



Universität Stuttgart Germany

**Institut für Mechanik (Bauwesen)** Lehrstuhl für Kontinuumsmechanik Prof. Dr.-Ing. Dr. h. c. W. Ehlers

## A quasi-double-porosity thermo-hydro-mechanical model with application to plant tissues

Jan Lukas Eurich





Report No.: II-38 (2021)

## A quasi-double-porosity thermo-hydro-mechanical model with application to plant tissues

Von der Fakultät Bau- und Umweltingenieurwissenschaften der Universität Stuttgart zur Erlangung der Würde eines Doktor-Ingenieurs (Dr.-Ing.) genehmigte Abhandlung

vorgelegt von

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aus Frankfurt am Main

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Tag der mündlichen Prüfung: 26. Februar 2021

Institut für Mechanik (Bauwesen) der Universität Stuttgart Lehrstuhl für Kontinuumsmechanik Prof. Dr.-Ing. H. Steeb

2021

Report No. II-38 Institut für Mechanik (Bauwesen) Lehrstuhl für Kontinuumsmechanik Universität Stuttgart, Germany, 2021

Editor: Prof. Dr.-Ing. Dr. h. c. W. Ehlers

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ISBN 978-3-937399-38-6 (D93 – Dissertation, Universität Stuttgart)

#### Acknowledgements

The research presented in this thesis has been carried out between the years 2014 and 2020 during my time as research associate at the Institute of Applied Mechanics, Chair of Continuum Mechanics at the University of Stuttgart. Several people contributed to the successful completion of this work in various ways, which I would like to acknowledge gratefully at this point.

First, I would like to express my gratitude towards my supervisor Wolfgang Ehlers for giving me the opportunity to work at his institute and sharing not only his knowledge in porous-media mechanics, but also his insights in the academic world in a broader sense. Especially his support during the past year is gratefully acknowledged. I would like to thank the co-examiner, Joachim Bluhm, for the quick preparation of the review report and for the discussions we had at various conferences.

Furthermore, I would like to thank Ronaldo Borja for hosting me at his chair at Stanford University for three months in summer/autumn 2018. A thank you also to the members of his group and the people at Blume Earthquake Engineering Center for making me feel so welcome.

Moreover, I would like to thank Rena Schott and Anita Roth-Nebelsick from the State Museum of Natural History in Stuttgart and all the other researchers from the Collaborative Research Center SFB-TRR 141 for the good collaboration. Also, I would like to thank Shahla Shahmoradi for giving me the opportunity to supervise her master's thesis.

A very warm thank you to my former and present colleagues from both chairs of the institute for the friendly atmosphere and the fruitful discussions on several topics. In particular, I would like to thank my officemates Davina Fink, Alixa Sonntag and Dominik Fauser for their support and interesting conversations. Furthermore, I would like to thank David Koch, Maik Schenke, Kai Häberle, Patrick Schröder and Malte Sauerwein for the cooperation and discussions on various PANDAS issues. Especially, I would like to express my gratitude to Arndt Wagner, Elten Polukhov, Aref Nateghi and Stephan Teichtmeister for proofreading parts of this thesis, but also for their support and pleasurable moments over the last years.

Last, but surely not least, I would like to express my deepest gratitude towards my family and friends for their dedication and support over all these years.

Stuttgart, March 2021

Jan Lukas Eurich

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## Zusammenfassung

Die Motivation für diese Dissertationsschrift ergibt sich aus der Beobachtung, dass verschiedene poröse Medien, wie zum Beispiel eine Vielzahl von herkömmlichen Baumaterialien, eine Schädigung erfahren, wenn sie Frost-Tau-Zyklen ausgesetzt werden, wohingegen andere poröse Medien, wie etwa verschiedene Pflanzengattungen, nicht geschädigt werden, wenn sie den gleichen Witterungen ausgesetzt werden. Daraus leiten sich die Fragestellungen ab, welche Strategien diese (frostresistenten) Pflanzen verwenden, wie sich diese mit einem biologisch motivierten Modell abbilden lassen und wie numerische Simulationen dazu beitragen können, die thermo-hydro-mechanischen Kopplungen zu verstehen und diese auch im Hinblick auf Baumaterialien zu deuten.

