n [\vec{v}_\alpha \cdot \mathbf{T}_\alpha]_-^+ \cdot \vec{n} da . \end{aligned} \quad (3.62)$$

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

$$\int_{\partial v} \vec{q} \cdot \vec{n} da = \int_{v \setminus \sigma(t)} \text{div } \vec{q} dv + \int_{\sigma(t)} [q]_-^+ \cdot \vec{n} da . \quad (3.63)$$

Substituting (3.61), (3.62) and (3.63) into (3.58) gives

$$\begin{aligned} 0 &= \int_{v \setminus \sigma(t)} \left(\sum_{\alpha=1}^n \left\{ \rho_\alpha \dot{\varepsilon}_\alpha^\alpha - \mathbf{T}_\alpha : \mathbf{D}_\alpha + \vec{v}_\alpha \cdot (\rho_\alpha \dot{\vec{v}}_\alpha^\alpha - \text{div } \mathbf{T}_\alpha - \rho_\alpha \vec{b}_\alpha) \right\} + \text{div } \vec{q} - Q \right) dv + \\ \int_{v \setminus \sigma(t)} \sum_{\alpha=1}^n \left\{ r_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) \right\} dv &+ \int_{\sigma(t)} \left[\sum_{\alpha=1}^n \left\{ \rho_\alpha (\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2) (\vec{v}_\alpha - \vec{v}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha \right\} + \vec{q} \right]_-^+ \cdot \vec{n} da . \end{aligned}$$

The term in parenthesis standing at $\vec{v}_\alpha \cdot$ in the first volume integral is equal to \vec{k}_α due to the linear momentum balance (3.39). Finally, postulating, that this result is valid for any arbitrary material volume v , we get

$$\begin{aligned} 0 &= \sum_{\alpha=1}^n \left\{ \rho_\alpha \dot{\varepsilon}_\alpha^\alpha - \mathbf{T}_\alpha : \mathbf{D}_\alpha + \vec{v}_\alpha \cdot \vec{k}_\alpha + r_\alpha \varepsilon_\alpha + \frac{1}{2} r_\alpha \vec{v}_\alpha^2 \right\} + \operatorname{div} \vec{q} - Q \quad \text{in } v \setminus \sigma(t), \\ 0 &= \left[\sum_{\alpha=1}^n \left\{ \rho_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) (\vec{v}_\alpha - \vec{v}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha \right\} + \vec{q} \right]_{-}^{+} \cdot \vec{n} \quad \text{at } \sigma(t). \end{aligned} \quad (3.64)$$

By summation of (3.56), we obtain

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

Subtracting these equation from (3.64) and with the use of (3.59) and (3.60) yields

$$\sum_{\alpha=1}^n \left\{ e_\alpha + \vec{v}_\alpha \cdot \vec{k}_\alpha + r_\alpha \varepsilon_\alpha + \frac{1}{2} r_\alpha \vec{v}_\alpha^2 \right\} = 0 \quad \text{in } v \setminus \sigma(t), \quad (3.65)$$

$$\sum_{\alpha=1}^n e_\alpha^S = 0 \quad \text{at } \sigma(t). \quad (3.66)$$

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:

$$\begin{aligned} & \sum_{\alpha=1}^n \vec{v}_\alpha \cdot \vec{k}_\alpha + \frac{1}{2} \sum_{\alpha=1}^n r_\alpha \vec{v}_\alpha^2 \\ &= \sum_{\alpha=1}^n (\vec{v}_n + \vec{u}_\alpha) \cdot \vec{k}_\alpha + \frac{1}{2} \sum_{\alpha=1}^n r_\alpha (\vec{v}_n^2 + 2\vec{v}_n \cdot \vec{u}_\alpha + \vec{u}_\alpha^2) \\ &= \vec{v}_n \cdot \sum_{\alpha=1}^n (\vec{k}_\alpha + r_\alpha \underbrace{\vec{u}_\alpha}_{\vec{v}_\alpha - \vec{v}_n}) + \sum_{\alpha=1}^n \vec{u}_\alpha \cdot \vec{k}_\alpha + \frac{1}{2} \vec{v}_n^2 \sum_{\alpha=1}^n r_\alpha + \frac{1}{2} \sum_{\alpha=1}^n r_\alpha \vec{u}_\alpha^2 \\ &= \vec{v}_n \cdot \sum_{\alpha=1}^n (\vec{k}_\alpha + r_\alpha \vec{v}_\alpha) - \frac{1}{2} \vec{v}_n^2 \sum_{\alpha=1}^n r_\alpha + \sum_{\alpha=1}^n \vec{u}_\alpha \cdot \vec{k}_\alpha + \frac{1}{2} \sum_{\alpha=1}^n r_\alpha \vec{u}_\alpha^2 \\ &= \sum_{\alpha=1}^n \vec{u}_\alpha \cdot \vec{k}_\alpha + \frac{1}{2} \sum_{\alpha=1}^n r_\alpha \vec{u}_\alpha^2 \\ &= \sum_{\beta=1}^{n-1} \vec{u}_\beta \cdot \vec{k}_\beta + \frac{1}{2} \sum_{\beta=1}^{n-1} r_\beta \vec{u}_\beta^2, \end{aligned} \quad (3.67)$$

where we have used the constraints $\sum_{\alpha=1}^n r_\alpha = 0$, $\sum_{\alpha=1}^n (\vec{k}_\alpha + r_\alpha \vec{v}_\alpha) = \vec{0}$, $\vec{u}_n = \vec{0}$, according to (3.32), (3.43) and (3.19), respectively.

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

$$\begin{array}{l}
 0 = \sum_{\alpha=1}^n \{e_{\alpha} + r_{\alpha}\varepsilon_{\alpha}\} + \sum_{\beta=1}^{n-1} \left\{ \vec{u}_{\beta} \cdot \vec{k}_{\beta} + \frac{1}{2} r_{\beta} \vec{u}_{\beta}^2 \right\} \quad \text{in} \quad v \setminus \sigma(t) , \\
 0 = \sum_{\alpha=1}^n e_{\alpha}^S \quad \text{at} \quad \sigma(t) .
 \end{array}
 \tag{3.68}$$

3.7 Entropy balance in a mixture

We introduce new quantities:

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

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

$$\sum_{\alpha=1}^n \frac{D_\alpha}{Dt} \int_v \rho_\alpha s_\alpha \, dv \geq - \int_{\partial v} \frac{1}{T} \vec{q} \cdot \vec{n} \, da + \int_{v \setminus \sigma(t)} \frac{Q}{T} \, dv . \quad (3.69)$$

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

$$\begin{aligned} 0 \leq & \int_{v \setminus \sigma(t)} \left\{ \sum_{\alpha=1}^n \rho_\alpha \dot{s}_\alpha^\alpha + \sum_{\alpha=1}^n r_\alpha s_\alpha + \operatorname{div} \left(\frac{\vec{q}}{T} \right) - \frac{Q}{T} \right\} \, dv + \\ & + \int_{\sigma(t)} \left[\sum_{\alpha=1}^n \rho_\alpha s_\alpha (\vec{v}_\alpha - \vec{v}) + \frac{\vec{q}}{T} \right]_+ \cdot \vec{n} \, da . \end{aligned} \quad (3.70)$$

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

$$\sum_{\alpha=1}^n \rho_\alpha \dot{s}_\alpha^\alpha + \sum_{\alpha=1}^n r_\alpha s_\alpha + \operatorname{div} \left(\frac{\vec{q}}{T} \right) - \frac{Q}{T} \geq 0 \quad \text{in} \quad v \setminus \sigma(t) , \quad (3.71)$$

$$\left[\sum_{\alpha=1}^n \rho_\alpha s_\alpha (\vec{v}_\alpha - \vec{v}) + \frac{\vec{q}}{T} \right]_+ \cdot \vec{n} \geq 0 \quad \text{at} \quad \sigma(t) . \quad (3.72)$$

Now we employ the energy balance of a mixture (3.64) and the formula (3.67) to express

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

Substituting this into the entropy inequality (3.71) yields

$$\begin{aligned} 0 \leq & \frac{1}{T} \left\{ - \sum_{\alpha=1}^n \rho_\alpha \dot{\varepsilon}_\alpha^\alpha - \sum_{\alpha=1}^n r_\alpha \varepsilon_\alpha + \sum_{\alpha=1}^n \mathbf{D}_\alpha : \mathbf{T}_\alpha - \sum_{\beta=1}^{n-1} \vec{u}_\beta \cdot \vec{k}_\beta - \frac{1}{2} \sum_{\beta=1}^{n-1} r_\beta \vec{u}_\beta^2 \right\} + \\ & + \sum_{\alpha=1}^n \rho_\alpha \dot{s}_\alpha^\alpha + \sum_{\alpha=1}^n r_\alpha s_\alpha - \frac{1}{T^2} \operatorname{grad} T \cdot \vec{q} \quad \text{in} \quad v \setminus \sigma(t) . \end{aligned} \quad (3.73)$$

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

- *free energy of the α -component*

$$f_\alpha = \varepsilon_\alpha - T s_\alpha , \quad \alpha = 1, \dots, n , \quad (3.74)$$

gives the Clausius-Duham inequality in the following form

$$\begin{aligned}
 0 &\geq \sum_{\alpha=1}^n \rho_{\alpha} \dot{f}_{\alpha}^{\alpha} + \sum_{\alpha=1}^n r_{\alpha} f_{\alpha} + \sum_{\alpha=1}^n \rho_{\alpha} s_{\alpha} \dot{T}^{\alpha} + T^{-1} \text{grad } T \cdot \vec{q} - \sum_{\alpha=1}^n \mathbf{D}_{\alpha} : \mathbf{T}_{\alpha} \\
 &+ \sum_{\beta=1}^{n-1} \vec{k}_{\beta} \cdot \vec{u}_{\beta} + \frac{1}{2} \sum_{\beta=1}^{n-1} r_{\beta} \vec{u}_{\beta}^2 \quad \text{in } v \setminus \sigma(t) .
 \end{aligned}
 \tag{3.75}$$

3.8 Constitutive equations of a mixture

Note: It is not 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 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 balance of mass of components and the mixture, the balance of linear momenta of components and the mixture, the balance of angular momenta of 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 mixture⁵. The missing equations should specify the material class by adding new relations among the kinematic, mechanical and thermal field variables. This task is handled by the *constitutive theory*.

We define a *process* as a set of all the fields that appear in the theory:

$$\chi_{\alpha}(X_{\alpha}, t), \rho_{\alpha}(X_{\alpha}, t), T(X_{\alpha}, t), \tag{3.76}$$

$$r_{\alpha}(\vec{x}, t), \varepsilon_{\alpha}(\vec{x}, t), s_{\alpha}(\vec{x}, t), \vec{q}(\vec{x}, t), \vec{k}_{\alpha}(\vec{x}, t), \mathbf{T}_{\alpha}(\vec{x}, t), \tag{3.77}$$

$$Q(\vec{x}, t), \vec{b}_{\alpha}(\vec{x}, t), \quad \alpha = 1, \dots, n, \tag{3.78}$$

and a *thermodynamic process* as the process, which satisfies the mass balance of reacting components, the linear momenta balance of components and the energy balance of mixture. *Note: The remaining balance laws will be satisfied by the use of the following principles of the constitutive theory, namely by the principle of determinism and by the entropy principle.*

The constitutive theory is based on several axioms, which will be briefly mentioned together with the most important conclusions they provide.

⁵The 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}_{α} and Q_{α} appear in the rest of balance laws only in \vec{q} , and Q , respectively (see Samohýl [1]).

- **The principle of determinism**

postulates that *the constitutive (response) functionals*:

$$r_\alpha, \varepsilon_\alpha, s_\alpha, \vec{q}, \vec{k}_\alpha, \mathbf{T}_\alpha, \quad \alpha = 1, \dots, n, \quad (3.79)$$

at a given place \vec{x} and at present time t , depend on the *thermo-kinetic process*, i.e. fields of motion (relative to the configuration κ_γ), density of components and temperature:

$$\vec{\chi}_{\kappa\gamma}(\vec{Y}_\gamma, \tau), \rho_\gamma(\vec{Y}_\gamma, \tau), T(\vec{Y}_\gamma, \tau), \quad \tau \leq t, \gamma = 1, \dots, n, \quad (3.80)$$

for which the mass balance of non-reacting components and mixture, the linear momentum balance of mixture and the angular momenta balance of components are satisfied.

- **The principle of local action**

states, that the responses (3.79) for a material particle at \vec{x} are most affected by the particles, being at present time t at place \vec{x} and in its nearest neighborhood.

- **The principle of differential memory**

states that the responses (3.79) are most affected by values of fields (3.80) at present time and in the nearest past.

The last two principles enable to reduce the functional form of (3.79) to a function of the Taylor expansion series of the fields (3.80). The order of the expansion specifies a particular material class.

- **The principle of equipresence**

states that a set of independent variables, i.e. appropriate Taylor expansion terms of (3.80), is the same for all response functionals (3.79) 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*:

$$\{r_\psi, \varepsilon_\alpha, s_\alpha, \vec{q}, \vec{k}_\beta, \mathbf{T}_\alpha\} = \mathcal{F}_\kappa[\vec{x}, \mathbf{F}_{\kappa\gamma}, \mathbf{G}_{\kappa\gamma}, \mathbf{L}_\gamma, \vec{v}_\gamma, \rho_\varphi, \vec{h}_\varphi, T, \vec{g}, X_\gamma, t]$$

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

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}_γ ... velocity gradient – see (3.15),
- \vec{v}_γ ... velocity of a material particle,
- ρ_φ ... density of a reacting component,
- \vec{h}_φ ... density gradient of a reacting component,

$$\vec{h}_\varphi = \text{grad } \rho_\varphi(\vec{x}, t), \quad (3.81)$$

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

$$\vec{g} = \text{grad } T(\vec{x}, t), \quad (3.82)$$

- X_γ ... material particle,
- t ... present time,
- m ... number of reacting components, i.e. $r_\epsilon \neq 0$ for $\epsilon \in (1 \dots m)$.

• **The principle of objectivity**

states that the shape of constitutive functionals \mathcal{F}_κ does not depend on a change of the frame. The general relation of two Cartesian frames can be expressed as⁶:

$$\vec{x}^* = \vec{c}(t) + \mathbf{Q}(t)\vec{\chi}_\alpha(\vec{X}_\alpha, t), \quad (3.83)$$

and

$$t^* = t + b, \quad (3.84)$$

where

$$\mathbf{Q}(t) \in Orth : \quad \mathbf{Q}(t)\mathbf{Q}^T(t) = \mathbf{Q}^T(t)\mathbf{Q}(t) = \mathbf{1}. \quad (3.85)$$

The velocity then transforms as

$$\vec{v}_\alpha^* = \mathbf{Q}(t)\vec{v}_\alpha + \dot{\vec{c}} + \mathbf{\Lambda}(\vec{x}^* - \vec{c}), \quad \text{with} \quad \mathbf{\Lambda} = \dot{\mathbf{Q}}\mathbf{Q}^T. \quad (3.86)$$

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

$$\{r_\psi, \varepsilon_\alpha, s_\alpha, \vec{q}, \vec{k}_\beta, \mathbf{T}_\alpha\} = \mathcal{F}_\kappa[\mathbf{F}_{\kappa\gamma}, \mathbf{G}_{\kappa\gamma}, \mathbf{D}_\gamma, \mathbf{\Omega}_\delta, \vec{u}_\delta, \rho_\varphi, \vec{h}_\varphi, T, \vec{g}, X_\gamma] \quad (3.87)$$

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

with considering

$$\begin{aligned} & \{r_\psi, \varepsilon_\alpha, s_\alpha, \mathbf{Q}\vec{q}, \mathbf{Q}\vec{k}_\beta, \mathbf{Q}\mathbf{T}_\alpha\mathbf{Q}^T\} = \\ & \mathcal{F}_\kappa[\mathbf{Q}\mathbf{F}_{\kappa\gamma}, \mathbf{Q}\mathbf{G}_{\kappa\gamma}, \mathbf{Q}\mathbf{D}_\gamma\mathbf{Q}^T, \mathbf{Q}\mathbf{\Omega}_\delta\mathbf{Q}^T, \mathbf{Q}\vec{u}_\delta, \rho_\varphi, \mathbf{Q}\vec{h}_\varphi, T, \mathbf{Q}\vec{g}, X_\gamma], \quad (3.88) \end{aligned}$$

for any orthogonal tensor \mathbf{Q} .

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

⁶Vectors are considered here as triplets of coordinates related to a "static" frame.

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

$$(\mathbf{H}, \mathbf{J}) \in \mathcal{G}_{\kappa\epsilon} \iff \mathcal{F}_{\kappa}[\mathbf{F}_{\kappa\epsilon}, \mathbf{G}_{\kappa\epsilon}, \Theta_{\epsilon}, X_{\epsilon}] = \mathcal{F}_{\kappa}[(\mathbf{F}_{\kappa\epsilon}, \mathbf{G}_{\kappa\epsilon}) \circ (\mathbf{H}, \mathbf{J}), \Theta_{\epsilon}, X_{\epsilon}] , \quad (3.89)$$

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 denoted

$$\begin{aligned} \Theta_{\epsilon} &= [\mathbf{F}_{\kappa\gamma \neq \epsilon}, \mathbf{G}_{\kappa\gamma \neq \epsilon}, \mathbf{D}_{\gamma}, \boldsymbol{\Omega}_{\delta}, \vec{u}_{\delta}, \rho_{\varphi}, \vec{h}_{\varphi}, T, \vec{g}, X_{\gamma \neq \epsilon}] , \\ \gamma &= 1, \dots, n; \quad \delta = 1, \dots, n-1; \quad \varphi = 1, \dots, m . \end{aligned}$$

Let g be the 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. The group operation \circ is defined as

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

where

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

The contracting operator \mathbf{C} is defined as

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

The inverse of group g is defined as

$$(\mathbf{P}, \mathbf{K})^{-1} = (\mathbf{P}^{-1}, \mathbf{K}^{-1}) , \quad \text{with} \quad \mathbf{K}^{-1} = -\mathbf{P}^{-1} \mathbf{C}(\mathbf{K} \otimes \mathbf{P}^{-1} \otimes \mathbf{P}^{-1}) . \quad (3.90)$$

– for a non-reacting component, $\epsilon \in (m+1, \dots, n)$, the definition of the symmetry group is the same as for a reacting component,

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

but, in addition, the tensors \mathbf{H} and \mathbf{J} have to satisfy the relations

$$|\det \mathbf{H}| = 1 \quad \dots \quad \mathbf{H} \text{ is unimodular} ,$$

and

$$\text{tr}(\mathbf{H}^{-1} \mathbf{J}) + \vec{k}_{\kappa\epsilon}(\mathbf{H} - \mathbf{1}) = \vec{0} , \quad (3.92)$$

where

$$\vec{k}_{\kappa\epsilon} = \rho_{\kappa\epsilon}^{-1} \text{Grad}_{\kappa\epsilon} \rho_{\kappa\epsilon} , \quad (3.93)$$

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

$$\rho_{\kappa\epsilon} = \rho_{\lambda\epsilon} , \quad \text{Grad}_{\kappa\epsilon} \rho_{\kappa\epsilon} = \text{Grad}_{\lambda\epsilon} \rho_{\lambda\epsilon} , \quad \epsilon \in (m+1, \dots, n) ,$$

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

Thus for any component ϵ of the mixture, reacting or non-reacting, we have defined a symmetry group $\mathcal{G}_{\kappa_\epsilon}$ with respect to the reference configuration κ_ϵ . When the reference configuration is changed to λ_ϵ , the symmetry group changes according to the 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 (3.75) is satisfied for all *admissible thermodynamic processes* – thermodynamic processes, taking place in a mixture of non-simple materials with differential memory and constitutive equations (3.87), (3.88), for which 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.

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

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

This inequality can then be rewritten by expanding the material time derivatives $\dot{\psi}_\alpha^\gamma$, 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 time derivatives of the form $\dot{\psi}_\alpha^\alpha$. The resulting inequality is very complicated and for sake of brevity we omit it here (see Samohýl [1]).