Die Strategien von frostresistenten Pflanzen lassen sich grob in zwei Bereiche unterteilen. Es gibt zum einen jene Strategien, die im Wesentlichen darauf beruhen, dass Pflanzen lebende Organismen sind. So gibt es beispielsweise Pflanzen, die ihre Frostresistenz unter anderem über eine Proteinproduktion gewährleisten. Es gibt aber auch eine Strategie, die überwiegend auf strukturellen Eigenschaften der Pflanzen basiert, was in Hinblick auf Baumaterialien von besonderer Bedeutung sein könnte. Tatsächlich ist diese auf dem strukturellen Bauplan einer Pflanze basierende Strategie überaus bedeutend, da in diesem Fall durch extrazelluläre Eisbildung die pflanzlichen Zellen dehydrieren, wodurch intrazelluläre Eisbildung vermieden werden kann, was eine irreparable Schädigung der Pflanzen zur Folge gehabt hätte. Extrazelluläre Eisbildung ist hingegen als unkritisch für die Pflanzen zu betrachten. Die Dehydrierung der Pflanzen wird maßgeblich bestimmt durch die Permeabilität der Zellen gegenüber Wasser, welche durch die Porosität der Zellwand bestimmt wird und somit eine strukturelle Eigenschaft ist.

Da darüber hinaus Interesse an einer auf verschiedene poröse Medien übertragbaren Theorie besteht, welche die makroskopische Skala adressiert, basiert das (Pflanzen-) Modell auf der Theorie Poröser Medien, einer kontinuumsmechanischen Theorie von überlagerten Partialkörpern, welche miteinander interagieren. Die Theorie wurde ursprünglich für Untersuchungen im Bereich der Bodenmechanik entwickelt, fand aber mittlerweile Anwendung in ganz unterschiedlichen Teilbereichen der Wissenschaft, in denen poröse Medien auftreten. Insbesondere auch im Bereich der Human-Biomechanik fand die Theorie breite Anwendung, in der Pflanzen-Biomechanik hingegen bislang weniger. Allerdings ist die Theorie Poröser Medien vor allem dann von großem Nutzen, wenn mehrphasige Kontinua mit einer sich deformierenden Festkörperstruktur beschrieben werden. So sind Pflanzen ein poröses Material, welches aus einem Festkörperskelett besteht, welches selbst ein Mehrphasenmaterial ist, da es zum einen verholzte Anteile enthalten kann, welche insbesondere über eine lokale Anisotropie die Lastabtragung ermöglichen, sowie pflanzliche Zellen, welche mit Wasser befüllt sind und so potenziell zur Tragfähigkeit beitragen können. Der Porenraum auf Makroebene, bei Pflanzen auch als der interzelluläre Bereich beschrieben, ist mit Luft und Wasser befüllt, welches unter geeigneten Zuständen gefrieren kann. Somit ergibt sich ein Modell mit vier Konstituierenden, diese sind das Festkörperskelett sowie im Makroporenraum Luft und Wasser, letzteres im flüssigen und festen Aggregatzustand.

Ein wesentlicher Teil der Dissertation widmet sich der bereits skizzierten Modellbildung für pflanzliches Gewebe und dem Beweis der thermodynamischen Konsistenz der Modellgleichungen. Insbesondere die Berücksichtigung der Phasentransformation von Wasser von flüssig zu fest im interzellulären Bereich der porösen Pflanze und der daraus resultierenden Dehydrierung der Zellen unter besonderer Berücksichtigung der internen Oberflächen ist von großem Interesse. Die Beschreibung der Phasentransformation von Wasser basiert konzeptionell auf der Einführung von singulären Flächen, so dass der Satz von Bilanzgleichungen (für Masse, Impuls, Drall, Energie und Entropie) erweitert wird um Sprungbedingungen über diese singulären Flächen. Die Phasentransformation von Wasser, wie auch die Dehydrierung der Zellen werden über so-genannte Masseninteraktionsterme in das Gleichungssystem eingebunden. Wie bereits erwähnt ist das zugrundeliegende Material ein poröses Material mit mehrskaliger Porositätseigenschaft, da es zusätzlich zu dem Porenraum auf Makroebene einen Porenraum auf Mikroebene gibt aufgrund der porösen Zellwand, welche durchlässig für Wasser ist; ein Austausch von Luft findet über die Zellwand allerdings nicht statt. Auf diese Weise wird das Wasser-Management auf der Mikroebene durch einen Masseninteraktionsterm zwischen dem Festkörperskelett und dem (Makro-) Porenwasser beschrieben, auf der Makroebene wird das Wasser-Management über ein erweitertes Darcy-Gesetz beschrieben. In diesem Zusammenhang sei anzumerken, dass die bestimmenden Gleichungen des Modells über volumenspezifische Größen gekoppelt sind, wobei Masseninteraktionsterme oberflächenbezogene Größen sind, so dass diese Größen über volumenspezifische Mittelungsprozesse zu homogenisieren sind.