Several new quantities are introduced:

- *specific free energy of a mixture*

$$f = \sum_{\alpha=1}^n \frac{\rho_\alpha}{\rho} f_\alpha , \quad (3.94)$$

- *specific entropy of a mixture*

$$s = \sum_{\alpha=1}^n \frac{\rho_\alpha}{\rho} s_\alpha , \quad (3.95)$$

– chemical potential g_φ and quantity \vec{p}_φ

$$g_\varphi = \frac{\partial(\rho f)}{\partial \rho_\varphi}, \quad \vec{p}_\varphi = \frac{\partial(\rho f)}{\partial \vec{h}_\varphi}, \quad \varphi = 1, \dots, m. \quad (3.96)$$

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 choices of the independent variables. Therefore coefficients standing at these "linear" variables must vanish. Namely:

– at $\frac{\partial T}{\partial t}$:

$$\frac{\partial f}{\partial T} = -s, \quad (3.97)$$

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

$$\frac{\partial f}{\partial \vec{g}} = \vec{0}, \quad (3.98)$$

– at $(\dot{\vec{v}}_\delta - \dot{\vec{v}}_n^n)$:

$$\frac{\partial f}{\partial \vec{u}_\delta} = \vec{0}, \quad \delta = 1, \dots, n-1, \quad (3.99)$$

– at $(\dot{\mathbf{F}})_\gamma$:

$$\frac{\partial f}{\partial \mathbf{D}_\gamma} = \mathbf{0}, \quad \frac{\partial f}{\partial \mathbf{\Omega}_\delta} = \mathbf{0}, \quad \gamma = 1, \dots, n; \quad \delta = 1, \dots, n-1. \quad (3.100)$$

Thus the free energy of a mixture depends only on

$$f = f(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T), \quad (3.101)$$

so does then, according to (3.96):

$$g_\nu = g_\nu(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T), \quad \vec{p}_\nu = \vec{p}_\nu(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T), \quad (3.102)$$

$$\gamma = 1, \dots, n, \quad \nu = 1, \dots, m,$$

and due to (3.97) also

$$s = s(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T). \quad (3.103)$$

Since the definition of the free energy f (3.94), with the use of (3.74), gives

$$f = \varepsilon - Ts, \quad (3.104)$$

we can immediately write that

$$\varepsilon = \varepsilon(\mathbf{F}_\gamma, \mathbf{G}_\gamma, \rho_\varphi, \vec{h}_\varphi, T). \quad (3.105)$$

– at $\text{grad } \vec{g}$:

$$A^{ij} + A^{ji} = 0 , \quad (3.106)$$

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 $\text{Grad } \vec{d}_{\varphi}$:

$$N_{\varphi}^{ij} + N_{\varphi}^{ji} = 0 , \quad \varphi = 1, \dots, m , \quad (3.107)$$

where

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

– at $\dot{\mathbf{G}}_{\gamma}^{iJK}$:

$$C_{\gamma}^{iJK} + C_{\gamma}^{iKJ} = 0 , \quad \gamma = 1, \dots, n , \quad (3.108)$$

with

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

– at $\text{Grad } \mathbf{G}_{\gamma}$:

$$\begin{aligned} D_{\gamma}^{iJKL} &= D_{\gamma}^{iKJL} , & D_{\gamma}^{iJJJ} &= 0 , & D_{\gamma}^{iJJK} + 2D_{\gamma}^{iJKJ} &= 0 , \\ D_{\gamma}^{i123} + D_{\gamma}^{i231} + D_{\gamma}^{i312} &= 0 , & \gamma &= 1, \dots, n; \quad i, J, K = 1, 2, 3 , \end{aligned} \quad (3.109)$$

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

$$D_{\gamma}^{iJKL} = \sum_{\alpha=1}^n \rho_{\alpha} \frac{\partial f_{\alpha}}{\partial G_{\gamma}^{iJK}} (u_{\alpha}^j - u_{\gamma}^j) F_{\gamma}^{-1Lj} + \sum_{\psi=1}^{m-1} (p_{\psi}^k - p_m^k) \frac{\partial r_{\psi}}{\partial G_{\gamma}^{iJK}} F_{\gamma}^{-1Lk} . \quad (3.110)$$

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

$$K^{ij} = K^{ji} , \quad (3.111)$$

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:

$$\begin{aligned}
0 &\geq \sum_{\alpha=1}^n \sum_{\gamma=1}^n \rho_\alpha \left[\frac{\partial f_\alpha}{\partial F_\gamma^{iJ}} F_\gamma^{jJ} + \frac{\partial f_\alpha}{\partial G_\gamma^{iJK}} G_\gamma^{jJK} \right] (D_\gamma^{ij} + \Omega_\gamma^{ij}) - \sum_{\varphi=1}^m p_\varphi^j h_\varphi^i (D_\varphi^{ij} + \Omega_\varphi^{ij}) \\
&+ \sum_{\alpha=1}^n \sum_{\gamma=1}^n \rho_\alpha \frac{\partial f_\alpha}{\partial F_\gamma^{iJ}} G_\gamma^{iJK} F_\gamma^{-1Kj} (u_\alpha^j - u_\gamma^j) + \sum_{\delta=1}^{n-1} \sum_{\alpha=1}^n \rho_\alpha \frac{\partial f_\alpha}{\partial u_\delta^i} u_\alpha^j (D_\delta^{ij} - D_n^{ij} + \Omega_\delta^{ij}) \\
&+ \sum_{\varphi=1}^m \sum_{\alpha=1}^n \rho_\alpha \frac{\partial f_\alpha}{\partial \rho_\varphi} u_\alpha^i h_\varphi^i - \sum_{\varphi=1}^m (u_\varphi^i h_\varphi^i + \rho_\varphi D_\varphi^{ii}) (g_\varphi - f_\varphi) - \sum_{\varphi=1}^m p_\varphi^i h_\varphi^i D_\varphi^{kk} \\
&+ \sum_{\psi=1}^{m-1} (p_\psi^k - p_m^k) \left\{ \sum_{\gamma=1}^n \frac{\partial r_\psi}{\partial F_\gamma^{iJ}} G_\gamma^{iJL} F_\gamma^{-1Lk} + \sum_{\delta=1}^{n-1} \frac{\partial r_\psi}{\partial u_\delta^i} (D_\delta^{ik} - D_n^{ik} + \Omega_\delta^{ik}) \right. \\
&+ \left. \sum_{\varphi=1}^m \frac{\partial r_\psi}{\partial \rho_\varphi} h_\varphi^k + \frac{\partial r_\psi}{\partial T} g^k \right\} + \sum_{\alpha=1}^n \rho_\alpha \left(\frac{\partial f_\alpha}{\partial T} + s_\alpha \right) u_\alpha^j g^j + \sum_{\psi=1}^{m-1} (g_\psi - g_m) r_\psi \\
&+ \frac{1}{T} q^i g^i - \sum_{\alpha=1}^n T_\alpha^{ij} D_\alpha^{ij} + \sum_{\beta=1}^{n-1} k_\beta^i u_\beta^i + \frac{1}{2} \sum_{\psi=1}^{m-1} (u_\psi^i u_\psi^i - u_m^i u_m^i) r_\psi . \tag{3.112}
\end{aligned}$$

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* $\epsilon \in (1, \dots, m)$,
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* $\epsilon \in (m+1, \dots, n)$,
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 (3.92).

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 (3.90), then

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

where $(\mathbf{1}, \mathbf{0})$ is the unit element of the group g . According to the definition of the symmetry group (3.89), we obtain

$$\mathcal{F}_\kappa[(\mathbf{F}_{\kappa\epsilon}, \mathbf{G}_{\kappa\epsilon}), \Theta_\epsilon, X_\epsilon] = \mathcal{F}_\kappa[(\mathbf{1}, \mathbf{0}), \Theta_\epsilon, X_\epsilon] = \mathcal{F}_\kappa[\Theta_\epsilon] . \tag{3.113}$$

The possibility to omit the dependence on X_ϵ in the last equality results from the fact that the first equality in (3.113) is valid for any reference configuration. We can choose the *homogeneous* configuration in which the dependence on X_ϵ vanishes.⁷

⁷The existence of such a configuration is discussed in Samohýl [1].

For a non-reacting component, we can choose

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

and

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

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

$$(\mathbf{A}^{sym.})^{ijk} \equiv \frac{1}{2} (A^{ijk} + A^{ikj}) . \quad (3.114)$$

It can be shown (Samohýl [1]) that the tensors \mathbf{H} and \mathbf{J} satisfy condition (3.92). Applying the definition of the symmetry group (3.91) yields

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

The last equality results from the fact that the previous formula can be derived for any reference configuration κ , particularly 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:

$$\{r_\psi, f_\alpha, s_\alpha, \vec{q}, \vec{k}_\beta, \mathbf{T}_\alpha\} = \hat{\mathcal{F}}[\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_\delta, \vec{u}_\delta, T, \vec{g}] , \quad (3.115)$$

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

where we replaced ε_α with f_α , since they are uniquely connected by the definition (3.74).

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

$$\{r_\psi, f_\alpha, s_\alpha, \mathbf{Q}\vec{q}, \mathbf{Q}\vec{k}_\beta, \mathbf{Q}\mathbf{T}_\alpha\mathbf{Q}^T\} = \hat{\mathcal{F}}[\rho_\gamma, \mathbf{Q}\vec{h}_\gamma, \mathbf{Q}\mathbf{D}_\gamma\mathbf{Q}^T, \mathbf{Q}\mathbf{\Omega}_\delta\mathbf{Q}^T, \mathbf{Q}\vec{u}_\delta, T, \mathbf{Q}\vec{g}] , \quad (3.116)$$

for any orthogonal tensor \mathbf{Q} .

Now we can rewrite the results (3.97) - (3.112) of the entropy principle for the case of fluid mixtures. We obtain:

$$f = f(\rho_\gamma, \vec{h}_\gamma, T) , \quad \gamma = 1, \dots, n , \quad (3.117)$$

$$\frac{\partial f}{\partial T} = -s . \quad (3.118)$$

For all components we define the *chemical potential* g_γ and the *vector* \vec{p}_γ :

$$g_\gamma = \frac{\partial(\rho f)}{\partial \rho_\gamma}, \quad \vec{p}_\gamma = \frac{\partial(\rho f)}{\partial \vec{h}_\gamma}, \quad \gamma = 1, \dots, n. \quad (3.119)$$

And we see that

$$s = s(\rho_\gamma, \vec{h}_\gamma, T), \quad g_\alpha = g_\alpha(\rho_\gamma, \vec{h}_\gamma, T), \quad \vec{p}_\alpha = \vec{p}_\alpha(\rho_\gamma, \vec{h}_\gamma, T), \quad \alpha, \gamma = 1, \dots, n. \quad (3.120)$$

$$\mathbf{0} = \left[\sum_{\delta=1}^{n-1} \rho_\delta \frac{\partial f_\delta}{\partial \vec{g}} \otimes \vec{u}_\delta + \sum_{\psi=1}^{m-1} \frac{\partial r_\psi}{\partial \vec{g}} \otimes (\vec{p}_\psi - \vec{p}_m) \right]^{sym.}, \quad (3.121)$$

$$\mathbf{0} = \left[\sum_{\delta=1}^{n-1} \rho_\delta \frac{\partial f_\delta}{\partial \vec{h}_\gamma} \otimes \vec{u}_\delta - \vec{p}_\gamma \otimes \vec{u}_\gamma + \sum_{\psi=1}^{m-1} \frac{\partial r_\psi}{\partial \vec{h}_\gamma} \otimes (\vec{p}_\psi - \vec{p}_m) \right]^{sym.}, \quad \gamma = 1, \dots, n, \quad (3.122)$$

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

$$\mathbf{0} = \sum_{\gamma=1}^n (\vec{p}_\gamma \otimes \vec{h}_\gamma - \vec{h}_\gamma \otimes \vec{p}_\gamma), \quad (3.124)$$

and the entropy inequality in a mixture of fluids reads:

$$0 \geq \sum_{\gamma=1}^n \sum_{\alpha=1}^n \rho_\alpha \frac{\partial f_\alpha}{\partial \rho_\gamma} \vec{h}_\gamma \cdot \vec{u}_\alpha - \sum_{\gamma=1}^n (g_\gamma - f_\gamma) \vec{h}_\gamma \cdot \vec{u}_\gamma - \sum_{\gamma=1}^n \rho_\gamma (g_\gamma - f_\gamma) \text{tr } \mathbf{D}_\gamma \\ - \sum_{\gamma=1}^n \vec{p}_\gamma \cdot \vec{h}_\gamma \text{tr } \mathbf{D}_\gamma - \sum_{\gamma=1}^n \vec{h}_\gamma \cdot (\mathbf{D}_\gamma + \Omega_\gamma) \vec{p}_\gamma + \sum_{\delta=1}^{n-1} \sum_{\alpha=1}^n \rho_\alpha \frac{\partial f_\alpha}{\partial \vec{u}_\delta} \cdot (\mathbf{D}_\delta - \mathbf{D}_n + \Omega_\delta) \vec{u}_\alpha \\ + \sum_{\psi=1}^{m-1} (\vec{p}_\psi - \vec{p}_m) \cdot \left[\sum_{\gamma=1}^n \frac{\partial r_\psi}{\partial \rho_\gamma} \vec{h}_\gamma + \frac{\partial r_\psi}{\partial T} \vec{g} + \sum_{\delta=1}^{n-1} \frac{\partial r_\psi}{\partial \vec{u}_\delta} \cdot (\mathbf{D}_\delta - \mathbf{D}_n + \Omega_\delta) \right] \\ + \sum_{\psi=1}^{m-1} (g_\psi - g_m) r_\psi + \sum_{\alpha=1}^n \rho_\alpha \left(\frac{\partial f_\alpha}{\partial T} + s_\alpha \right) \vec{u}_\alpha \cdot \vec{g} + \frac{1}{T} \vec{q} \cdot \vec{g} - \sum_{\alpha=1}^n \text{tr } \mathbf{T}_\alpha \mathbf{D}_\alpha \\ + \sum_{\beta=1}^{n-1} \vec{k}_\beta \cdot \vec{u}_\beta + \frac{1}{2} \sum_{\psi=1}^{m-1} (\vec{u}_\psi^2 - \vec{u}_m^2) r_\psi. \quad (3.125)$$

In the following text, we will be inspecting the constitutive equations for a two-component reacting mixture of fluids in the vicinity of equilibrium. Thus we will first handle the problem of an equilibrium in fluid mixtures in general.

3.10 Equilibrium in a mixture of fluids

The equilibrium is defined as a thermodynamic process with a zero entropy production. This means that there is equality in the reduced entropy inequality (3.125). This is

satisfied for a process, in which

$$\mathbf{D}_\gamma^+ = \mathbf{0} , \quad \boldsymbol{\Omega}_\delta^+ = \mathbf{0} , \quad \vec{u}_\delta^+ = \vec{0} , \quad \vec{g}^+ = \vec{0} , \quad (3.126)$$

$$\sum_{\psi=1}^{m-1} \sum_{\gamma=1}^n \left(\frac{\partial r_\psi}{\partial \rho_\gamma} \right)^+ (\vec{p}_\psi^+ - \vec{p}_m^+) \cdot \vec{h}_\gamma^+ = 0 , \quad (3.127)$$

$$\sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) r_\psi^+ = 0 , \quad \gamma = 1, \dots, n; \delta = 1, \dots, n-1 , \quad (3.128)$$

where the equilibrated quantities are denoted by symbol + .

Let symbol Σ denote the right-hand side of the entropy inequality (3.125),

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

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

$$\frac{d}{d\lambda} \Sigma(\rho_\gamma^+ + \lambda\alpha_\gamma, \vec{h}_\gamma^+ + \lambda\vec{\gamma}_\gamma, \lambda\mathbf{D}_\gamma, \lambda\boldsymbol{\Omega}_\delta, \lambda\vec{u}_\delta, T^+ + \lambda\beta, \lambda\vec{g}) \Big|_{\lambda=0} = 0 , \quad (3.129)$$

$$\frac{d^2}{d\lambda^2} \Sigma(\rho_\gamma^+ + \lambda\alpha_\gamma, \vec{h}_\gamma^+ + \lambda\vec{\gamma}_\gamma, \lambda\mathbf{D}_\gamma, \lambda\boldsymbol{\Omega}_\delta, \lambda\vec{u}_\delta, T^+ + \lambda\beta, \lambda\vec{g}) \Big|_{\lambda=0} \leq 0 , \quad (3.130)$$

for a real parameter λ , arbitrary, but fixed quantities

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

and equilibrated

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

which satisfy (3.127) and (3.128).

We will consider only the extremal condition (3.129). Applying it on the reduced entropy inequality (3.125) yields:

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

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

Since $\alpha_\eta, \vec{\gamma}_\alpha, \mathbf{D}_\gamma, \Omega_\delta, \vec{u}_\delta, \beta, \vec{g}$, are arbitrary constants, the terms standing at them must vanish. We obtain the following seven constraints:

The terms at α_η must vanish

$$\begin{aligned}
0 & = \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \rho_\gamma} \right)^+ \left(\frac{\partial(\vec{p}_\psi - \vec{p}_m)}{\partial \rho_\eta} \right)^+ \cdot \vec{h}_\gamma^+ + \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \rho_\eta} \right)^+ (\vec{p}_\psi^+ - \vec{p}_m^+) \cdot \vec{h}_\gamma^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \rho_\eta} \right)^+ + \sum_{\psi=1}^{m-1} \left(\frac{\partial(g_\psi - g_m)}{\partial \rho_\eta} \right)^+ r_\psi^+ , \quad \eta = 1, \dots, n ,
\end{aligned} \tag{3.131}$$

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

$$\begin{aligned}
\vec{0} & = \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \rho_\eta} \right)^+ (\vec{p}_\psi^+ - \vec{p}_m^+) + \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \rho_\gamma} \right)^+ \vec{h}_\gamma^+ \cdot \left(\frac{\partial(\vec{p}_\psi - \vec{p}_m)}{\partial \vec{h}_\eta} \right)^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{h}_\eta} \right)^+ + \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} [(\vec{p}_\psi^+ - \vec{p}_m^+) \cdot \vec{h}_\gamma^+] \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \vec{h}_\eta} \right)^+ \\
& + \sum_{\psi=1}^{m-1} \left(\frac{\partial(g_\psi - g_m)}{\partial \vec{h}_\eta} \right)^+ r_\psi^+ , \quad \eta = 1, \dots, n .
\end{aligned} \tag{3.132}$$

The terms at \mathbf{D}_γ must vanish after symmetrization:

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

$$\begin{aligned}
& - \rho_\gamma^+ (g_\gamma^+ - f_\gamma^+) \mathbf{1} - (\vec{p}_\gamma^+ \cdot \vec{h}_\gamma^+) \mathbf{1} - \vec{h}_\gamma^+ \otimes \vec{p}_\gamma^+ \\
& + \left[\sum_{\psi=1}^{m-1} \sum_{\delta=1}^{n-1} (\delta_{\delta\gamma} - \delta_{\gamma n}) \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+ \otimes (\vec{p}_\psi^+ - \vec{p}_m^+) - \mathbf{T}_\gamma^+ \right]^{sym.}, \quad \gamma = 1, \dots, n.
\end{aligned} \tag{3.133}$$

The terms at Ω_δ must vanish after antisymmetrization:

$$\begin{aligned}
\mathbf{0} & = \left[\sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+ \otimes (\vec{p}_\psi^+ - \vec{p}_m^+) - \vec{h}_\delta^+ \otimes \vec{p}_\delta^+ + \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} ((\vec{p}_\psi^+ - \vec{p}_m^+) \cdot \vec{h}_\gamma^+) \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \Omega_\delta} \right)^+ \right. \\
& \left. + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \Omega_\delta} \right)^+ \right]^{antis.}, \quad \delta = 1, \dots, n-1.
\end{aligned} \tag{3.134}$$

The terms at \vec{u}_δ must vanish:

$$\begin{aligned}
\vec{0} & = \sum_{\gamma=1}^n \rho_\delta^+ \left(\frac{\partial f_\delta}{\partial \rho_\gamma} \right)^+ \vec{h}_\gamma^+ - (g_\delta^+ - f_\delta^+) \vec{h}_\delta^+ + \vec{k}_\delta^+ + \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} ((\vec{p}_\psi^+ - \vec{p}_m^+) \cdot \vec{h}_\gamma^+) \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \vec{u}_\delta} \right)^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+, \quad \delta = 1, \dots, n-1.
\end{aligned} \tag{3.135}$$

The term at β must vanish:

$$\begin{aligned}
0 & = \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} \left(\frac{\partial (\vec{p}_\psi - \vec{p}_m)}{\partial T} \right)^+ \cdot \vec{h}_\gamma^+ \left(\frac{\partial r_\psi}{\partial \rho_\gamma} \right)^+ + \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial T} \right)^+ (\vec{p}_\psi^+ - \vec{p}_m^+) \cdot \vec{h}_\gamma^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial T} \right)^+ + \sum_{\psi=1}^{m-1} \left(\frac{\partial (g_\psi - g_m)}{\partial T} \right)^+ r_\psi^+.
\end{aligned} \tag{3.136}$$

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

$$\begin{aligned}
\vec{0} & = \frac{1}{T^+} \vec{q}^+ + \sum_{\psi=1}^{m-1} \left(\frac{\partial r_\psi}{\partial T} \right)^+ (\vec{p}_\psi^+ - \vec{p}_m^+) + \sum_{\gamma=1}^n \sum_{\psi=1}^{m-1} ((\vec{p}_\psi^+ - \vec{p}_m^+) \cdot \vec{h}_\gamma^+) \left(\frac{\partial^2 r_\psi}{\partial \rho_\gamma \partial \vec{g}} \right)^+ \\
& + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{g}} \right)^+.
\end{aligned} \tag{3.137}$$

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

$$r_\psi^+ = r_\psi(\rho_\gamma^+, \vec{h}_\gamma^+, \mathbf{0}, \mathbf{0}, \vec{0}, T^+, \vec{0}) = 0, \quad \psi = 1, \dots, m-1, \tag{3.138}$$

and that the density gradient in equilibrium is equal to zero,

$$\vec{h}_\gamma^+ = \vec{0}, \quad \gamma = 1, \dots, n. \tag{3.139}$$

As a result of these assumptions, conditions (3.127) and (3.128) are satisfied automatically. It might be a bit questionable to assert the condition (3.139) when working in the

field of external volume force (e.g. gravity), but we will assume that due to low compressibility of ice, the resulting equilibrium density gradient would be negligible, see measured density profiles (Paterson, [7]). In a temperate ice zone, there might be expected a non-zero equilibrium density gradient resulting from variations of equilibrium water fraction. Again according to the measurements, the resulting density variations can be neglected and the assumption (3.139) may be regarded valid.

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,

$$\vec{p}_\gamma = \frac{\partial(\rho f)}{\partial \vec{h}_\gamma} \equiv \vec{0}, \quad (3.140)$$

the equilibrium conditions (3.131) – (3.137) reduce considerably to the form:

$$0 = \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \rho_\alpha} \right)^+, \quad \alpha = 1, \dots, n, \quad (3.141)$$

$$\vec{0} = \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{h}_\alpha} \right)^+, \quad \alpha = 1, \dots, n, \quad (3.142)$$

$$\mathbf{0} = \left[\sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \mathbf{D}_\gamma} \right)^+ - \rho_\gamma^+ (g_\gamma^+ - f_\gamma^+) \mathbf{1} - \mathbf{T}_\gamma^+ \right]^{sym.}, \quad \gamma = 1, \dots, n, \quad (3.143)$$

$$\mathbf{0} = \left[\sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \mathbf{\Omega}_\delta} \right)^+ \right]^{antis.}, \quad \delta = 1, \dots, n-1, \quad (3.144)$$

$$\vec{0} = \vec{k}_\delta^+ + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{u}_\delta} \right)^+, \quad \delta = 1, \dots, n-1, \quad (3.145)$$

$$0 = \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial T} \right)^+, \quad (3.146)$$

$$\vec{0} = \frac{1}{T^+} \vec{q}^+ + \sum_{\psi=1}^{m-1} (g_\psi^+ - g_m^+) \left(\frac{\partial r_\psi}{\partial \vec{g}} \right)^+. \quad (3.147)$$

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 is distinctly separated from ice, both being different phases of the same material and 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 which handles this topic and 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 ($\alpha = 2$), will be considered as non-simple fluids of the constitutive model (3.115):

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

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

For further simplifications of this constitutive model, several assumptions are to be introduced. Guided by an effort 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

$$\{r_1, f_\alpha, s_\alpha, \vec{q}, \vec{k}_1\} , \quad \alpha = 1, 2 , \quad (4.2)$$

will be linearized in the vicinity of equilibrium, defined by eq. (3.126) – (3.147), in variables $\{\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, \vec{g}\}$, without imposing any restrictions on the functional dependence on the remaining variables, ρ_γ, T .

The stress-tensor functionals \mathbf{T}_α 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 of \mathbf{T}_α .

Now we will make use of the *principle of objectivity* (3.116), which states:

$$\{r_1, f_\alpha, s_\alpha, \mathbf{Q}\vec{q}, \mathbf{Q}\vec{k}_1, \mathbf{Q}\mathbf{T}_\alpha\mathbf{Q}^T\} = \hat{\mathcal{F}}[\rho_\gamma, \mathbf{Q}\vec{h}_\gamma, \mathbf{Q}\mathbf{D}_\gamma\mathbf{Q}^T, \mathbf{Q}\Omega_1\mathbf{Q}^T, \mathbf{Q}\vec{u}_1, T, \mathbf{Q}\vec{g}] , \quad (4.3)$$

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}_β and second-order tensors \mathbf{Y}_γ respectively if they satisfy:

$$a = a(y_\alpha, \vec{y}_\beta, \mathbf{Y}_\gamma) = a(y_\alpha, \mathbf{Q}\vec{y}_\beta, \mathbf{Q}\mathbf{Y}_\gamma\mathbf{Q}^T) , \quad (4.4)$$

$$\vec{a} = \vec{a}(y_\alpha, \vec{y}_\beta, \mathbf{Y}_\gamma) = \mathbf{Q}^T\vec{a}(y_\alpha, \mathbf{Q}\vec{y}_\beta, \mathbf{Q}\mathbf{Y}_\gamma\mathbf{Q}^T) , \quad (4.5)$$

$$\mathbf{A} = \mathbf{A}(y_\alpha, \vec{y}_\beta, \mathbf{Y}_\gamma) = \mathbf{Q}^T\mathbf{A}(y_\alpha, \mathbf{Q}\vec{y}_\beta, \mathbf{Q}\mathbf{Y}_\gamma\mathbf{Q}^T)\mathbf{Q} , \quad (4.6)$$

for any orthogonal tensor \mathbf{Q} . Now we 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}_β , ($\beta = 1, \dots, r$), and s second-order tensors \mathbf{Y}_γ , ($\gamma = 1, \dots, s$), it is sufficient and necessary to represent them in the forms

$$a = a_0 + \sum_{\gamma=1}^s \vartheta_\gamma \text{tr } \mathbf{Y}_\gamma , \quad (4.7)$$

$$\vec{a} = \sum_{\beta=1}^r \zeta_\beta \vec{y}_\beta , \quad (4.8)$$

$$\mathbf{A} = \tau \mathbf{1} + \sum_{\gamma=1}^s \alpha_\gamma (\text{tr } \mathbf{Y}_\gamma) \mathbf{1} + \sum_{\gamma=1}^s (\eta_\gamma \mathbf{Y}_\gamma + \xi_\gamma \mathbf{Y}_\gamma^T) , \quad (4.9)$$

where $a_0, \vartheta_\gamma, \zeta_\beta, \tau, \alpha_\gamma, \eta_\gamma$, and ξ_γ are scalar constants.

The linearization of the constitutive equations (4.2) with respect to $\{\vec{h}_\gamma, \mathbf{D}_\gamma, \Omega_1, \vec{u}_1, \vec{g}\}$, 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 of the following form,

$$r_1 = r_1^{(0)}(\rho_\gamma, T) + r_1^{(1)}(\rho_\gamma, T) \text{tr} \mathbf{D}_1 + r_1^{(2)}(\rho_\gamma, T) \text{tr} \mathbf{D}_2, \quad (4.10)$$

$$f_\alpha = f_\alpha^{(0)}(\rho_\gamma, T) + f_\alpha^{(1)}(\rho_\gamma, T) \text{tr} \mathbf{D}_1 + f_\alpha^{(2)}(\rho_\gamma, T) \text{tr} \mathbf{D}_2, \quad (4.11)$$

$$s_\alpha = s_\alpha^{(0)}(\rho_\gamma, T) + s_\alpha^{(1)}(\rho_\gamma, T) \text{tr} \mathbf{D}_1 + s_\alpha^{(2)}(\rho_\gamma, T) \text{tr} \mathbf{D}_2, \quad (4.12)$$

$$\vec{q} = -k(\rho_\gamma, T)\vec{g} - \lambda(\rho_\gamma, T)\vec{u}_1 + \sum_{\psi=1}^2 \chi_\psi(\rho_\gamma, T)\vec{h}_\psi , \quad (4.13)$$

$$\vec{k}_1 = -\xi(\rho_\gamma, T)\vec{g} - \nu(\rho_\gamma, T)\vec{u}_1 + \sum_{\psi=1}^2 \omega_\psi(\rho_\gamma, T)\vec{h}_\psi , \quad (4.14)$$

while the stress tensors \mathbf{T}_α are represented by nonlinear functionals as

$$\mathbf{T}_\alpha = \mathbf{T}_\alpha(\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \Omega_1, \vec{u}_1, T, \vec{g}) , \quad (4.15)$$

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

4.3 Equilibrium in the water-ice mixture

We have simplified our material model by the 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:

$$\mathbf{D}_\gamma^+ = \mathbf{0}, \quad \boldsymbol{\Omega}_1^+ = \mathbf{0}, \quad \vec{u}_1^+ = \vec{0}, \quad \vec{g}^+ = \vec{0}, \quad (4.16)$$

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

$$(g_1^+ - g_2^+) r_1^+ = 0, \quad (4.18)$$

$$\gamma = 1, 2.$$

We postulated by (3.138) that:

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

and by (3.139) that:

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

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 density gradients \vec{h}_γ . The same holds for the free energy f of a mixture, because of its definition (3.94). Consequently, (3.119), yields

$$\vec{p}_\gamma \equiv \vec{0}, \quad \gamma = 1, 2, \quad (4.19)$$

and the equilibrium conditions (3.131)-(3.137) can be reduced to the form (3.141)-(3.147). In the case of a 2-component mixture, they read:

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

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

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

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

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

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

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

We have omitted the superscripts *sym.* and *antis.* in (4.22) and (4.23), respectively, since (4.22) is already symmetric (see (3.47)) 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 neither on \vec{h}_1 , nor $\mathbf{\Omega}_1$. Moreover, r_1 does not depend on \vec{u}_1 and \vec{g} , so equations (4.24) and (4.26), yield

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

If we assume that either

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

then (4.20) or (4.25) imply that

$$g_1^+ = g_2^+. \quad (4.27)$$

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

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

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 (3.121)-(3.124) we can see that they are satisfied identically due to (4.10)-(4.15), (4.19), except (3.123) which now reads

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

According to (4.11) we have

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

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

$$\begin{aligned} \left(\frac{\partial f_1}{\partial \mathbf{D}_1}\right)_{ij} &= \frac{\partial f_1}{\partial D_{1ij}} \\ &= f_1^{(1)}(\rho_\gamma, T) \delta_{ij}. \end{aligned} \quad (4.31)$$

Then, according to (3.114), the first condition in (4.29) reads

$$\frac{1}{2} \rho_1 f_1^{(1)} (\delta_{ij} u_{1k} + \delta_{ik} u_{1j}) = 0, \quad \forall i, j, k. \quad (4.32)$$

Provided that $\vec{u}_1 \neq \vec{0}$, we can always achieve by a suitable choice of the coordinate system that

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

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

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

For a non-zero water-density ρ_1 (or, equivalently, non-zero water fraction w) we immediately find

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

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

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

and thus obtain

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

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

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

To conclude, eq. (4.29) yields

$$f_1 = f_1(\rho_\gamma, T), \quad (4.37)$$

where we omitted the superscript ⁽⁰⁾.

Let us recall (3.117), which implies that

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

where f is the free energy of mixture, defined by (3.94) as $\rho f = \rho_1 f_1 + \rho_2 f_2$. Having shown that f_1 is independent of \mathbf{D}_γ , we see that

$$\frac{\partial f_2}{\partial \mathbf{D}_\gamma} \equiv \mathbf{0} , \quad \gamma = 1, 2 . \quad (4.38)$$

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

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

and the constraint (4.38), we have

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

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

and, consequently,

$$f_2 = f_2(\rho_\gamma, T) , \quad (4.41)$$

where the superscript ⁽⁰⁾ has been omitted.

The reduced entropy inequality (3.125) has the following form:

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

This inequality must hold for any values of independent variables, particularly for any arbitrary \vec{h}_1 , \vec{h}_2 , \vec{u}_1 , \vec{g} , \mathbf{D}_1 , \mathbf{D}_2 . Now we will 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 be always non-positive:

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

- 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 positive quantity, it must hold

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

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

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

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

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

- 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

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

Having exploited the entropy principle, we arrived at:

$$r_1 = r_1^{(0)}(\rho_\gamma, T) + r_1^{(1)}(\rho_\gamma, T) \operatorname{tr} \mathbf{D}_1 + r_1^{(2)}(\rho_\gamma, T) \operatorname{tr} \mathbf{D}_2, \quad (4.57)$$

$$f_\alpha = f_\alpha^{(0)}(\rho_\gamma, T), \quad (4.58)$$

$$s_\alpha = s_\alpha^{(0)}(\rho_\gamma, T) + s_\alpha^{(1)}(\rho_\gamma, T) \operatorname{tr} \mathbf{D}_1 + s_\alpha^{(2)}(\rho_\gamma, T) \operatorname{tr} \mathbf{D}_2, \quad (4.59)$$

$$\vec{q} = -k(\rho_\gamma, T) \vec{g} - \lambda(\rho_\gamma, T) \vec{u}_1, \quad (4.60)$$

$$\vec{k}_1 = -\xi(\rho_\gamma, T) \vec{g} - \nu(\rho_\gamma, T) \vec{u}_1 + \sum_{\psi=1}^2 \omega_\psi(\rho_\gamma, T) \vec{h}_\psi, \quad (4.61)$$

$$\mathbf{T}_\alpha = \mathbf{T}_\alpha(\rho_\gamma, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}), \quad (4.62)$$

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 a few percent only (Hutter, [4]). If we assume that the constitutive functionals are continuous and differentiable in densities ρ_1, ρ_2 , it seems us reasonable to expand constitutive functionals into a Taylor series with respect to the water content. 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)-(4.62). Defining the *water mass fraction* w

$$w = \frac{\rho_1}{\rho}, \quad (4.63)$$

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

$$\rho_1 = w \rho, \quad (4.64)$$

$$\rho_2 = (1 - w) \rho, \quad (4.65)$$

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 make the Taylor expansion in the vicinity of $w = 0$:

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

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

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

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

• r_1 :

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

In view of linearization, we also omit the last two terms $w \operatorname{tr} \mathbf{D}_1$ and $w \operatorname{tr} \mathbf{D}_2$:

$$r_1 = \tilde{r}_1^{(0)}(\rho, T) + w \hat{r}_1^{(0)}(\rho, T) + \tilde{r}_1^{(1)}(\rho, T) \operatorname{tr} \mathbf{D}_1 + \tilde{r}_1^{(2)}(\rho, T) \operatorname{tr} \mathbf{D}_2. \quad (4.68)$$

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

- f_α , $\alpha = 1, 2$:

$$f_\alpha = \tilde{f}_\alpha(\rho, T) + w \hat{f}_\alpha(\rho, T) . \quad (4.69)$$

- s_α , $\alpha = 1, 2$:

$$\begin{aligned} s_\alpha &= \tilde{s}_\alpha^{(0)}(\rho, T) + \tilde{s}_\alpha^{(1)}(\rho, T) \operatorname{tr} \mathbf{D}_1 + \tilde{s}_\alpha^{(2)}(\rho, T) \operatorname{tr} \mathbf{D}_2 \\ &+ w(\hat{s}_\alpha^{(0)}(\rho, T) + \hat{s}_\alpha^{(1)}(\rho, T) \operatorname{tr} \mathbf{D}_1 + \hat{s}_\alpha^{(2)}(\rho, T) \operatorname{tr} \mathbf{D}_2) . \end{aligned} \quad (4.70)$$

Following the same argumentation as for r_1 , we omit the terms $w \operatorname{tr} \mathbf{D}_1$, $w \operatorname{tr} \mathbf{D}_2$:

$$s_\alpha = \tilde{s}_\alpha^{(0)}(\rho, T) + w \hat{s}_\alpha^{(0)}(\rho, T) + \tilde{s}_\alpha^{(1)}(\rho, T) \operatorname{tr} \mathbf{D}_1 + \tilde{s}_\alpha^{(2)}(\rho, T) \operatorname{tr} \mathbf{D}_2 . \quad (4.71)$$

The entropy of the mixture was defined in (3.95) 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 (4.71), we have

$$\begin{aligned} s &= w(\tilde{s}_1^{(0)} + w \hat{s}_1^{(0)} + \tilde{s}_1^{(1)} \operatorname{tr} \mathbf{D}_1 + \tilde{s}_1^{(2)} \operatorname{tr} \mathbf{D}_2) \\ &+ (1 - w)(\tilde{s}_2^{(0)} + w \hat{s}_2^{(0)} + \tilde{s}_2^{(1)} \operatorname{tr} \mathbf{D}_1 + \tilde{s}_2^{(2)} \operatorname{tr} \mathbf{D}_2) , \end{aligned} \quad (4.72)$$

or with the help of an auxiliary quantity \mathcal{S} :

$$\begin{aligned} \mathcal{S} &= (\tilde{s}_1^{(0)} + w \hat{s}_1^{(0)} + \tilde{s}_1^{(1)} \operatorname{tr} \mathbf{D}_1 + \tilde{s}_1^{(2)} \operatorname{tr} \mathbf{D}_2 + \hat{s}_2^{(0)} - \tilde{s}_2^{(0)} - w \hat{s}_2^{(0)} \\ &- \tilde{s}_2^{(1)} \operatorname{tr} \mathbf{D}_1 - \tilde{s}_2^{(2)} \operatorname{tr} \mathbf{D}_2) , \end{aligned}$$

we may write

$$s = \tilde{s}_2^{(0)}(\rho, T) + \tilde{s}_2^{(1)}(\rho, T) \operatorname{tr} \mathbf{D}_1 + \tilde{s}_2^{(2)}(\rho, T) \operatorname{tr} \mathbf{D}_2 + w \mathcal{S}(w, \rho, T, \operatorname{tr} \mathbf{D}_1, \operatorname{tr} \mathbf{D}_2) . \quad (4.73)$$

Now let us recall the result (3.120), which implies

$$\frac{\partial s}{\partial \mathbf{D}_1} \equiv 0 , \quad \frac{\partial s}{\partial \mathbf{D}_2} \equiv 0 , \quad (4.74)$$

or with the use of (4.73)

$$\begin{aligned} \tilde{s}_2^{(1)}(\rho, T) \mathbf{1} + w \frac{\partial \mathcal{S}(w, \rho, T, \operatorname{tr} \mathbf{D}_1, \operatorname{tr} \mathbf{D}_2)}{\partial \mathbf{D}_1} &\equiv \mathbf{0} , \\ \tilde{s}_2^{(2)}(\rho, T) \mathbf{1} + w \frac{\partial \mathcal{S}(w, \rho, T, \operatorname{tr} \mathbf{D}_1, \operatorname{tr} \mathbf{D}_2)}{\partial \mathbf{D}_2} &\equiv \mathbf{0} , \end{aligned}$$

Taking the limit of these two identities for $w \rightarrow 0$ yields

$$\tilde{s}_2^{(1)}(\rho, T) \equiv \mathbf{0} , \quad (4.75)$$

and

$$\tilde{s}_2^{(2)}(\rho, T) \equiv \mathbf{0} , \quad (4.76)$$

respectively. Equation (4.71) for $\alpha = 2$ reduces to the form:

$$s_2 = \tilde{s}_2(\rho, T) + w \hat{s}_2(\rho, T) , \quad (4.77)$$

where we omitted the superscript (0) . Since we now have

$$\frac{\partial s_2}{\partial \mathbf{D}_\gamma} \equiv \mathbf{0} , \quad \gamma = 1, 2 ,$$

and concerning (4.74) and the definition of the mixture entropy density (3.95), we immediately conclude that

$$\frac{\partial s_1}{\partial \mathbf{D}_1} \equiv \mathbf{0} \quad \longrightarrow \quad \tilde{s}_1^{(1)}(\rho, T) \equiv 0 ,$$

and

$$\frac{\partial s_1}{\partial \mathbf{D}_2} \equiv \mathbf{0} \quad \longrightarrow \quad \tilde{s}_1^{(2)}(\rho, T) \equiv 0 ,$$

and equation (4.71) for $\alpha = 1$ reduces to the form:

$$s_1 = \tilde{s}_1(\rho, T) + w \hat{s}_1(\rho, T) . \quad (4.78)$$

- \vec{q} :

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

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

In view of linearization, we omit the terms $w\vec{g}$ and $w\vec{u}_1$:

$$\vec{q} = -k(\rho, T)\vec{g} - \lambda(\rho, T)\vec{u}_1 , \quad (4.79)$$

where the label $\tilde{}$ was dropped out.

- \vec{k}_1 :

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

$$\omega_1 = g_1 - f_1 - \rho_1 \frac{\partial f_1}{\partial \rho_1} . \quad (4.80)$$

The chemical potential g_1 was defined by (3.119):

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

so

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

But

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

and ω_1 then reads

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

Using (4.53) we have

$$\begin{aligned} \omega_2 &= -\rho w \frac{\partial f_1(\rho_\gamma, T)}{\partial \rho_2} \\ &= -\rho w \left. \frac{\partial (\tilde{f}_1(\rho, T) + w \hat{f}_1(\rho, T))}{\partial \rho_2} \right|_{\rho_1, T} \\ &= -\rho w \left. \frac{\partial}{\partial \rho_2} \right|_{\rho_1, T} \left(\tilde{f}_1(\rho_1 + \rho_2, T) + \frac{\rho_1}{\rho_1 + \rho_2} \hat{f}_1(\rho_1 + \rho_2, T) \right) \\ &= -\rho w \left(\frac{\partial \tilde{f}_1(\rho, T)}{\partial \rho} - \frac{\rho_1}{(\rho_1 + \rho_2)^2} \hat{f}_1(\rho, T) + \frac{\rho_1}{\rho_1 + \rho_2} \frac{\partial \hat{f}_1(\rho, T)}{\partial \rho} \right) \\ &= -\rho w \left(\frac{\partial \tilde{f}_1(\rho, T)}{\partial \rho} - w \frac{\hat{f}_1(\rho, T)}{\rho} + w \frac{\partial \hat{f}_1(\rho, T)}{\partial \rho} \right). \end{aligned} \tag{4.82}$$

Substituting the expansions (4.81), (4.82), and the expansions of the coefficients

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

into the constitutive equation (4.61) for \vec{k}_1 , neglecting the nonlinear terms proportional to $w\vec{g}$, $w\vec{u}_1$, $w\vec{h}_1$, $w\vec{h}_2$, results in

$$\vec{k}_1 = -\xi(\rho, T) \vec{g} - \nu(\rho, T) \vec{u}_1 - \omega(\rho, T) \vec{h}_1 , \quad (4.83)$$

where we omitted the label \sim and introduced

$$\omega = - \left(\rho \frac{\partial \tilde{f}_2(\rho, T)}{\partial \rho} + \hat{f}_2(\rho, T) \right) . \quad (4.84)$$

- \mathbf{T}_1 :

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

$$\mathbf{T}_1 = \tilde{\mathbf{T}}_1(\rho, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) + w \hat{\mathbf{T}}_1(\rho, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) . \quad (4.85)$$

It is not obvious that the constitutive relation for the stress tensor is continuous or even differentiable in the water fraction. However, following traditional approach in glaciology, we assume differentiability of the constitutive functional.

- \mathbf{T}_2 :

Similarly, we expand

$$\mathbf{T}_2 = \tilde{\mathbf{T}}_2(\rho, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) + w \hat{\mathbf{T}}_2(\rho, \vec{h}_\gamma, \mathbf{D}_\gamma, \mathbf{\Omega}_1, \vec{u}_1, T, \vec{g}) . \quad (4.86)$$

In the next step, we will introduce an incompressibility condition into the constitutive model. To do it we firstly rewrite the entropy inequality in terms of the barycentric velocity and the diffusive velocity with respect to the barycentre.

4.5.1 Entropy inequality in terms of the barycentric velocity

Considering $r_2 = -r_1$, due to (3.32), the entropy inequality (3.75) for a two-component reacting mixture reads:

$$\begin{aligned}0 &\geq \rho_1 \dot{f}_1^1 + \rho_2 \dot{f}_2^2 + r_1(f_1 - f_2) + \rho_1 s_1 \dot{T}^1 + \rho_2 s_2 \dot{T}^2 + \frac{\vec{q} \cdot \vec{g}}{T} \\ &\quad - \mathbf{T}_1 : \mathbf{D}_1 - \mathbf{T}_2 : \mathbf{D}_2 + \vec{k}_1 \cdot \vec{u}_1 + \frac{1}{2} r_1 \vec{u}_1^2 .\end{aligned} \quad (4.87)$$

We recall that the superscript $^\alpha$ denotes the material time derivative with respect to the velocity of the α component. For what it follows, 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

$$\vec{u}_1^B = \vec{v}_1 - \vec{v}^B , \quad \vec{u}_2^B = \vec{v}_2 - \vec{v}^B . \quad (4.88)$$

Consequently,

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

and

$$\vec{u}_2^B = -\frac{\rho_1}{\rho_2} \vec{u}_1^B . \quad (4.89)$$

Now we can rewrite

$$\begin{aligned} \dot{f}_1^1 &= \frac{\partial f_1}{\partial t} + \text{grad } f_1 \cdot \vec{v}_1 \\ &= \frac{\partial f_1}{\partial t} + \text{grad } f_1 \cdot \vec{v}^B + \text{grad } f_1 \cdot \vec{u}_1^B \\ &= \dot{f}_1^B + \text{grad } f_1 \cdot \vec{u}_1^B , \end{aligned} \quad (4.90)$$

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

$$\begin{aligned} \dot{f}_2^2 &= \dot{f}_2^B + \text{grad } f_2 \cdot \vec{u}_2^B \\ &= \dot{f}_2^B - \frac{\rho_1}{\rho_2} \text{grad } f_2 \cdot \vec{u}_1^B , \end{aligned} \quad (4.91)$$

where we made use of (4.89). Analogously, it holds

$$\hat{T}^1 = \hat{T}^B + \vec{g} \cdot \vec{u}_1^B , \quad (4.92)$$

$$\hat{T}^2 = \hat{T}^B - \frac{\rho_1}{\rho_2} \vec{g} \cdot \vec{u}_1^B , \quad (4.93)$$

We can also write

$$\begin{aligned} \mathbf{D}_1 &= \{\text{grad } \vec{v}_1\}^{sym.} \\ &= \{\text{grad } \vec{v}^B + \text{grad } \vec{u}_1^B\}^{sym.} \\ &= \mathbf{D}^B + \mathbf{D}_1^B , \end{aligned} \quad (4.94)$$

with

$$\mathbf{D}^B = \{\text{grad } \vec{v}^B\}^{sym.} , \quad \mathbf{D}_1^B = \{\text{grad } \vec{u}_1^B\}^{sym.} , \quad (4.95)$$

and similarly

$$\begin{aligned} \mathbf{D}_2 &= \{\text{grad } \vec{v}_2\}^{sym.} \\ &= \{\text{grad } \vec{v}^B + \text{grad } \vec{u}_2^B\}^{sym.} \\ &= \left\{ \text{grad } \vec{v}^B - \frac{\rho_1}{\rho_2} \text{grad } \vec{u}_1^B \right\}^{sym.} \\ &= \mathbf{D}^B - \frac{\rho_1}{\rho_2} \mathbf{D}_1^B . \end{aligned} \quad (4.96)$$

Finally

$$\begin{aligned}
\vec{u}_1 &= \vec{v}_1 - \vec{v}_2 \\
&= (\vec{v}^B + \vec{u}_1^B) - (\vec{v}^B + \vec{u}_2^B) \\
&= \left(1 + \frac{\rho_1}{\rho_2}\right) \vec{u}_1^B.
\end{aligned} \tag{4.97}$$

We insert the expressions (4.90) – (4.97) into the entropy inequality (4.87) and arrive at the form:

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

which, after slight rearranging the terms, reads

$$\begin{aligned}
0 &\geq \rho_1 \dot{f}_1^B + \rho_2 \dot{f}_2^B + \rho_1 \vec{u}_1^B \cdot \text{grad}(f_1 - f_2) + r_1(f_1 - f_2) + (\rho_1 s_1 + \rho_2 s_2) \dot{T}^B \\
&+ \rho_1 (s_1 - s_2) \vec{g} \cdot \vec{u}_1^B + \frac{\vec{q} \cdot \vec{g}}{T} - (\mathbf{T}_1 + \mathbf{T}_2) : \mathbf{D}^B - \left(\mathbf{T}_1 - \frac{\rho_1}{\rho_2} \mathbf{T}_2\right) : \mathbf{D}_1^B \\
&+ \left(1 + \frac{\rho_1}{\rho_2}\right) \vec{k}_1 \cdot \vec{u}_1^B + \frac{1}{2} \left(1 + \frac{\rho_1}{\rho_2}\right)^2 r_1 (\vec{u}_1^B)^2.
\end{aligned} \tag{4.98}$$

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

$$\tilde{\rho}_1 = \frac{dm_1}{dV_1}, \quad \tilde{\rho}_2 = \frac{dm_2}{dV_2}, \tag{4.99}$$

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

$$\tilde{w} = \frac{dV_1}{dV}. \tag{4.100}$$

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

$$dV_1 + dV_2 = dV. \tag{4.101}$$

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

$$\begin{aligned}\rho_1 &= \frac{dm_1}{dV} \\ &= \tilde{\rho}_1 \tilde{w} ,\end{aligned}\tag{4.102}$$

$$\begin{aligned}\rho_2 &= \frac{dm_2}{dV} \\ &= \tilde{\rho}_2(1 - \tilde{w}) .\end{aligned}\tag{4.103}$$

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

$$\begin{aligned}\delta\rho &= \delta\rho_1 + \delta\rho_2 \\ &= \tilde{\rho}_1 \delta\tilde{w} - \tilde{\rho}_2 \delta\tilde{w} \\ &= (\tilde{\rho}_1 - \tilde{\rho}_2) \delta\tilde{w} .\end{aligned}\tag{4.104}$$

The values $\tilde{\rho}_1$ and $\tilde{\rho}_2$ differ approximately within 10% (Hutter, [4]), the variation of the water volume fraction is of the order of 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

$$\rho = \rho_1 + \rho_2 \equiv \text{const.} ,\tag{4.105}$$

where the equivalence symbol in (4.105) 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, constitutive functional \mathcal{F} of a constrained material will be considered in the form (Gurtin & Guidugli, [5]):

$$\mathcal{F} = \mathcal{F}^E + \bar{\mathcal{F}} ,\tag{4.106}$$

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 constitutive functions by the *reaction set* $\left\{ \bar{r}_1, \bar{f}_\alpha, \bar{s}_\alpha, \bar{q}, \bar{k}_1, \bar{\mathbf{T}}_\alpha \right\}$ in the form:

$$r_1 = r_1^E + \bar{r}_1 ,\tag{4.107}$$

$$f_\alpha = f_\alpha^E + \bar{f}_\alpha ,\tag{4.108}$$

$$s_\alpha = s_\alpha^E + \bar{s}_\alpha ,\tag{4.109}$$

$$\vec{q} = \vec{q}^E + \bar{\vec{q}}, \quad (4.110)$$

$$\vec{k}_1 = \vec{k}_1^E + \bar{\vec{k}}_1, \quad (4.111)$$

$$\mathbf{T}_\alpha = \mathbf{T}_\alpha^E + \bar{\mathbf{T}}_\alpha, \quad (4.112)$$

$$\alpha = 1, 2.$$

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* $\mathcal{R}_\mathcal{C}$

$$\{\bar{r}_1, \bar{f}_\alpha, \bar{s}_\alpha, \bar{\vec{q}}, \bar{\vec{k}}_1, \bar{\mathbf{T}}_\alpha\} = \mathcal{R}_\mathcal{C}(\rho_1, \rho_2, \mathbf{F}_1, \mathbf{F}_2, T), \quad (4.113)$$

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 (4.113) will be determined with the use of entropy inequality (4.98). Inserting the expansion (4.107)-(4.112) of the functionals $\{r_1, f_\alpha, s_\alpha, \vec{q}, \vec{k}_1, \mathbf{T}_\alpha\}$ into the inequality (4.98) yields

$$\begin{aligned} 0 \geq & \sigma^E + \rho_1 \dot{\check{f}}_1^B + \rho_2 \dot{\check{f}}_2^B + \rho_1 \vec{u}_1^B \cdot \text{grad}(\bar{f}_1 - \bar{f}_2) + \bar{r}_1 (f_1^E - f_2^E) + r_1^E (\bar{f}_1 - \bar{f}_2) \\ & + \bar{r}_1 (\bar{f}_1 - \bar{f}_2) + (\rho_1 \bar{s}_1 + \rho_2 \bar{s}_2) \dot{I}^B + \rho_1 (\bar{s}_1 - \bar{s}_2) \vec{g} \cdot \vec{u}_1^B + \frac{\bar{\vec{q}} \cdot \vec{g}}{T} \\ & - (\bar{\mathbf{T}}_1 + \bar{\mathbf{T}}_2) : \mathbf{D}^B - \left(\bar{\mathbf{T}}_1 - \frac{\rho_1}{\rho_2} \bar{\mathbf{T}}_2 \right) : \mathbf{D}_1^B + \left(1 + \frac{\rho_1}{\rho_2} \right) \bar{\vec{k}}_1 \cdot \vec{u}_1^B \\ & + \frac{1}{2} \left(1 + \frac{\rho_1}{\rho_2} \right)^2 \bar{r}_1 (\vec{u}_1^B)^2, \end{aligned} \quad (4.114)$$

where for brevity we introduced quantity σ^E , which is equal to the right-hand side of (4.98) 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 (4.114), let us remind the balance of mass of a mixture (3.29), which now reads

$$\dot{\rho}_1 + \dot{\rho}_2 + \rho_1 \text{div} \vec{v}_1 + \rho_2 \text{div} \vec{v}_2 = 0,$$

and can be rewritten as

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

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

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

Finally, with the use of the incompressibility condition (4.105), we arrive at a constraint for \vec{v}^B :

$$\operatorname{div} \vec{v}^B = 0, \quad (4.115)$$

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

$$\operatorname{tr} \mathbf{D}^B = 0. \quad (4.116)$$

Thus the mass balance of a mixture under the incompressibility condition (4.105) constrains \mathbf{D}^B by (4.116). Since the rest of the independent variables in (4.114) is not constrained by the remaining balance laws, (linear momentum, angular momentum and energy), conditions (4.105) and (4.116) represent the only additional restrictions on the admissible thermodynamic process.

In accordance with the rational-thermodynamics approach, we assert that the inequality (4.114) 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 $\dot{T}^B = 0$, $\vec{u}_1^B = \vec{g} = \vec{0}$, $\mathbf{D}^B = \mathbf{D}_1^B = \mathbf{0}$ and the remaining variables be arbitrary, then the inequality (4.114) reads

$$0 \geq \sigma^E + \rho_1 \check{f}_1^B + \rho_2 \check{f}_2^B + \bar{r}_1(f_1^E - f_2^E) + r_1^E(\bar{f}_1 - \bar{f}_2) + \bar{r}_1(\bar{f}_1 - \bar{f}_2). \quad (4.117)$$

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

$$0 \geq \sigma^E + \lambda \left(\rho_1 \check{f}_1^B + \rho_2 \check{f}_2^B + \bar{r}_1(f_1^E - f_2^E) + r_1^E(\bar{f}_1 - \bar{f}_2) \right) + \lambda^2 \left(\bar{r}_1(\bar{f}_1 - \bar{f}_2) \right), \quad (4.118)$$

for arbitrary real λ . Moreover we will assume that

$$\bar{f}_1 = \bar{f}_2. \quad (4.119)$$

Note: 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 (4.119) for a 2-component mixture is somewhat weaker, however, needed for the following considerations.

The inequality (4.118) then reads

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

and it holds for any real λ . Thus

$$0 \equiv \rho \check{f}_1^B + \bar{r}_1(f_1^E - f_2^E). \quad (4.120)$$

The entropy inequality (4.114) is now reduced to

$$\begin{aligned} 0 \geq \sigma^E &+ (\rho_1 \bar{s}_1 + \rho_2 \bar{s}_2) \dot{T}^B + \rho_1(\bar{s}_1 - \bar{s}_2) \vec{g} \cdot \vec{u}_1^B + \frac{\vec{q} \cdot \vec{g}}{T} - (\bar{\mathbf{T}}_1 + \bar{\mathbf{T}}_2) : \mathbf{D}^B \\ &- \left(\bar{\mathbf{T}}_1 - \frac{\rho_1}{\rho_2} \bar{\mathbf{T}}_2 \right) : \mathbf{D}_1^B + \left(1 + \frac{\rho_1}{\rho_2} \right) \bar{k}_1 \cdot \vec{u}_1^B + \frac{1}{2} \left(1 + \frac{\rho_1}{\rho_2} \right)^2 \bar{r}_1 (\vec{u}_1^B)^2. \end{aligned} \quad (4.121)$$

It will be convenient to rewrite (4.121) as:

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

where the operation \star has the following meaning:

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

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

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

for any real λ . This immediately yields

$$0 \equiv \left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{q}, \bar{k}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2 \right) \star \left(\frac{1}{2} \left(1 + \frac{\rho_1}{\rho_2} \right)^2 (\bar{u}_1^B)^2, \rho_1 \dot{T}^B + \rho_1 \bar{g} \cdot \bar{u}_1^B, \right. \\ \left. \rho_2 \dot{T}^B - \rho_1 \bar{g} \cdot \bar{u}_1^B, \frac{\bar{g}}{T}, \left(1 + \frac{\rho_1}{\rho_2} \right) \bar{u}_1^B, -\mathbf{D}^B - \mathbf{D}_1^B, -\mathbf{D}^B + \frac{\rho_1}{\rho_2} \mathbf{D}_1^B \right). \quad (4.122)$$

The reactions $\left\{ \bar{r}_1, \bar{f}_\alpha, \bar{s}_\alpha, \bar{q}, \bar{k}_1, \bar{\mathbf{T}}_\alpha \right\}$ are functions of $\{\rho_1, \rho_2, \mathbf{F}_1, \mathbf{F}_2, T\}$ only, see (4.113), hence, for special choices of $\bar{u}_1^B, \bar{g}, \mathbf{D}, \mathbf{D}_1^B, \dot{T}$, we obtain:

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

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

thus

$$\rho_1 \bar{s}_1 + \rho_2 \bar{s}_2 \equiv 0, \quad (4.123)$$

and (4.122) now reads

$$0 \equiv \left(\bar{r}_1, \bar{s}_1, \bar{s}_2, \bar{q}, \bar{k}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2 \right) \star \left(\frac{1}{2} \left(1 + \frac{\rho_1}{\rho_2} \right)^2 (\bar{u}_1^B)^2, \rho_1 \bar{g} \cdot \bar{u}_1^B, -\rho_1 \bar{g} \cdot \bar{u}_1^B, \right. \\ \left. \frac{\bar{g}}{T}, \left(1 + \frac{\rho_1}{\rho_2} \right) \bar{u}_1^B, -\mathbf{D}^B - \mathbf{D}_1^B, -\mathbf{D}^B + \frac{\rho_1}{\rho_2} \mathbf{D}_1^B \right), \quad (4.124)$$

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

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

thus

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

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

$$\bar{r}_1 \equiv 0, \quad (4.125)$$

$$\vec{k}_1 \equiv \vec{0}. \quad (4.126)$$

In view of (4.125), equation (4.120) yields

$$\check{f}_1^B \equiv 0,$$

thus in view of (4.119):

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

in order to keep the reaction functional closed to scalar multiplication (at each time), we must put

$$\bar{f}_1 \equiv \bar{f}_2 \equiv 0. \quad (4.127)$$

Now (4.124) reduces to

$$0 \equiv \left(\bar{s}_1, \bar{s}_2, \vec{q}, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2 \right) \star \left(\rho_1 \vec{g} \cdot \vec{u}_1^B, -\rho_1 \vec{g} \cdot \vec{u}_1^B, \frac{\vec{g}}{T}, -\mathbf{D}^B - \mathbf{D}_1^B, -\mathbf{D}^B + \frac{\rho_1}{\rho_2} \mathbf{D}_1^B \right), \quad (4.128)$$

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

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

thus

$$\bar{\mathbf{T}}_1 \equiv \frac{\rho_1}{\rho_2} \bar{\mathbf{T}}_2, \quad (4.129)$$

and (4.128) reduces to

$$0 \equiv \left(\bar{s}_1, \bar{s}_2, \vec{q}, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2 \right) \star \left(\rho_1 \vec{g} \cdot \vec{u}_1^B, -\rho_1 \vec{g} \cdot \vec{u}_1^B, \frac{\vec{g}}{T}, -\mathbf{D}^B, -\mathbf{D}^B \right), \quad (4.130)$$

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

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

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

$$\vec{q} \equiv \vec{0}, \quad (4.131)$$

and (4.130) reduces to

$$0 \equiv (\bar{s}_1, \bar{s}_2, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2) \star (\rho_1 \vec{g} \cdot \vec{u}_1^B, -\rho_1 \vec{g} \cdot \vec{u}_1^B, -\mathbf{D}^B, -\mathbf{D}^B), \quad (4.132)$$

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

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

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

$$\bar{s}_1 \equiv \bar{s}_2, \quad (4.133)$$

which together with (4.123) immediately yields

$$\bar{s}_1 \equiv 0, \quad (4.134)$$

$$\bar{s}_2 \equiv 0, \quad (4.135)$$

and (4.132) reduces to

$$0 \equiv (\bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2) \star (-\mathbf{D}^B, -\mathbf{D}^B), \quad (4.136)$$

or

$$(\bar{\mathbf{T}}_1 + \bar{\mathbf{T}}_2) : \mathbf{D}^B \equiv 0. \quad (4.137)$$

The tensor \mathbf{D}^B does not have arbitrary values, but according to (4.116), it must be trace-free:

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

thus (4.137) 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 (4.129) we obtain

$$\bar{\mathbf{T}}_1 \equiv -p \frac{\rho_1}{\rho} \mathbf{1}, \quad (4.138)$$

$$\bar{\mathbf{T}}_2 \equiv -p \frac{\rho_2}{\rho} \mathbf{1}. \quad (4.139)$$

In summary, we have found that the form of the reaction functionals in our 2-component mixture, for the constraint (4.105), are of the form

$$\left\{ \bar{r}_1, \bar{f}_\alpha, \bar{s}_\alpha, \bar{q}, \bar{k}_1, \bar{\mathbf{T}}_1, \bar{\mathbf{T}}_2 \right\} = \left\{ 0, 0, 0, \vec{0}, \vec{0}, -pw\mathbf{1}, -p(1-w)\mathbf{1} \right\}, \quad (4.140)$$

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

Now, with the help of the incompressibility condition (4.105), we can further reduce the constitutive equations for the *extra functionals* (see (4.106)): $\{r_1^E, f_\alpha^E, s_\alpha^E, \vec{q}^E, \vec{k}_1^E, \mathbf{T}_\alpha^E\}$. In the case of $\{r_1^E, f_\alpha^E, s_\alpha^E, \vec{q}^E\}$ we only omit the dependence on ρ , since ρ is now a constant parameter. In the case of \vec{k}_1^E , we can moreover replace \vec{h}_1 by definition (3.81):

$$\begin{aligned} \vec{h}_1 &= \text{grad } \rho_1 \\ &= \rho \text{grad } w, \end{aligned} \quad (4.141)$$

and write

$$\vec{k}_1 = -\xi(T)\vec{g} - \nu(T)\vec{u}_1 - \rho\omega(T)\text{grad } w. \quad (4.142)$$

More information can be obtained about the extra stress functionals $\mathbf{T}_1^E, \mathbf{T}_2^E$.

- \mathbf{T}_1^E

According to (4.85), we have (omitting the dependence on ρ)

$$\mathbf{T}_1^E = \tilde{\mathbf{T}}_1(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}) + w\hat{\mathbf{T}}_1(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}). \quad (4.143)$$

The case $w = 0$ corresponds to pure ice, where no extra "water-stress" should be exerted, thus we assert

$$\mathbf{T}_1^E|_{w=0} \equiv \mathbf{0}, \quad (4.144)$$

and conclude

$$\mathbf{T}_1^E = w\hat{\mathbf{T}}_1(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}). \quad (4.145)$$

- \mathbf{T}_2^E

According to (4.86), we have

$$\mathbf{T}_2^E = \tilde{\mathbf{T}}_2(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}) + w\hat{\mathbf{T}}_2(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}). \quad (4.146)$$

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

$$\tilde{\mathbf{T}}_2 = -\Pi_2(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g})\mathbf{1} + \overset{\circ}{\tilde{\mathbf{T}}}_2(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}). \quad (4.147)$$

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

$$\overset{\circ}{\tilde{\mathbf{T}}}_2 \Big|_{w=0} = \mathcal{B}(T)h(D_{2II}^\circ) \overset{\circ}{\mathbf{D}}_2, \quad (4.148)$$

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

In view of (4.112) and (4.140), we have

$$\mathbf{T}_2 = -p(1-w)\mathbf{1} + \mathbf{T}_2^E. \quad (4.149)$$

Using (4.146) and (4.147), equation (4.148) implies that

$$\tilde{\overset{\circ}{\mathbf{T}}}_2 = \mathcal{B}(T)h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2. \quad (4.150)$$

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

$$\mathbf{D}_2 = \mathcal{A}(T)f(\sigma) \overset{\circ}{\mathbf{T}}_2, \quad (4.151)$$

where

$$\sigma = \sqrt{\frac{1}{2}\text{tr}(\overset{\circ}{\mathbf{T}}_2)^2}. \quad (4.152)$$

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

$$\overset{\circ}{\mathbf{D}}_2 = \mathbf{D}_2.$$

Hence the relation (4.151) may also be written as

$$\overset{\circ}{\mathbf{D}}_2 = \mathcal{A}(T)f(\sigma) \overset{\circ}{\mathbf{T}}_2. \quad (4.153)$$

We now intend to express the inverse relation, i.e. to express $\overset{\circ}{\mathbf{T}}_2$ as a function of $\overset{\circ}{\mathbf{D}}_2$ and its invariants. The double-dot product of (4.153) is

$$\overset{\circ}{\mathbf{D}}_2 \cdot \overset{\circ}{\mathbf{D}}_2 = (\mathcal{A}(T)f(\sigma))^2 \overset{\circ}{\mathbf{T}}_2 \cdot \overset{\circ}{\mathbf{T}}_2. \quad (4.154)$$

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

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

and considering (4.152), we obtain

$$\overset{\circ}{D}_{2II} = -(\mathcal{A}(T)f(\sigma))^2 \sigma^2.$$

Provided that the function $f(\sigma)$ is invertible², we may express σ by means of $\overset{\circ}{D}_{2II}$ and T . As a result, we have

$$\overset{\circ}{\mathbf{T}}_2 = \mathcal{B}(T)h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2. \quad (4.155)$$

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

The expression (4.150) 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 (4.150), we can write (4.146) as

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

To summarize, the constitutive equations of ice-water mixture, after applying the partial linearization, the entropy principle, and the incompressibility constraint, and requiring that the model of ice-water mixture reduces to the model of pure ice in the limit $w \rightarrow 0$, we have

$$r_1 = \tilde{r}_1^{(0)}(T) + w\hat{r}_1^{(0)}(T) + \tilde{r}_1^{(1)}(T) \operatorname{tr}\mathbf{D}_1 + \tilde{r}_1^{(2)}(T) \operatorname{tr}\mathbf{D}_2 , \quad (4.156)$$

$$f_\alpha = \tilde{f}_\alpha(T) + w\hat{f}_\alpha(T) , \quad (4.157)$$

$$s_\alpha = \tilde{s}_\alpha(T) + w\hat{s}_\alpha(T) , \quad (4.158)$$

$$\vec{q} = -k(T)\vec{g} - \lambda(T)\vec{u}_1 , \quad (4.159)$$

$$\vec{k}_1 = -\xi(T)\vec{g} - \nu(T)\vec{u}_1 - \rho\omega(T) \operatorname{grad} w , \quad (4.160)$$

$$\mathbf{T}_1 = -pw\mathbf{1} + w\hat{\mathbf{T}}_1(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}) , \quad (4.161)$$

$$\begin{aligned} \mathbf{T}_2 &= -p(1-w)\mathbf{1} - \Pi_2(w, \vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g})\mathbf{1} + \mathcal{B}(T)h(\overset{\circ}{D}_{2II})\overset{\circ}{\mathbf{D}}_2 \\ &+ w\hat{\mathbf{T}}_2(\vec{h}_\gamma, \mathbf{D}_\gamma, \boldsymbol{\Omega}_1, \vec{u}_1, T, \vec{g}) , \end{aligned} \quad (4.162)$$

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

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 (4.156)-(4.162).

4.6.1 Mass balance

The ice component

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

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

Since

$$r_2 = -r_1 ,$$

as follows from (3.32), we can write

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

Assuming ρ constant, we further have

$$\frac{\partial w}{\partial t} + \text{grad } w \cdot \vec{v}_2 - (1 - w) \text{div } \vec{v}_2 = \frac{r_1}{\rho} . \quad (4.163)$$

The water component

The mass balance for the water component reads

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

or,

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

and assuming additionally ρ to be constant, we have

$$\frac{\partial w}{\partial t} + \text{grad } w \cdot \vec{v}_1 + w \text{div } \vec{v}_1 = \frac{r_1}{\rho} . \quad (4.164)$$

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 (4.164) will be further rearranged by (4.163):

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

or

$$\text{grad } w \cdot \vec{u}_1 + \text{div } \vec{v}_2 + w \text{div } \vec{u}_1 = 0 . \quad (4.165)$$

4.6.2 Linear momentum balance

The ice component

With the use of the general linear momentum balance for a mixture component (3.39), we arrive at

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

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

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

following from (3.43), and using (4.160), we obtain

$$\rho(1 - w) \frac{D_2 \vec{v}_2}{Dt} = \text{div } \mathbf{T}_2 + \rho(1 - w) \vec{g}_F + \xi \vec{g} + \nu \vec{u}_1 + \rho \omega \text{grad } w - r_1 \vec{u}_1 . \quad (4.166)$$

The water component

Similarly, for the water component:

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

or, if we express \vec{b}_1 and \vec{k}_1 from (4.160), we obtain

$$\rho w \frac{D_1 \vec{v}_1}{Dt} = \operatorname{div} \mathbf{T}_1 + \rho w \vec{g}_F - \xi \vec{g} - \nu \vec{u}_1 - \rho \omega \operatorname{grad} w . \quad (4.167)$$

Note that neither here, nor in the previous case of ice momentum balance, we do not 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 (3.47) implies the symmetry of the constitutive functionals for \mathbf{T}_1 and \mathbf{T}_2 :

$$\mathbf{T}_1 = \mathbf{T}_1^T , \quad \mathbf{T}_2 = \mathbf{T}_2^T ,$$

which, in view of (4.161) and (4.162) means

$$\hat{\mathbf{T}}_1 = \hat{\mathbf{T}}_1^T, \quad \text{and} \quad \hat{\mathbf{T}}_2 = \hat{\mathbf{T}}_2^T . \quad (4.168)$$

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 (3.64), has the form

$$\begin{aligned} \rho_1 \frac{D_1 \varepsilon_1}{Dt} + \rho_2 \frac{D_2 \varepsilon_2}{Dt} &= \mathbf{T}_1 : \mathbf{D}_1 + \mathbf{T}_2 : \mathbf{D}_2 - \operatorname{div} \vec{q} - r_1 \varepsilon_1 - r_2 \varepsilon_2 \\ &\quad - \vec{v}_1 \cdot \vec{k}_1 - \vec{v}_2 \cdot \vec{k}_2 - \frac{1}{2} r_1 \vec{v}_1^2 - \frac{1}{2} r_2 \vec{v}_2^2 , \end{aligned}$$

where we do not consider any internal heating Q . By (3.67), it holds

$$\vec{v}_1 \cdot \vec{k}_1 + \vec{v}_2 \cdot \vec{k}_2 + \frac{1}{2} r_1 \vec{v}_1^2 + \frac{1}{2} r_2 \vec{v}_2^2 = \vec{u}_1 \cdot \vec{k}_1 + \frac{1}{2} r_1 \vec{u}_1^2 .$$

By (3.32), it holds

$$r_2 = -r_1 .$$

Hence, using the constitutive equations for \vec{q} , see (4.159), and \vec{k}_1 , see (4.160), we arrive at

$$\begin{aligned} \rho w \frac{D_1 \varepsilon_1}{Dt} + \rho(1-w) \frac{D_2 \varepsilon_2}{Dt} &= \mathbf{T}_1 : \mathbf{D}_1 + \mathbf{T}_2 : \mathbf{D}_2 + \operatorname{div} (k \vec{g} + \lambda \vec{u}_1) - r_1 (\varepsilon_1 - \varepsilon_2) \\ &\quad + \vec{u}_1 \cdot (\xi \vec{g} + \nu \vec{u}_1 + \rho \omega \operatorname{grad} w) - \frac{1}{2} r_1 \vec{u}_1^2 . \end{aligned} \quad (4.169)$$

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 it numerically for a 2-D case with a simple geometry to study the role of particular processes involved. To achieve this aim, we 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 (4.163), since it is small compared to $\operatorname{div} \vec{v}_2$, and write

$$\frac{\partial w}{\partial t} + \operatorname{grad} w \cdot \vec{v}_2 - \operatorname{div} \vec{v}_2 = \frac{r_1}{\rho}. \quad (4.170)$$

The mass balance of water (4.165) will be kept unchanged

$$\operatorname{grad} w \cdot \vec{u}_1 + \operatorname{div} \vec{v}_2 + w \operatorname{div} \vec{u}_1 = 0. \quad (4.171)$$

4.7.3 Linear momentum balance

We start with the linear momentum balance for the water component (4.167):

$$\rho w \frac{D_1 \vec{v}_1}{Dt} = \operatorname{div} \mathbf{T}_1 + \rho w \vec{g}_F - \xi \vec{g} - \nu \vec{u}_1 - \rho w \operatorname{grad} w. \quad (4.172)$$

In the first approximation, we omit the inertia term on the left-hand side and the term $\operatorname{div}(w \hat{\mathbf{T}}_1)$ occurring in the expansion

$$\operatorname{div} \mathbf{T}_1 = \operatorname{div}(-pw \mathbf{1} + w \hat{\mathbf{T}}_1).$$

Hence, we arrive at

$$\nu \vec{u}_1 = -\operatorname{grad}(pw) - \xi \vec{g} - \rho w \operatorname{grad} w + \rho w \vec{g}_F \quad (4.173)$$

which may be interpreted as the equation for the diffusive water velocity \vec{u}_1 .

The linear momentum balance for the ice component (4.166) reads,

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

We again neglect the inertia term on the left-hand side and also the term $r_1 \vec{u}_1$, corresponding to linear-momentum change induced by the mass exchange between the components. We further expand \mathbf{T}_2 , according to (4.162):

$$\mathbf{T}_2 = -p(1-w) \mathbf{1} - \Pi_2 \mathbf{1} + \mathcal{B}(T) h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 + w \hat{\mathbf{T}}_2.$$

Since the constitutive functional for the thermodynamic pressure Π_2 is not known, we neglect Π_2 term and keep only the reaction pressure p . Following (Larson, [9]), we specify the constitutive functional \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, (4.174) becomes

$$\begin{aligned} \vec{0} &= \operatorname{grad}(pw) + \xi \vec{g} + \nu \vec{u}_1 + \rho w \operatorname{grad} w - \rho w \vec{g}_F \\ &\quad - \operatorname{grad} p + \operatorname{div}(\mathcal{B}(T, w) h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2) + \rho \vec{g}_F, \end{aligned}$$

which, due to (4.173), reads

$$\vec{0} = -\operatorname{grad} p + \operatorname{div}(\mathcal{B}(T, w) h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2) + \rho \vec{g}_F. \quad (4.175)$$

4.7.4 Energy balance

Let us recall the constitutive equations for free energy and entropy. By (4.157) and (4.158), we have

$$f_\alpha = \tilde{f}_\alpha(T) + w\hat{f}_\alpha(T), \quad (4.176)$$

$$s_\alpha = \tilde{s}_\alpha(T) + w\hat{s}_\alpha(T). \quad (4.177)$$

For the following derivations, it will be convenient to omit the terms $\hat{f}_\alpha, \hat{s}_\alpha$. This step can only be justified in view of the approach commonly applied in glaciology, that internal energy and entropy only depend on temperature. In fact, there is not any knowledge of possible dependencies on the omitted functions. Thus, we will consider

$$f_\alpha = f_\alpha(T), \quad (4.178)$$

$$s_\alpha = s_\alpha(T), \quad (4.179)$$

where we omitted the $\tilde{}$ label.

On the left-hand side of the equation (4.169), we neglect terms $\rho w \dot{\varepsilon}_1^1, \rho w \dot{\varepsilon}_2^2$, being small compared to $\rho \dot{\varepsilon}_2^2$. We expand

$$\begin{aligned} \mathbf{T}_1 : \mathbf{D}_1 + \mathbf{T}_2 : \mathbf{D}_2 &= (-pw\mathbf{1} + w\hat{\mathbf{T}}_1) : \mathbf{D}_1 + \left(-p(1-w)\mathbf{1} + \mathcal{B}(T, w)h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 \right) : \mathbf{D}_2 \\ &= -pw \operatorname{div} \vec{u}_1 - p \operatorname{div} \vec{v}_2 + w\hat{\mathbf{T}}_1 : \mathbf{D}_1 + \mathcal{B}(T, w)h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2, \end{aligned}$$

where we have already omitted the term $\Pi_2\mathbf{1}$ from the same reasons as before, and made use of

$$\overset{\circ}{\mathbf{D}}_2 : \mathbf{D}_2 = \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2,$$

which follows from the fact that the deviator $\overset{\circ}{\mathbf{D}}_2$ is traceless. Moreover, we will neglect the work $w\hat{\mathbf{T}}_1 : \mathbf{D}_1$ and the term corresponding to the kinetic energy changes $\frac{1}{2}r_1\vec{u}_1^2$. We will use (4.173) and write

$$\vec{u}_1 \cdot (\xi\vec{g} + \nu\vec{u}_1 + \rho\omega \operatorname{grad}w) = \vec{u}_1 \cdot (-\operatorname{grad}(pw) + \rho w\vec{g}_F).$$

The equation (4.169) becomes

$$\begin{aligned} \rho \frac{D_2\varepsilon_2}{Dt} &= -pw \operatorname{div} \vec{u}_1 - p \operatorname{div} \vec{v}_2 + \mathcal{B}(T, w)h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 + \operatorname{div}(k\vec{g} + \lambda\vec{u}_1) \\ &\quad - r_1(\varepsilon_1 - \varepsilon_2) + \vec{u}_1 \cdot (-\operatorname{grad}(pw) + \rho w\vec{g}_F). \end{aligned} \quad (4.180)$$

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,

$$T_M = T_M(p). \quad (4.181)$$

By (4.181), we implicitly assume that the mixture is close to the thermodynamic equilibrium, since relation (4.181) follows from the equilibrium analysis, namely from equality of chemical potentials. Strictly speaking, relation (4.181) 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 interpretation may justify the Clausius-Clapeyron relation, in (4.181) 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 mistake introduced by such an assumption, but, following (Hutter [4]), we expect it to be small.

As according to (3.74)

$$\varepsilon_\alpha = f_\alpha + T s_\alpha ,$$

and according to (4.178), (4.179),

$$\varepsilon_\alpha = \varepsilon_\alpha(T) , \quad (4.182)$$

we have

$$\frac{D_2\varepsilon_2}{Dt} = c_\rho \frac{D_2T_M(p)}{Dt} , \quad (4.183)$$

where we introduced

$$c_\rho = \frac{d\varepsilon_2}{dT} . \quad (4.184)$$

The energy balance (4.180) can now be rewritten as a constitutive relation for the water production term r_1

$$\begin{aligned} r_1(\varepsilon_1 - \varepsilon_2) = & - \operatorname{div}(pw\vec{u}_1) - p \operatorname{div}\vec{v}_2 + \mathcal{B}(T, w)h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 + \operatorname{div}(k\vec{g} + \lambda\vec{u}_1) \\ & - \rho c_\rho \frac{D_2T_M(p)}{Dt} + \rho w\vec{u}_1 \cdot \vec{g}_F . \end{aligned} \quad (4.185)$$

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 that, consider a system which contains ice mass m of volume V_2 , which melts to water of the same mass and volume V_1 . Let us 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 was during the process in thermodynamic equilibrium, the first law of thermodynamics (Kvasnica [12]) states that

$$[U] = T[S] - W ,$$

where

$$[U] = U_1 - U_2 , \quad [S] = S_1 - S_2 ,$$

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, which can be shown to be continuous across the surface of phase equilibrium (see (3.39) and note that in equilibrium the velocities and surface linear momenta production terms are equal to zero), and we thus arrive at

$$[U] = T[S] - p[V] ,$$

or dividing this equation by the mass m

$$[\varepsilon] = T[s] - p \left[\frac{1}{\tilde{\rho}} \right], \quad (4.186)$$

where ε is the internal energy density (related to mass),

$$T[s] = L \quad (4.187)$$

is the *specific latent heat of melting* and $\tilde{\rho}$ denotes the "material" density.

Thus under the simplifying assumptions (quasi-static melting, equilibrium pressure equal to the reaction stress), we arrive at

$$r_1 = \frac{1}{(L - p\Delta)} \left\{ \begin{aligned} & - \operatorname{div}(pw\vec{u}_1) - p \operatorname{div}\vec{v}_2 + \mathcal{B}(T, w)h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 + \operatorname{div}(k\vec{g} + \lambda\vec{u}_1) \\ & - \rho c_\rho \frac{D_2 T_M(p)}{Dt} + \rho w \vec{u}_1 \cdot \vec{g}_F \end{aligned} \right\}, \quad (4.188)$$

where we introduced

$$\Delta = \frac{1}{\tilde{\rho}_1} - \frac{1}{\tilde{\rho}_2}. \quad (4.189)$$

Chapter 5

The polythermal ice-sheet model

The aim of this chapter is to summarize the knowledge obtained so far, introducing the boundary and transition conditions and set up the description of a typical polythermal ice-sheet configuration as depicted in Fig. 2.1.

5.1 Field equations

5.1.1 Cold region

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

$$\operatorname{div} \vec{v} = 0, \quad (5.1)$$

$$\rho \dot{\vec{v}} = -\operatorname{grad} p + \operatorname{div} \overset{\circ}{\mathbf{T}} + \rho \vec{g}_F, \quad (5.2)$$

$$\rho \dot{\varepsilon} = \mathbf{T} : \mathbf{D} - \operatorname{div} \vec{q}, \quad (5.3)$$

with the constitutive relations

$$\mathbf{T} = -p\mathbf{1} + \overset{\circ}{\mathbf{T}}, \quad (5.4)$$

$$\varepsilon = c_V T, \quad (5.5)$$

$$\vec{q} = -k(T) \operatorname{grad} T, \quad (5.6)$$

$$\mathbf{D} = \mathcal{A}(T)f(\sigma) \overset{\circ}{\mathbf{T}}. \quad (5.7)$$

5.1.2 The temperate ice region

In the previous chapter, we arrived at the set of equations for the temperate ice-zone behaviour in the view the mixture theory. Namely, two *mass balance laws* (4.170), (4.171):

$$\frac{\partial w}{\partial t} + \operatorname{grad} w \cdot \vec{v}_2 - \operatorname{div} \vec{v}_2 = \frac{r_1}{\rho}, \quad (5.8)$$

$$\operatorname{grad} w \cdot \vec{u}_1 + \operatorname{div} \vec{v}_2 + w \operatorname{div} \vec{u}_1 = 0, \quad (5.9)$$

two *linear momentum balance laws* (4.173) and (4.175):

$$\nu \vec{u}_1 = -\text{grad}(pw) - \xi \vec{g} - \rho \omega \text{grad} w + \rho w \vec{g}_F \quad (5.10)$$

$$\vec{0} = -\text{grad} p + \text{div} \left(\mathcal{B}(T, w) h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 \right) + \rho \vec{g}_F, \quad (5.11)$$

and *the energy balance* (4.188)

$$r_1 = \frac{1}{(L - p\Delta)} \left\{ \begin{aligned} & - \text{div}(pw\vec{u}_1) - p \text{div}\vec{v}_2 + \mathcal{B}(T, w) h(\overset{\circ}{D}_{2II}) \overset{\circ}{\mathbf{D}}_2 : \overset{\circ}{\mathbf{D}}_2 + \text{div}(k\vec{g} + \lambda\vec{u}_1) \\ & - \rho c_\rho \frac{D_2 T_M(p)}{Dt} + \rho w \vec{u}_1 \cdot \vec{g}_F \end{aligned} \right\}. \quad (5.12)$$

5.2 Boundary and transition conditions

So far we have assumed the investigated quantities are continuous, mostly also differentiable. However, in the 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 the consequence of the balance laws. We will also arrange them to a form applicable in numerical computations. To complete the description, we have to add appropriate boundary conditions, both on the free surface (ice-air boundary) and at the base (ice-bedrock boundary). In all of the 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 be 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 physical processes at mixture boundaries.

5.2.1 Free surface

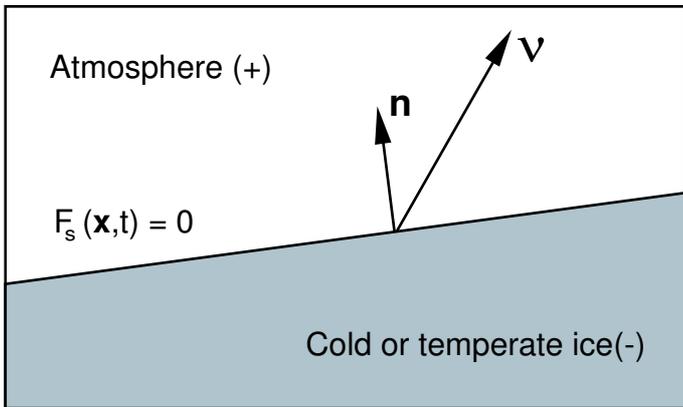


Figure 5.1: Free surface geometry.

Free surface is a cold or temperate-ice – air boundary. The two cases differ according to the processes that take place at the surface. At the *cold-ice – air boundary* accumulation of the ice component due to snowfalls may occur, as well as ablation. At the *temperate-ice – air boundary* we may, in addition, expect melting or refreezing of the meltwater. Due to these processes, a free surface is generally not material and therefore *kinematic conditions* have to 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

$$F_S(\vec{x}, t) = 0 \quad (5.13)$$

for a certain function F_S . Let

$$\mathcal{S}_t = \{\vec{x} \in E^3 : F_S(\vec{x}, t) = 0\}$$

be the free surface at time t . Let us assume that there exist a one-parametric one-to-one mapping

$$\chi_S : \mathcal{S}_0 \times E \longrightarrow \mathcal{S}_t ,$$

such that for any $\vec{x} \in \mathcal{S}_t$ there exists $\vec{x}_0 \in \mathcal{S}_0$ that

$$\vec{x} = \chi_S(\vec{x}_0, t) .$$

Then we can define the *surface velocity* \vec{v} (the mapping is assumed to be sufficiently smooth) by

$$\vec{v} = \left. \frac{\partial \chi_S(\vec{x}_0, t)}{\partial t} \right|_{\vec{x}_0} . \quad (5.14)$$

The time derivative at constant \vec{x}_0 of the implicit equation (5.13) then yields

$$\frac{\partial F_S}{\partial t} + \vec{v} \cdot \text{grad} F_S = 0 , \quad (5.15)$$

which is the evolution equation for the free surface. It might be convenient to rewrite this equation as

$$\frac{\partial F_S}{\partial t} + \vec{v}_2^- \cdot \text{grad} F_S = (\vec{v}_2^- - \vec{v}) \cdot \text{grad} F_S , \quad (5.16)$$

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} :

$$\vec{n}(\vec{x}, t) = \frac{\text{grad} F_S(\vec{x}, t)}{\|\text{grad} F_S(\vec{x}, t)\|} , \quad \vec{x} \in \mathcal{S}_t , \quad (5.17)$$

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

$$\frac{\partial F_S}{\partial t} + \vec{v}_2^- \cdot \text{grad} F_S = (\vec{v}_2^- - \vec{v}) \cdot \vec{n} \|\text{grad} F_S\| . \quad (5.18)$$

The evolution equation (5.15) represents a *kinematic* constraint for the free surface. Apart from that, the analysis of the balance laws yields a set of *dynamic constraints*.

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 will assume that air at the negative side of the free surface (in glacier) is highly diluted, and its density is sufficiently small that it cannot affect the behaviour of the ice-water mixture. To express that, we will here and henceforth adopt the following notation

$$\rho_3^- \rightarrow 0. \quad (5.19)$$

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 in the atmosphere, are assumed to be small, 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 $\rho_1^- \rightarrow 0$ (water is not present in 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

$$[\rho_\alpha(\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} = r_\alpha^s, \quad \sum_{\alpha=1}^n r_\alpha^s = 0. \quad (5.20)$$

At the free surface we further assume that there is not surface air production,

$$r_3^s \equiv 0. \quad (5.21)$$

Eq. (5.20) then implies that

$$r_1^s = -r_2^s, \quad (5.22)$$

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

$$[\rho_2(\vec{v}_2 - \vec{v})]_-^+ \cdot \vec{n} = r_2^s. \quad (5.23)$$

The term $\rho_2^+(\vec{v}_2 - \vec{v})^+ \cdot \vec{n}$, means the mass influx or outflow of ice through the free surface from 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 ablation-accumulation function* (positive for ablation):

$$a_{2\perp}^s = \rho_2^+(\vec{v}_2^+ - \vec{v}) \cdot \vec{n}. \quad (5.24)$$

With (5.24), equation (5.23) becomes

$$\rho_2^-(\vec{v}_2^- - \vec{v}) \cdot \vec{n} = a_{2\perp}^s - r_2^s, \quad (5.25)$$

or expressed in terms of the water content w and ice-water mixture density ρ , we have

$$(1 - w^-)(\vec{v}_2^- - \vec{v}) \cdot \vec{n} = \frac{a_{2\perp}^s - r_2^s}{\rho}. \quad (5.26)$$

The water component

The jump condition (5.20) for water ($\alpha = 1$) reads:

$$[\rho_1(\vec{v}_1 - \vec{v})]_{-}^{+} \cdot \vec{n} = r_1^s. \quad (5.27)$$

Introducing the *free-surface water accumulation function* by $a_{1\perp}^s$:

$$a_{1\perp}^s = \rho_1^+(\vec{v}_1^+ - \vec{v}) \cdot \vec{n}. \quad (5.28)$$

Equation (5.27) becomes

$$\rho_1^-(\vec{v}_1^- - \vec{v}) \cdot \vec{n} = a_{1\perp}^s - r_1^s. \quad (5.29)$$

In the following, we put

$$a_{1\perp}^s = r_1^s, \quad (5.30)$$

which means that all the water outflow to the atmosphere comes from the ice melted at the free surface. In other words evaporation or liquid precipitation is not considered. In view of (5.30), eq. (5.27) reads

$$\rho_1^-(\vec{v}_1^- - \vec{v}) \cdot \vec{n} = 0, \quad (5.31)$$

or, equivalently,

$$\rho w^-(\vec{v}_2^- - \vec{v}) \cdot \vec{n} + \rho w^- \vec{u}_1^- \cdot \vec{n} = 0.$$

Substituting for $(\vec{v}_2^- - \vec{v}) \cdot \vec{n}$ from (5.26), we find

$$w^- \frac{a_{2\perp}^s - r_2^s}{1 - w^-} + \rho w^- \vec{u}_1^- \cdot \vec{n} = 0. \quad (5.32)$$

Provided that $w^- \neq 0$ (only possible at the temperate-ice – air boundary), we obtain

$$\vec{u}_1^- \cdot \vec{n} = \frac{r_2^s - a_{2\perp}^s}{\rho(1 - w^-)}. \quad (5.33)$$

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

$$\rho_3^-(\vec{v}_3^- - \vec{v}) \cdot \vec{n} = 0, \quad (5.34)$$

we obtain

$$\rho_3^+(\vec{v}_3^+ - \vec{v}) \cdot \vec{n} = 0. \quad (5.35)$$

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 $r_1^s = r_2^s = 0$, i.e. there is no surface melting or refreezing (the ice is below melting temperature), and also $\rho_1^- \rightarrow 0$, i.e. $w^- \rightarrow 0$. Then the mass balance for *the ice component* (5.26) reads

$$(\vec{v}_2^- - \vec{v}) \cdot \vec{n} = \frac{a_\perp^s}{\rho}, \quad (5.36)$$

mass balance for *the water component* (5.27) concerning (5.30) is satisfied identically, and for *the air component* (5.34) and (5.35) remain unaltered.

Linear momentum jump conditions

The general form of these conditions follows from (3.39) and (3.43):

$$[\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} = -\vec{f}_\alpha^s, \quad \sum_{\alpha=1}^n \vec{f}_\alpha^s = \vec{0}. \quad (5.37)$$

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:

$$\sum_{\alpha=1}^n [\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} = \vec{0}.$$

Since the accumulation velocities at the free surface are small, we neglect the terms $[\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n}$, corresponding to the linear momentum jumps across the free surface. We arrive at

$$[\mathbf{T}_1 + \mathbf{T}_2 + \mathbf{T}_3]_-^+ \cdot \vec{n} = 0, \quad (5.38)$$

Additionally, we will assume

$$\mathbf{T}_3^- = \mathbf{0}, \quad (5.39)$$

since air is not considered to be present in the glacier. Likewise, for a *cold-ice – air boundary*, we assume

$$\mathbf{T}_1^- = \mathbf{0}. \quad (5.40)$$

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,

$$[T]_-^+ = 0. \quad (5.41)$$

The energy jump condition for a mixture (3.64) is

$$\left[\sum_{\alpha=1}^n \left\{ \rho_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) (\vec{v}_\alpha - \vec{v}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha \right\} + \vec{q} \right]_-^+ \cdot \vec{n} = 0.$$

For our case $n = 3$:

$$0 = \left[\rho_1 \left(\varepsilon_1 + \frac{1}{2} \vec{v}_1^2 \right) (\vec{v}_1 - \vec{v}) + \rho_2 \left(\varepsilon_2 + \frac{1}{2} \vec{v}_2^2 \right) (\vec{v}_2 - \vec{v}) + \rho_3 \left(\varepsilon_3 + \frac{1}{2} \vec{v}_3^2 \right) (\vec{v}_3 - \vec{v}) - \vec{v}_1 \cdot \mathbf{T}_1 - \vec{v}_2 \cdot \mathbf{T}_2 - \vec{v}_3 \cdot \mathbf{T}_3 + \vec{q} \right]_{-}^{+} \cdot \vec{n}. \quad (5.42)$$

Since the accumulation velocities at the free surface are small, we neglect $\frac{1}{2}(\rho_1 \vec{v}_1^2)^{\pm}$, $\frac{1}{2}(\rho_2 \vec{v}_2^2)^{\pm}$, $\frac{1}{2}(\rho_3 \vec{v}_3^2)^{\pm}$, which describe the jump in kinetic energies. Moreover, ε_1 and ε_2 are functions of temperature only (see (4.182)) and the temperature is continuous across the surface, which implies continuity of ε_1 , ε_2 across the free surface, and (5.42) reads:

$$0 = \varepsilon_1 [\rho_1 (\vec{v}_1 - \vec{v})]_{-}^{+} \cdot \vec{n} + \varepsilon_2 [\rho_2 (\vec{v}_2 - \vec{v})]_{-}^{+} \cdot \vec{n} + [\varepsilon_3 \rho_3 (\vec{v}_3 - \vec{v})]_{-}^{+} \cdot \vec{n} - [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + \vec{v}_3 \cdot \mathbf{T}_3]_{-}^{+} \cdot \vec{n} + [\vec{q}]_{-}^{+} \cdot \vec{n}.$$

Using (5.22), (5.23), (5.27), (5.34) and (5.35), we find:

$$0 = r_2^s (\varepsilon_2 - \varepsilon_1) - [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + \vec{v}_3 \cdot \mathbf{T}_3]_{-}^{+} \cdot \vec{n} + [\vec{q}]_{-}^{+} \cdot \vec{n}. \quad (5.43)$$

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 (+) or (-) side). In view of this interpretation, we can put

$$\vec{v}_3^{-} \cdot \mathbf{T}_3^{-} \cdot \vec{n} = 0, \quad (5.44)$$

keeping in mind the assumption that the air is not present at the negative side of the surface, in the glacier.

In the special case of a *cold-ice - air surface*, in addition to the above conditions, it holds $\vec{v}_1^{-} \cdot \mathbf{T}_1^{-} \cdot \vec{n} = 0$. Moreover, the surface production terms r_1^s and r_2^s vanish (ice is below melting temperature).

Entropy jump condition

The general condition (3.72) at the singular surface is

$$0 \leq \left[\sum_{\alpha=1}^n \rho_{\alpha} s_{\alpha} (\vec{v}_{\alpha} - \vec{v}) + \frac{\vec{q}}{T} \right]_{-}^{+} \cdot \vec{n}.$$

In accordance with Hutter [4], we further assume that the total surface entropy production at the singular surface is equal to zero:

$$0 = \left[\rho_1 s_1 (\vec{v}_1 - \vec{v}) + \rho_2 s_2 (\vec{v}_2 - \vec{v}) + \rho_3 s_3 (\vec{v}_3 - \vec{v}) + \frac{\vec{q}}{T} \right]_{-}^{+} \cdot \vec{n}. \quad (5.45)$$

Since s_1 and s_1 are again continuous across the free surface, being functions of T only (see (4.179)), we obtain:

$$0 = s_1 [\rho_1 (\vec{v}_1 - \vec{v})]_{-}^{+} \cdot \vec{n} + s_2 [\rho_2 (\vec{v}_2 - \vec{v})]_{-}^{+} \cdot \vec{n} + [s_3 \rho_3 (\vec{v}_3 - \vec{v})]_{-}^{+} \cdot \vec{n} + \left[\frac{\vec{q}}{T} \right]_{-}^{+} \cdot \vec{n}.$$

Using (5.22), (5.23), (5.27), (5.34) and (5.35), we finally have

$$0 = r_2^s T(s_2 - s_1) + [\vec{q}]_-^+ \cdot \vec{n}. \quad (5.46)$$

For a *cold-ice – air* surface, at which $r_1^s = r_2^s = 0$, this condition reduces to

$$0 = [\vec{q}]_-^+ \cdot \vec{n}, \quad (5.47)$$

that is the normal component of the heat flux is continuous across the cold-ice – air surface.

5.2.2 Ice-bedrock interface

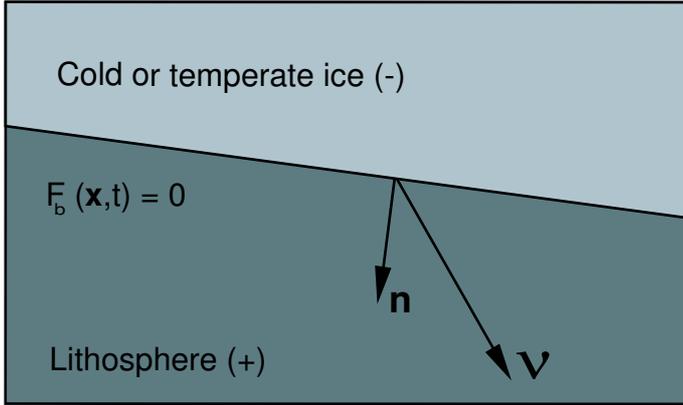


Figure 5.2: Ice-bedrock boundary.

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

$$\rho_2^+ \rightarrow 0, \quad \rho_3^- \rightarrow 0, \quad (5.48)$$

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 the temperate ice at one side, the case with cold ice can be obtained by considering $\rho_1^- \rightarrow 0$.

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{v} is again well defined.

The dynamic constraints are derived from the balance as follows.

Mass jump condition

The mass jump conditions (3.28) and (3.32) are:

$$[\rho_\alpha(\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} = r_\alpha^b, \quad \sum_{\alpha=1}^n r_\alpha^b = 0. \quad (5.49)$$

We assume that the bedrock material is not produced at ice-bedrock interface, that is

$$r_3^b \equiv 0 . \quad (5.50)$$

Thus, (5.49) yields

$$r_1^b = -r_2^b , \quad (5.51)$$

where the surface production terms r_1^b, r_2^b , describe the mass exchange between ice and water, caused by melting of ice or refreezing of water at the ice-bedrock interface.

Ice component

The general jump condition (5.49) for $\alpha = 2$ reads

$$[\rho_2(\vec{v}_2 - \vec{v})]_{-}^{+} \cdot \vec{n} = r_2^b . \quad (5.52)$$

We will consider the bedrock is impermeable for ice, thus

$$\rho_2^{+}(\vec{v}_2^{+} - \vec{v}) \cdot \vec{n} = 0 . \quad (5.53)$$

Hence it holds

$$\rho_2^{-}(\vec{v}_2^{-} - \vec{v}) \cdot \vec{n} = -r_2^b , \quad (5.54)$$

or,

$$\rho(1 - w^{-})(\vec{v}_2^{-} - \vec{v}) \cdot \vec{n} = -r_2^b . \quad (5.55)$$

Water component

The jump condition (5.49) for the water component ($\alpha = 1$) reads

$$[\rho_1(\vec{v}_1 - \vec{v})]_{-}^{+} \cdot \vec{n} = r_1^b \quad (5.56)$$

We define function

$$o_{1\perp}^b = \rho_1^{+}(\vec{v}_1^{+} - \vec{v}) \cdot \vec{n} , \quad (5.57)$$

that describes the outflow (inflow) of water from the glacier to the bedrock. Inspecting (5.51), eq. (5.56) becomes

$$\rho_1^{-}(\vec{v}_1^{-} - \vec{v}) \cdot \vec{n} = o_{1\perp}^b + r_2^b , \quad (5.58)$$

or, equivalently,

$$\rho w^{-}(\vec{v}_2^{-} - \vec{v}) \cdot \vec{n} + \rho w^{-} \vec{u}_1^{-} \cdot \vec{n} = o_{1\perp}^b + r_2^b . \quad (5.59)$$

Using (5.55), we get

$$\begin{aligned} -r_2^b \frac{w^{-}}{1 - w^{-}} + \rho w^{-} \vec{u}_1^{-} \cdot \vec{n} &= o_{1\perp}^b + r_2^b , \\ \rho w^{-} \vec{u}_1^{-} \cdot \vec{n} &= o_{1\perp}^b + \frac{r_2^b}{1 - w^{-}} . \end{aligned} \quad (5.60)$$

Bedrock-material component

The mass jump condition (5.49) the bedrock-material component ($\alpha = 3$) reads

$$[\rho_3(\vec{v}_3 - \vec{v})]_{-}^+ \cdot \vec{n} = 0 . \quad (5.61)$$

The bedrock-material does not penetrate to the glacier, hence

$$\rho_3^-(\vec{v}_3^- - \vec{v}) \cdot \vec{n} = 0 . \quad (5.62)$$

Thus (5.61) yields

$$\rho_3^+(\vec{v}_3^+ - \vec{v}) \cdot \vec{n} = 0 . \quad (5.63)$$

Here again we summarize the above results for the special case of *the cold-ice – bedrock boundary*, where, in addition, $\rho_1^- \rightarrow 0$, and $r_1^b = r_2^b = 0$, since the ice temperature is lower than its melting point. The mass balance for *the ice component* (5.54) reduces to

$$\rho(\vec{v}_2^- - \vec{v}) \cdot \vec{n} = 0 . \quad (5.64)$$

The mass balance (5.60) for *the water component* simplifies to

$$o_{1\perp}^b = 0 . \quad (5.65)$$

The mass balance (5.63) 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* $\vec{t}_{2\parallel}^-$. The sliding velocity is defined as the tangential velocity of ice relative to the bedrock:

$$\vec{v}_{2sl} = \vec{v}_{2\parallel}^- - \vec{v}_{3\parallel}^+ , \quad (5.66)$$

where

$$\vec{v}_{\alpha\parallel}^{\pm} = \vec{v}_{\alpha}^{\pm} - \vec{n}(\vec{v}_{\alpha}^{\pm} \cdot \vec{n}) .$$

The basal shear stress is defined as

$$\vec{t}_{2\parallel}^- = \mathbf{T}_2^- \cdot \vec{n} - \vec{n}(\vec{n} \cdot \mathbf{T}_2^- \cdot \vec{n}) .$$

The sliding law has then the form

$$\vec{v}_{2sl} = -C(\vec{n} \cdot \mathbf{T}_2^- \cdot \vec{n}, \dots) \vec{t}_{2\parallel}^- . \quad (5.67)$$

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 (see Greve [6]).

Linear momentum jump conditions

The situation is analogous to the free surface, so we discuss it briefly. The linear momentum jump conditions (3.39) and (3.43) read:

$$[\mathbf{T}_{\alpha} - \rho_{\alpha} \vec{v}_{\alpha} \otimes (\vec{v}_{\alpha} - \vec{v})]_{-}^+ \cdot \vec{n} = -\vec{f}_{\alpha}^b , \quad \sum_{\alpha=1}^n \vec{f}_{\alpha}^b = \vec{0} . \quad (5.68)$$

We will again make use of only the linear momentum jump condition for the mixture as a whole:

$$\sum_{\alpha=1}^n [\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_{-}^{\pm} \cdot \vec{n} = \vec{0}. \quad (5.69)$$

We neglect the terms with $[\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_{-}^{\pm} \cdot \vec{n}$, that correspond to the linear momentum jumps across the free surface since they are assumed to be small:

$$[\mathbf{T}_1 + \mathbf{T}_2 + \mathbf{T}_3]_{-}^{\pm} \cdot \vec{n} = 0.$$

In view of the density limits (5.48):

$$\mathbf{T}_2^+ = \mathbf{T}_3^- = \mathbf{0}, \quad (5.70)$$

and the linear momentum jump condition reads:

$$(\mathbf{T}_3^+ + \mathbf{T}_1^+) \cdot \vec{n} = (\mathbf{T}_1^- + \mathbf{T}_2^-) \cdot \vec{n}. \quad (5.71)$$

Energy jump condition

Analogously to the free surface, the temperature is considered continuous across ice-bedrock interface:

$$[T]_{-}^{\pm} = 0. \quad (5.72)$$

The general energy jump condition for the mixture (3.64) are

$$0 = \left[\sum_{\alpha=1}^n \left\{ \rho_\alpha \left(\varepsilon_\alpha + \frac{1}{2} \vec{v}_\alpha^2 \right) (\vec{v}_\alpha - \vec{v}) - \vec{v}_\alpha \cdot \mathbf{T}_\alpha \right\} + \vec{q} \right]_{-}^{\pm} \cdot \vec{n}.$$

For a 3-component mixture:

$$\begin{aligned} 0 &= \left[\rho_1 \left(\varepsilon_1 + \frac{1}{2} \vec{v}_1^2 \right) (\vec{v}_1 - \vec{v}) + \rho_2 \left(\varepsilon_2 + \frac{1}{2} \vec{v}_2^2 \right) (\vec{v}_2 - \vec{v}) + \rho_3 \left(\varepsilon_3 + \frac{1}{2} \vec{v}_3^2 \right) (\vec{v}_3 - \vec{v}) \right. \\ &\quad \left. - \vec{v}_1 \cdot \mathbf{T}_1 - \vec{v}_2 \cdot \mathbf{T}_2 - \vec{v}_3 \cdot \mathbf{T}_3 + \vec{q} \right]_{-}^{\pm} \cdot \vec{n}. \end{aligned}$$

We omit the terms $\frac{1}{2}(\rho_1 \vec{v}_1^2)_{-}^{\pm}$, $\frac{1}{2}(\rho_2 \vec{v}_2^2)_{-}^{\pm}$, $\frac{1}{2}(\rho_3 \vec{v}_3^2)_{-}^{\pm}$, describing jumps in kinetic energies, and since ε_1 and ε_2 are continuous being functions of temperature only, we obtain

$$\begin{aligned} 0 &= \varepsilon_1 [\rho_1 (\vec{v}_1 - \vec{v})]_{-}^{\pm} \cdot \vec{n} + \varepsilon_2 [\rho_2 (\vec{v}_2 - \vec{v})]_{-}^{\pm} \cdot \vec{n} + [\varepsilon_3 \rho_3 (\vec{v}_3 - \vec{v})]_{-}^{\pm} \cdot \vec{n} \\ &\quad - [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + \vec{v}_3 \cdot \mathbf{T}_3]_{-}^{\pm} \cdot \vec{n} + [\vec{q}]_{-}^{\pm} \cdot \vec{n}. \end{aligned}$$

Using (5.51), (5.52), (5.56), (5.62) and (5.63):

$$0 = r_2^b (\varepsilon_2 - \varepsilon_1) - [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + \vec{v}_3 \cdot \mathbf{T}_3]_{-}^{\pm} \cdot \vec{n} + [\vec{q}]_{-}^{\pm} \cdot \vec{n}. \quad (5.73)$$

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 ice-bedrock interface are highly diluted. As a result, we have

$$0 = r_2^b(\varepsilon_2 - \varepsilon_1) + \vec{v}_1^- \cdot \mathbf{T}_1^- \cdot \vec{n} + \vec{v}_2^- \cdot \mathbf{T}_2^- \cdot \vec{n} - \vec{v}_3^+ \cdot \mathbf{T}_3^+ \cdot \vec{n} - \vec{v}_1^+ \cdot \mathbf{T}_1^+ \cdot \vec{n} + [\vec{q}]_-^+ \cdot \vec{n}. \quad (5.74)$$

The special case of cold ice–bedrock interface follows the same procedure, but assuming $\vec{v}_1^- \cdot \mathbf{T}_1^- \cdot \vec{n} = 0$, and putting the surface mass production terms equal to zero, $r_1^b = r_2^b = 0$. Since no melting or refreezing then occurs and the energy jump condition reduces to:

$$0 = \vec{v}_2^- \cdot \mathbf{T}_2^- \cdot \vec{n} - \vec{v}_3^+ \cdot \mathbf{T}_3^+ \cdot \vec{n} - \vec{v}_1^+ \cdot \mathbf{T}_1^+ \cdot \vec{n} + [\vec{q}]_-^+ \cdot \vec{n}. \quad (5.75)$$

Entropy jump condition

From (3.72), we have

$$0 \leq \left[\sum_{\alpha=1}^n \rho_\alpha s_\alpha (\vec{v}_\alpha - \vec{v}) + \frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n}.$$

We assume that the total surface entropy production at the singular surface is zero (Hutter [4]):

$$0 = \left[\rho_1 s_1 (\vec{v}_1 - \vec{v}) + \rho_2 s_2 (\vec{v}_2 - \vec{v}) + \rho_3 s_3 (\vec{v}_3 - \vec{v}) + \frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n}. \quad (5.76)$$

Since T is continuous, so are s_1, s_2 , being functions of T only (see (4.179)). Thus it holds

$$0 = s_1 [\rho_1 (\vec{v}_1 - \vec{v})]_-^+ \cdot \vec{n} + s_2 [\rho_2 (\vec{v}_2 - \vec{v})]_-^+ \cdot \vec{n} + [s_3 \rho_3 (\vec{v}_3 - \vec{v})]_-^+ \cdot \vec{n} + \left[\frac{\vec{q}}{T} \right]_-^+ \cdot \vec{n},$$

and finally using (5.51), (5.52), (5.56), (5.62) and (5.63), we find

$$0 = r_2^b T (s_2 - s_1) + [\vec{q}]_-^+ \cdot \vec{n}. \quad (5.77)$$

In the special case of *the cold-ice–bedrock* surface, we additionally assume $r_1^b = r_2^b = 0$, since the ice temperature is lower than the melting temperature and, therefore, no melting or refreezing occurs. We obtain:

$$0 = [\vec{q}]_-^+ \cdot \vec{n}, \quad (5.78)$$

that is, the normal component of heat flux is continuous across the cold-ice – bedrock interface.

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. At the CTS, 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:

$$\rho_1^+ \rightarrow 0. \quad (5.79)$$

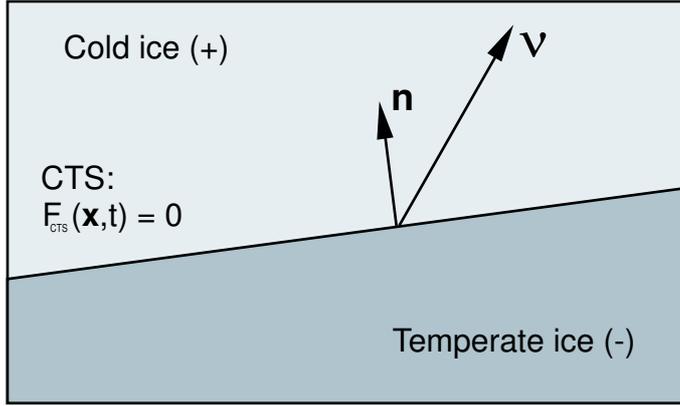


Figure 5.3: Cold-temperate ice transition surface geometry.

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{v} is defined, the evolution equation for the CTS is

$$\frac{\partial F_{CTS}}{\partial t} + \vec{v}_2^+ \cdot \text{grad} F_{CTS} = (\vec{v}_2^+ - \vec{v}) \cdot \vec{n} \|\text{grad} F_{CTS}\|, \quad (5.80)$$

where

$$\vec{n}(\vec{x}, t) = \frac{\text{grad} F_{CTS}(\vec{x}, t)}{\|\text{grad} F_{CTS}(\vec{x}, t)\|}, \quad \vec{x} \in \text{CTS}, \quad (5.81)$$

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 density jump conditions (3.28) and (3.32) read

$$[\rho_\alpha(\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} = r_\alpha^{cts}, \quad \sum_{\alpha=1}^n r_\alpha^{cts} = 0. \quad (5.82)$$

For the 2-component ice-water mixture:

$$r_1^{cts} = -r_2^{cts}. \quad (5.83)$$

The surface production terms r_1^{cts}, r_2^{cts} , describe the mass exchange between the ice and water component, i.e. melting of ice or refreezing of water at the CTS.

The ice component

The jump condition (5.82) for the ice component ($\alpha = 2$) implies

$$[\rho_2(\vec{v}_2 - \vec{v})]_-^+ \cdot \vec{n} = r_2^{cts}. \quad (5.84)$$

Introducing the *ablation-accumulation function*

$$a_{2\perp}^{cts} = \rho_2^+(\vec{v}_2^+ - \vec{v}) \cdot \vec{n}, \quad (5.85)$$

which represents the ice mass inflow (outflow) to the cold-ice zone, we arrive at

$$\rho_2^- (\vec{v}_2^- - \vec{v}) \cdot \vec{n} = a_{2\perp}^{cts} - r_2^{cts}. \quad (5.86)$$

In terms of the water content w , and the ice-water mixture density ρ :

$$(1 - w^-) (\vec{v}_2^- - \vec{v}) \cdot \vec{n} = \frac{a_{2\perp}^{cts} - r_2^{cts}}{\rho}. \quad (5.87)$$

The water component

The jump condition (5.82) for the water component ($\alpha = 1$) reads

$$[\rho_1 (\vec{v}_1 - \vec{v})]_-^+ \cdot \vec{n} = r_1^{cts}. \quad (5.88)$$

We have

$$\rho_1^+ (\vec{v}_1^+ - \vec{v}) \cdot \vec{n} = 0,$$

since there is no meltwater in the cold-ice zone. By this and (5.83), we conclude that

$$\rho_1^- (\vec{v}_1^- - \vec{v}) \cdot \vec{n} = r_2^{cts}, \quad (5.89)$$

or,

$$\rho w^- (\vec{v}_2^- - \vec{v}) \cdot \vec{n} + \rho w^- \vec{u}_1^- \cdot \vec{n} = r_2^{cts},$$

which, in view of (5.87) may be written as

$$w^- \frac{a_{2\perp}^{cts} - r_2^{cts}}{1 - w^-} + \rho w^- \vec{u}_1^- \cdot \vec{n} = r_2^{cts},$$

or,

$$\rho w^- \vec{u}_1^- \cdot \vec{n} = \frac{r_2^{cts} - w^- a_{2\perp}^{cts}}{1 - w^-}. \quad (5.90)$$

Linear momentum jump conditions

The linear momentum jump condition at the CTS follows from (3.39) and (3.43):

$$[\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} = -\vec{f}_\alpha^{cts}, \quad \sum_{\alpha=1}^n \vec{f}_\alpha^{cts} = \vec{0}. \quad (5.91)$$

We again use only the linear momentum jump condition for the mixture as a whole:

$$\sum_{\alpha=1}^n [\mathbf{T}_\alpha - \rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n} = \vec{0}. \quad (5.92)$$

Neglecting the terms $[\rho_\alpha \vec{v}_\alpha \otimes (\vec{v}_\alpha - \vec{v})]_-^+ \cdot \vec{n}$, corresponding to the linear momentum jumps across the CTS, which are considered to be small, we arrive at

$$[\mathbf{T}_1 + \mathbf{T}_2]_-^+ \cdot \vec{n} = 0. \quad (5.93)$$

According to (5.79), we assume:

$$\mathbf{T}_1^+ = \mathbf{0} .$$

Hence, we obtain

$$\mathbf{T}_2^+ \cdot \vec{n} = (\mathbf{T}_1^- + \mathbf{T}_2^-) \cdot \vec{n} . \quad (5.94)$$

Energy jump condition

The temperature is considered to be continuous across the CTS:

$$[T]_{-}^{+} = 0 . \quad (5.95)$$

The general energy jump condition (3.64) for the mixture reads:

$$0 = \sum_{\alpha=1}^n \left[\rho_{\alpha} (\varepsilon_{\alpha} + \frac{1}{2} \vec{v}_{\alpha}^2) (\vec{v}_{\alpha} - \vec{v}) - \vec{v}_{\alpha} \cdot \mathbf{T}_{\alpha} + \vec{q}_{\alpha} \right]_{-}^{+} \cdot \vec{n} .$$

In our particular case $n = 2$:

$$\begin{aligned} 0 &= \left[\rho_1 \left(\varepsilon_1 + \frac{1}{2} \vec{v}_1^2 \right) (\vec{v}_1 - \vec{v}) + \rho_2 \left(\varepsilon_2 + \frac{1}{2} \vec{v}_2^2 \right) (\vec{v}_2 - \vec{v}) \right. \\ &\quad \left. - \vec{v}_1 \cdot \mathbf{T}_1 - \vec{v}_2 \cdot \mathbf{T}_2 + \vec{q} \right]_{-}^{+} \cdot \vec{n} . \end{aligned}$$

We omit $\frac{1}{2}(\rho_1 \vec{v}_1^2)_{-}^{\pm}$, $\frac{1}{2}(\rho_2 \vec{v}_2^2)_{-}^{\pm}$, describing the jump in kinetic energies, since they are small. Moreover ε_1 and ε_2 are continuous across the CTS, being functions of temperature only, then

$$\begin{aligned} 0 &= \varepsilon_1 [\rho_1 (\vec{v}_1 - \vec{v})]_{-}^{+} \cdot \vec{n} + \varepsilon_2 [\rho_2 (\vec{v}_2 - \vec{v})]_{-}^{+} \cdot \vec{n} \\ &\quad - [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2 + [\vec{q}]_{-}^{+} \cdot \vec{n} . \end{aligned}$$

Using (5.83), (5.84) and (5.88):

$$0 = r_2^{cts} (\varepsilon_2 - \varepsilon_1) - [\vec{v}_1 \cdot \mathbf{T}_1 + \vec{v}_2 \cdot \mathbf{T}_2]_{-}^{+} \cdot \vec{n} + [\vec{q}]_{-}^{+} \cdot \vec{n} . \quad (5.96)$$

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 we have

$$0 = r_2^{cts} (\varepsilon_2 - \varepsilon_1) + \vec{v}_1^- \cdot \mathbf{T}_1^- \cdot \vec{n} + \vec{v}_2^- \cdot \mathbf{T}_2^- \cdot \vec{n} - \vec{v}_2^+ \cdot \mathbf{T}_2^+ \cdot \vec{n} + [\vec{q}]_{-}^{+} \cdot \vec{n} . \quad (5.97)$$

Entropy jump condition

The general entropy jump condition (3.72) reads:

$$0 \leq \left[\sum_{\alpha=1}^n \rho_{\alpha} s_{\alpha} (\vec{v}_{\alpha} - \vec{v}) + \frac{\vec{q}}{T} \right]_{-}^{+} \cdot \vec{n} .$$

As for the free surface or the ice-bedrock boundary, we assume the total surface entropy production at the singular surface to be zero (Hutter [4]), thus:

$$0 = \left[\rho_1 s_1 (\vec{v}_1 - \vec{v}) + \rho_2 s_2 (\vec{v}_2 - \vec{v}) + \frac{\vec{q}}{T} \right]_{-}^{+} \cdot \vec{n} . \quad (5.98)$$

Temperature T is continuous across the CTS, which implies continuity of s_1 and s_2 , since they are functions of T only (according to (4.179)). Then

$$0 = s_1 [\rho_1 (\vec{v}_1 - \vec{v})]_{-}^{+} \cdot \vec{n} + s_2 [\rho_2 (\vec{v}_2 - \vec{v})]_{-}^{+} \cdot \vec{n} + \left[\frac{\vec{q}}{T} \right]_{-}^{+} \cdot \vec{n} ,$$

and finally using (5.83), (5.84) and (5.88), we find

$$0 = r_2^{cts} T (s_2 - s_1) + [\vec{q}]_{-}^{+} \cdot \vec{n} . \quad (5.99)$$

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 study of the differences in physical behaviour in the present and the traditional formulation, outlined in the second chapter. However numerical problems with connecting the two solutions, in the cold zone with the solution in the temperate zone at the CTS, prevented us from reaching this goal. The main difficulty is the fact that the CTS interface is a free surface, which position must be determined too. If, in addition, the nonlinearity of the field equations and the uncertainty of several material parameters and boundary conditions are considered, the resulting problem is numerically ill-conditioned. We, therefore confined ourselves and numerically solved 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, the uniformity in x -direction:

$$\frac{\partial}{\partial x}(\cdot) = 0 . \quad (6.1)$$

- Steady-state configuration:

$$\frac{\partial}{\partial t}(\cdot) = 0 . \quad (6.2)$$

- Neglect of the pressure dependence of the melting point of ice,

$$T_M \equiv 0^\circ\text{C} . \tag{6.3}$$

- Parameter values:

$$\begin{aligned} \rho &= 910 \text{ kg m}^{-3}, \quad k = 2.1 \text{ W m}^{-1} \text{ K}^{-1}, \quad c_V = 2009 \text{ J kg}^{-1} \text{ K}^{-1}, \quad L = 335 \text{ kJ kg}^{-1}, \\ g_F &= 9.81 \text{ m s}^{-2}. \end{aligned}$$

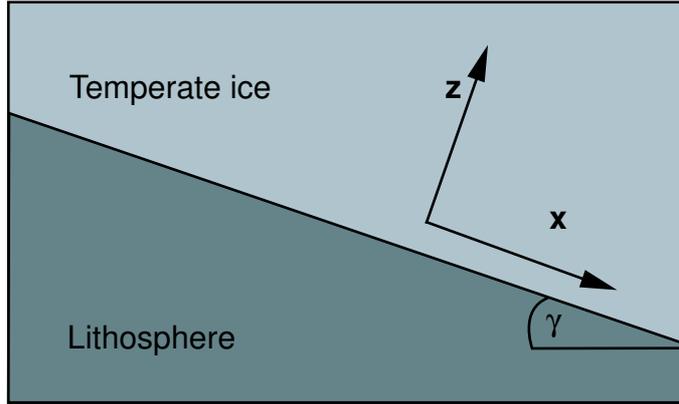


Figure 6.1: Inclined temperate-ice layer – the coordinate system.

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 $\rho \dot{v}^B$ (Greve, [6]), (2.17) reads:

$$-\frac{dp}{dz} + \frac{d(\overset{\circ}{\mathbf{T}})_{zz}}{dz} - \rho g_F \cos \gamma = 0 , \tag{6.5}$$

$$\frac{d(\overset{\circ}{\mathbf{T}})_{xz}}{dz} + \rho g_F \sin \gamma = 0 . \tag{6.6}$$

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):

With the use of (6.4) and (6.1) we obtain

$$(\overset{\circ}{\mathbf{T}})_{xx} = 0, \quad (6.8)$$

$$(\overset{\circ}{\mathbf{T}})_{zz} = 0, \quad (6.9)$$

$$\frac{dv_x^B}{dz} = 2\mathcal{A}(T, w)f(\sigma)(\overset{\circ}{\mathbf{T}})_{xz}, \quad (6.10)$$

the temperature T_M is assumed equal to zero, see (6.3), and for the function $f(\sigma)$ we adopt the *Glen's flow law* with $n = 3$:

$$f(\sigma) = \sigma^2. \quad (6.11)$$

The σ variable was defined (see (2.26)) as

$$\sigma = \sqrt{\frac{1}{2}\text{tr}(\overset{\circ}{\mathbf{T}})^2}, \quad (6.12)$$

which now yields

$$\sigma^2 = (\overset{\circ}{\mathbf{T}})_{xz}^2. \quad (6.13)$$

The dependence of $\mathcal{A}(w)$ on w is restricted to a linear function (see Lliboutry&Duval [11])

$$\mathcal{A}(w) = A(1 + \alpha w), \quad (6.14)$$

with

$$A = 5.3 \cdot 10^{-24} \text{s}^{-1} \text{Pa}^{-3}, \quad \alpha = 184. \quad (6.15)$$

Thus, the stress-strain rate relation (6.10) can be rewritten as

$$\frac{dv_x^B}{dz} = 2A(1 + \alpha w)((\overset{\circ}{\mathbf{T}})_{xz})^3. \quad (6.16)$$

Constitutive equation for the diffusive water flux \vec{j} (see (2.22)):

$$j_z = -\nu \frac{dw}{dz}, \quad (6.17)$$

and constitutive relation for water mass-production term M (see (2.23)):

$$\begin{aligned} M &= 2 \frac{\mathcal{A}(w)f(\sigma)\sigma^2}{L} \\ &= 2 \frac{A(1 + \alpha w)(\overset{\circ}{\mathbf{T}})_{xz}^4}{L}. \end{aligned} \quad (6.18)$$

The present formulation:

We rewrite the field equations, listed at the beginning of Chapter 5;

Mass balance for the ice component (see (5.8)):

$$\frac{dw}{dz}v_{2z} - \frac{dv_{2z}}{dz} = \frac{r_1}{\rho}. \quad (6.19)$$

Mass balance for the water component (see (5.9)):

$$\frac{dw}{dz}u_{1z} + \frac{dv_{2z}}{dz} + w\frac{du_{1z}}{dz} = 0. \quad (6.20)$$

Linear momentum balance for the water component (see (5.10)):

$$\tilde{\nu}u_{1x} = w\rho g_F \sin \gamma, \quad (6.21)$$

$$\tilde{\nu}u_{1z} = -\frac{d(pw)}{dz} - w\rho g_F \cos \gamma - \rho\omega\frac{dw}{dz}. \quad (6.22)$$

Note: we marked diffusivity ν by tilde to distinguish it from ν considered in the traditional formulation. In general, ν and $\tilde{\nu}$ have different meaning

Linear momentum balance for the ice component

For numerical implementation, we consider $\overset{\circ}{\mathbf{T}}_2$ instead of $\overset{\circ}{\mathbf{D}}_2$ an independent variable in the stress-strain rate relation. The linear momentum balance for the ice component (5.11) is then written as

$$\frac{(\overset{\circ}{\mathbf{T}}_2)_{xz}}{dz} + \rho g_F \sin \gamma = 0, \quad (6.23)$$

$$-\frac{dp}{dz} + \frac{(\overset{\circ}{\mathbf{T}}_2)_{zz}}{dz} - \rho g_F \cos \gamma = 0. \quad (6.24)$$

The *stress – strain-rate relation* adopted for numerical implementation is of the form discussed in Chapter 4 (see (4.153)):

$$\overset{\circ}{\mathbf{D}}_2 = \mathcal{A}(w)f(\sigma)\overset{\circ}{\mathbf{T}}_2, \quad (6.25)$$

that is, inverse to the relation considered in theoretical investigations. We will also use linear dependence of $\mathcal{A}(w)$ on w :

$$\mathcal{A}(w) = A(1 + \alpha w), \quad (6.26)$$

and apply Glen's flow law:

$$f(\sigma) = \sigma^2. \quad (6.27)$$

For the purpose of modelling we need to specify the values of parameters A and α . Due to the lack of reliable estimates, we decide to use the same values as in the traditional relations. 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 2-D case,

$$\mathbf{D}_2 = \begin{pmatrix} 0 & \frac{1}{2} \frac{dv_{2x}}{dz} \\ \frac{1}{2} \frac{dv_{2x}}{dz} & \frac{dv_{2z}}{dz} \end{pmatrix}, \quad (6.28)$$

and¹

$$\overset{\circ}{\mathbf{D}}_2 = \mathbf{D}_2 - \frac{1}{2} \text{tr}(\mathbf{D}_2) \mathbf{1}, \quad (6.29)$$

the relation (6.25) reads

$$\frac{1}{2} \begin{pmatrix} -\frac{dv_{2z}}{dz} & \frac{dv_{2x}}{dz} \\ \frac{dv_{2x}}{dz} & \frac{dv_{2z}}{dz} \end{pmatrix} = \mathcal{A}(w) f(\sigma) \begin{pmatrix} \overset{\circ}{T}_{2xx} & \overset{\circ}{T}_{2xz} \\ \overset{\circ}{T}_{2xz} & \overset{\circ}{T}_{2zz} \end{pmatrix}. \quad (6.30)$$

In view of (4.152), we have

$$\begin{aligned} 2\sigma^2 &= \text{tr}(\overset{\circ}{\mathbf{T}}_2)^2 \\ &= (\overset{\circ}{\mathbf{T}}_2)_{xx}^2 + (\overset{\circ}{\mathbf{T}}_2)_{zz}^2 + 2(\overset{\circ}{\mathbf{T}}_2)_{xz}^2 \\ &= 2 \left((\overset{\circ}{\mathbf{T}}_2)_{zz}^2 + (\overset{\circ}{\mathbf{T}}_2)_{xz}^2 \right). \end{aligned} \quad (6.31)$$

In addition, using the Glen's flow law (6.27) and (6.26), eq. (6.30) implies:

$$\frac{dv_{2z}}{dz} = 2A(1 + \alpha w) \left((\overset{\circ}{\mathbf{T}}_2)_{zz}^2 + (\overset{\circ}{\mathbf{T}}_2)_{xz}^2 \right) (\overset{\circ}{\mathbf{T}}_2)_{zz}, \quad (6.32)$$

$$\frac{dv_{2x}}{dz} = 2A(1 + \alpha w) \left((\overset{\circ}{\mathbf{T}}_2)_{zz}^2 + (\overset{\circ}{\mathbf{T}}_2)_{xz}^2 \right) (\overset{\circ}{\mathbf{T}}_2)_{xz}. \quad (6.33)$$

Finally, the balance of energy (see (4.188)):

$$\begin{aligned} (L - p\Delta)r_1 &= -\frac{d(pwu_{1z})}{dz} - p\frac{v_{2z}}{dz} + 2A(1 + \alpha w) \left((\overset{\circ}{\mathbf{T}}_2)_{zz}^2 + (\overset{\circ}{\mathbf{T}}_2)_{xz}^2 \right)^2 \\ &\quad + \lambda \frac{u_{1z}}{dz} + w\rho g_F (u_{1x} \sin \gamma - u_{1z} \cos \gamma). \end{aligned} \quad (6.34)$$

Moreover, we will put $\lambda = 0$, since the physical interpretation of the term $\lambda \frac{du_{1z}}{dz}$ is unclear.

¹This definition of the deviator corresponds to the traceless part of a second-order tensor in two dimensions. It is not clear, whether the flow law in the form (6.25) is still valid for the 2-D case (it is valid in the 3-D case), but we adopt it here. The difference induced by the deviator definition in 2-D and 3-D case is, however, only connected with the numeral standing at the term $\text{tr}\mathbf{D}_2$ in (6.29). This term is equal to zero in the traditional formulation and assumed to be small in the present formulation.

6.3 Solution

The equations from the preceding section were solved numerically by a program `t_ice.f90` written in Fortran 90 (see the attachment). 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 were solving an initial-value problem, the ice-bedrock boundary as the initial point. The temperate layer thickness was $H = 200m$.

The initial values are:

$$\begin{aligned} w(0) &= 0, \\ p(0) &= H\rho g_F \text{ [Pa]}, \\ \overset{\circ}{T}_{xz}(0) &= 0.07 \cdot H\rho g_F \text{ [Pa]}, \\ \overset{\circ}{T}_{zz}(0) &= 0 \text{ [Pa]}, \\ u_{1z}(0) &= 0 \text{ [m a}^{-1}\text{]}, \\ v_{2x}(0) &= 5 \text{ [m a}^{-1}\text{]}, \\ v_{2x}(0) &= -0.2 \text{ [m a}^{-1}\text{]}, \\ j_z(0) &= 0 \text{ [kg m a}^{-1}\text{]}. \end{aligned}$$

We introduce the parameters

$$a = \frac{1}{\tilde{\nu}}, \quad b = \frac{\rho\omega}{\tilde{\nu}}, \quad c = \nu, \quad (6.35)$$

where the first two are diffusion parameters of the present formulation and c is the diffusivity considered in the traditional model.

The physical dimensions are

$$[a] = \text{kg}^{-1} \text{m}^{-3} \text{s}, \quad [b] = \text{m s}^{-1}, \quad [c] = \text{kg m}^{-2} \text{s}^{-1}.$$

Figure 6.2 shows the case

$$a = 0, \quad b = 0, \quad c = 0.$$

We can see that both solutions coincide.

Figure 6.3 shows 4 different choices:

$$\begin{aligned} \text{A1:} & \quad a = 10^{-11}, & b = 10^{-4}, & c = 0, \\ \text{A2:} & \quad a = 10^{-10}, & b = 10^{-4}, & c = 0, \\ \text{A3:} & \quad a = 10^{-9}, & b = 10^{-4}, & c = 0, \\ \text{A4:} & \quad a = 10^{-8}, & b = 10^{-4}, & c = 0. \end{aligned}$$

Figure 6.4 complementary shows:

$$\begin{array}{lll} \text{B1 :} & a = 10^{-8}, & b = 10^{-5}, & c = 0, \\ \text{B2 :} & a = 10^{-8}, & b = 10^{-4}, & c = 0, \\ \text{B3 :} & a = 10^{-8}, & b = 10^{-3}, & c = 0, \\ \text{B4 :} & a = 10^{-8}, & b = 10^{-2}, & c = 0. \end{array}$$

From Figures 6.3 and 6.4 we see that the two diffusivities a and b , introduced in the present formulation significantly influence the water-content profiles w (the panels in the third rows) and the longitudinal velocity profiles v_{2x} (the panels in the second rows).

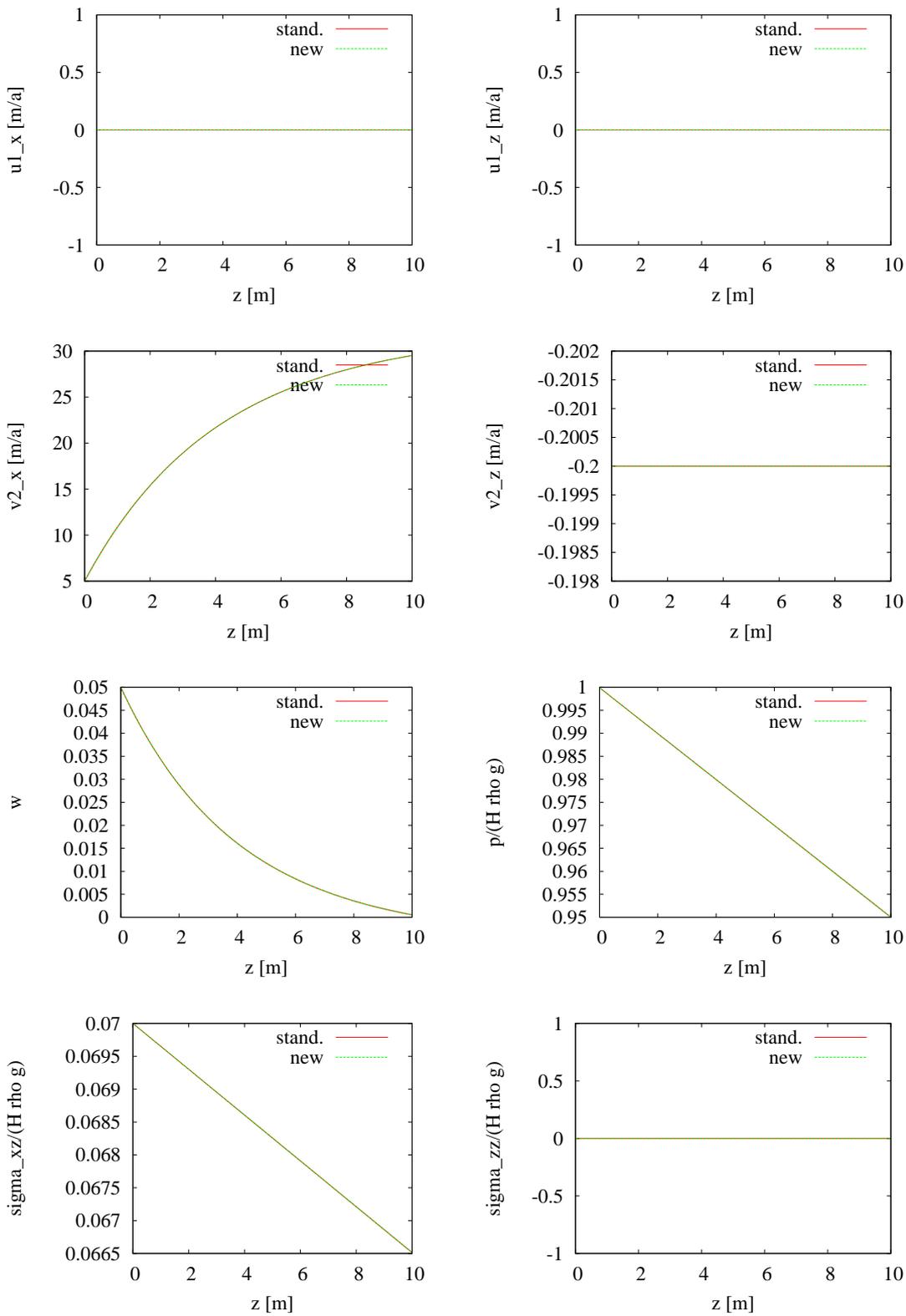


Figure 6.2: The solutions of the initial-value problem in the temperate-ice zone for the traditional approach 'stand' and the present formulation 'new' for the case $a = b = c = 0$, i.e. no water diffusion is allowed in ice. We denoted \dot{T}_{xz} by "sigma_xz" and \dot{T}_{zz} by "sigma_zz". Both solutions coincide.

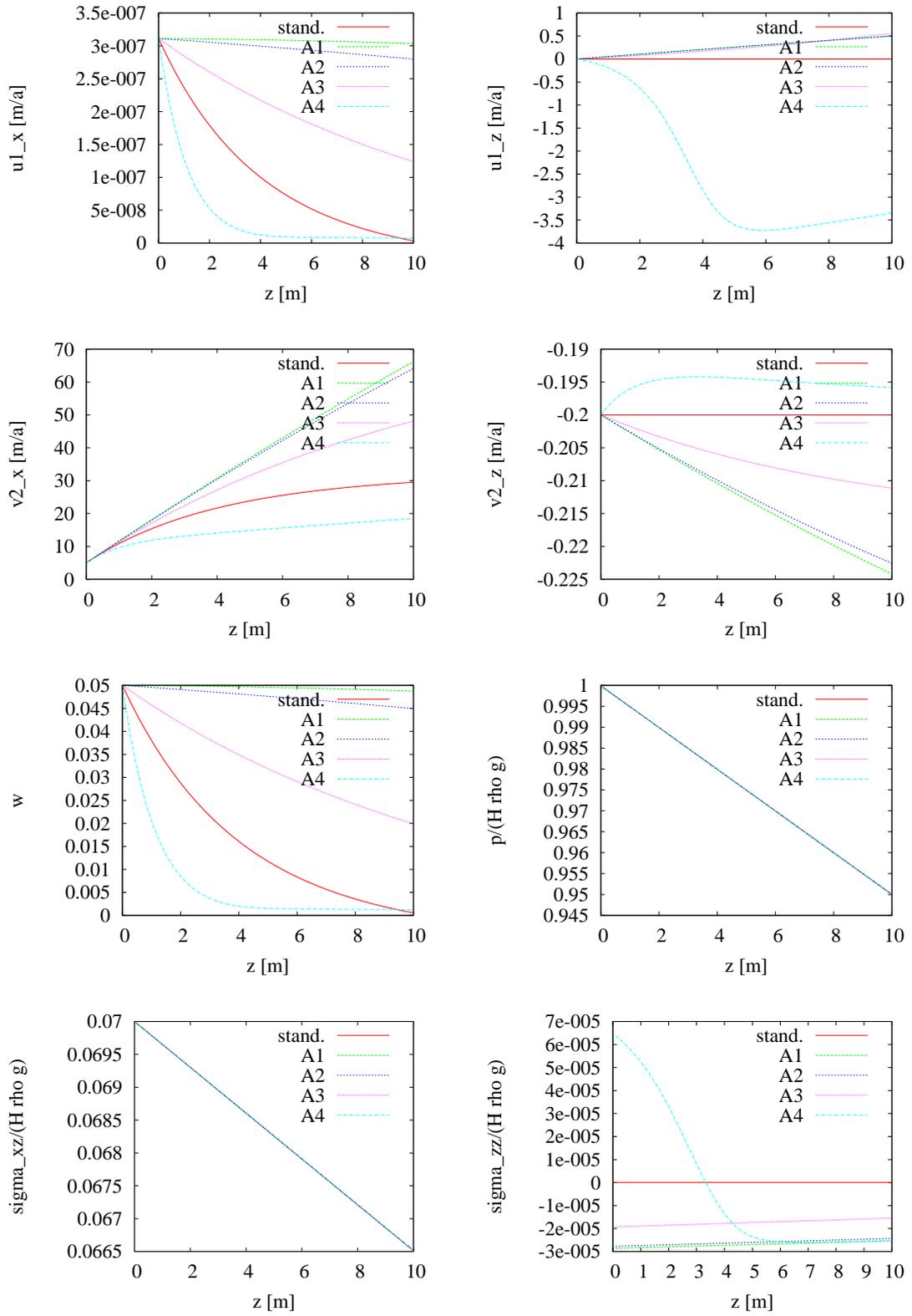


Figure 6.3: The solutions of the initial-value problem in the temperate-ice zone for the traditional formulation without diffusion ($c = 0$) and the present formulation, with $b = 10^{-4}$, A1: $a = 10^{-11}$, A2: $a = 10^{-10}$, A3: $a = 10^{-9}$, A4: $a = 10^{-8}$, respectively. We denoted $\overset{\circ}{T}_{xz}$ by "sigma_xz" and $\overset{\circ}{T}_{zz}$ by "sigma_zz".

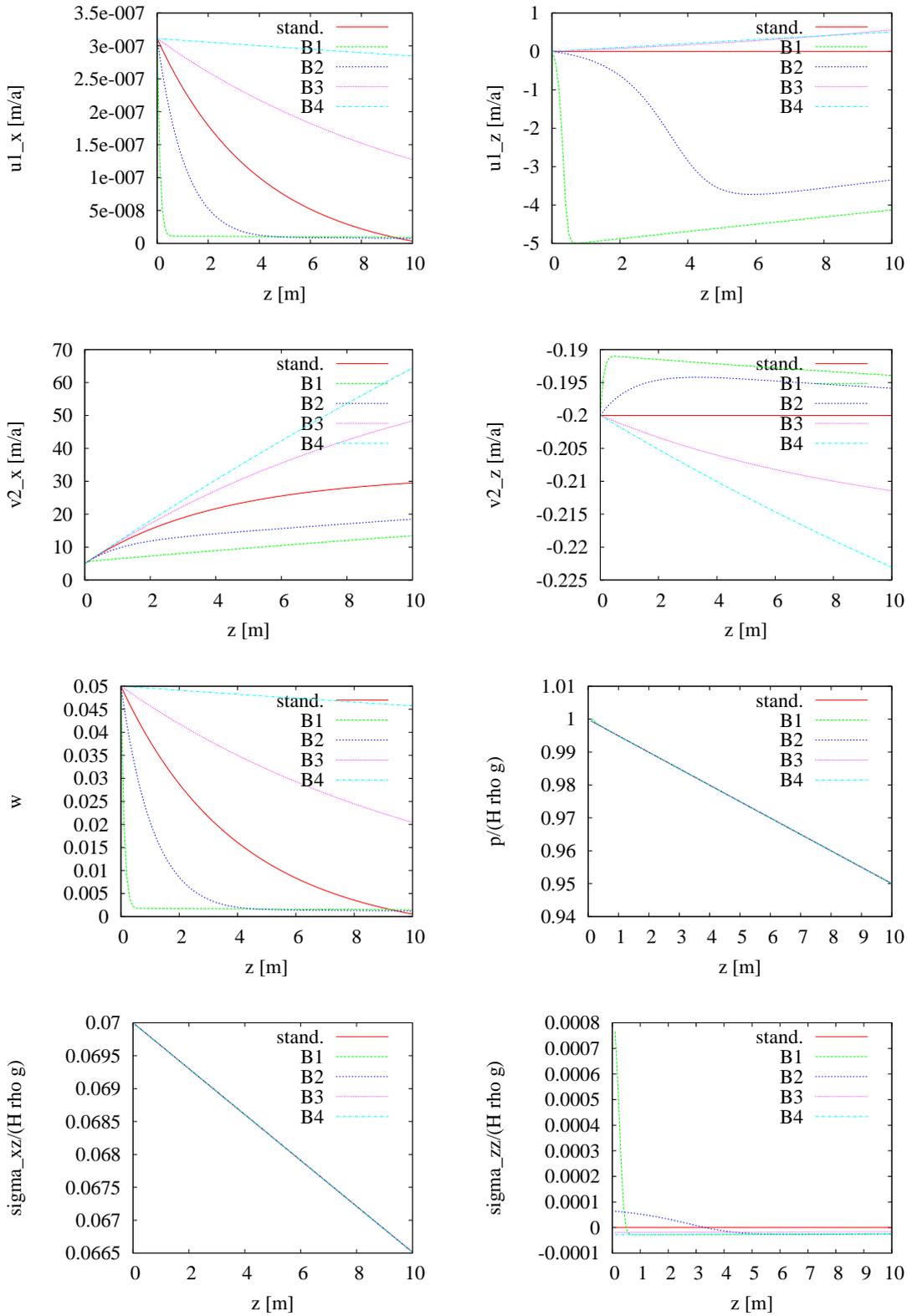


Figure 6.4: The solutions of the initial-value problem in the temperate-ice zone for the traditional formulation without diffusion ($c = 0$) and the present formulation, with $a = 10^{-8}$, B1: $b = 10^{-5}$, B2: $b = 10^{-4}$, B3: $b = 10^{-3}$, B4: $b = 10^{-2}$, respectively. We denoted $\overset{\circ}{T}_{xz}$ by "sigma_xz" and $\overset{\circ}{T}_{zz}$ by "sigma_zz".

Chapter 7

Summary

We were dealing with the formulation of a physical model of a polythermal ice sheet. For the temperate-ice zone, we applied the mixture approach on the basis of the rational thermodynamics of reacting mixtures. We derived the balance laws for reacting mixtures containing discontinuity surface with including surface production terms at this 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 the means of rational thermodynamics, firstly by inspecting the entropy principle, then by partial linearization of the material model with respect to the equilibrium state.

According to 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 the 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 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 a uniform thickness under steady 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. The stress – strain-rate relation is assumed to be sensitive to the water content, which implies considerable variations in the velocity profiles. There is a lack of knowledge about the real values of the diffusive parameters, which makes difficult to quantify the difference between the fully-mixture formulation, presented here, and the traditional formulation. Nevertheless, both formulations coincide if the diffusion of water is neglected. To decide the importance of our present formulation is a question of more experimental data on water diffusion in glaciers.

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 Recipes in FORTRAN: The Art of Scientific Computing, Second edition, Cambridge University Press