Die gekoppelten Differentialgleichungen des Modells werden monolithisch mittels Finite-Elemente-Methode gelöst über sogenannte gemischte Taylor-Hood-Elemente durch Implementierung in das Programmpaket PANDAS. In den numerischen Beispielen wird zunächst auf die Art der Eisbildung eingegangen, welche entweder diffus im kompletten Querschnitt der Pflanze auftreten kann oder an Oberflächen größerer Hohlräume innerhalb der Pflanze. Im letztgenannten Fall ist die Anwendung eines reduzierten Modells von Vorteil, welches ohne Eis-Konstituierende auskommt, und die Wirkung der Eisbildung in den Hohlräumen der Pflanze über geeignete Randbedingungen abbildet. Diese sind insbesondere über Dirichlet-Randbedingungen des Wasserdrucks gegeben, welche auf experimentellen Untersuchungen basieren. Im Fokus dieses numerischen Beispiels steht das Verhältnis des Wasser-Managements auf der Mikroskala und der Makroskala sowie daraus folgend die Orte maximaler Eis-Akkumulation. Für den Fall der diffusen Eisbildung ist die Berücksichtigung des kompletten Modells mit vier Konstituierenden notwendig. Hier bildet sich Eis über den kompletten Querschnitt der Pflanze aus, was eine Druckänderung des Wassers zur Folge hat, was wiederum die Pflanze dehydriert. Auch hier steht neben der Phasentransformation das Wasser-Management im Zentrum des numerischen Beispiels. Abschließend werden Gemeinsamkeiten und Unterschiede der Modelle erläutert sowie einen Ausblick gegeben, wie diese Ergebnisse vor dem Hintergrund der ursprünglichen Fragestellungen zu bewerten sind.

Daraus ergibt sich eine Gliederung der Monographie, welche sich wie folgt ausgestaltet: In Kapitel 1 erfolgt eine generelle Verortung des Themas der Dissertationsschrift, in Kapitel 2 werden die biologischen Grundlagen von frostresistenten Pflanzen und deren Strategien näher beleuchtet, in Kapitel 3 wird die zugrundeliegende makroskopische Theorie Poröser Medien eingeführt mit Angabe eines Modells für Pflanzen, was auch die Einführung der Kinematik, des Spannungsbegriffs sowie der gekoppelten Bilanzgleichungen umfasst, auch für den Spezialfall von singulären Flächen im Gebiet. In Kapitel 4 werden die Modellannahmen und Modellgleichungen im Detail eingeführt und diskutiert sowie deren thermodynamische Konsistenz bewiesen, ferner wird ein reduziertes Modell motiviert und eingeführt. Kapitel 5 widmet sich der Finite-Elemente-Methode, welche zur Lösung der gekoppelten Modellgleichungen in schwacher Formulierung herangezogen wird. Dies beinhaltet die Herleitung der schwachen Formulierung der bestimmenden Gleichungen sowie die Angabe einer räumlichen und zeitlichen Diskretisierung. In Kapitel 6 werden zwei numerische Beispiele gezeigt, eines für das komplette Modell mit diffuser Eisbildung im Querschnitt der Pflanze, eines für das reduzierte Modell zur Beschreibung der Auswirkung einer lokalisierten Eisbildung in größeren Hohlräumen. In Kapitel 7 erfolgt eine Zusammenfassung der Arbeit sowie ein Ausblick über mögliche weitere Schritte. Die Monographie schließt mit der Überprüfung der thermodynamischen Konsistenz des reduzierten Modells in Anhang A.

### Abstract

The motivation for this doctoral thesis is based on the observation that certain porous media, such as conventional construction materials, get damaged in case they are exposed to freeze-thaw cycles, whereas other porous materials, such as a variety of porous plants, do not exhibit any damage under the same ambient conditions. This raises a number of questions: Which properties and strategies of plants lead to their frost resistance? How can these strategies be captured by a biologically motivated model? And how can simulations contribute to a better understanding of the involved thermo-hydro-mechanical couplings - in plant tissues, but also with regard to construction materials?

With regard to frost resistance, plants utilise essentially two kinds of strategies. There are these types of strategies that are related to the fact that plants are living organisms. For instance, there are plants that ensure their frost resistance, among other factors, by a production of proteins, when they are exposed to subzero environments. But there are also strategies that are based on the blueprints of plants, which is particularly of interest with regard to construction materials. In fact, this structural property of plants is of high importance, as it works in a way that the formation of extracellular ice leads to a dehydration of plant cells. By this, intracellular ice formation, which is lethal for plant cells, can be avoided, extracellular ice formation is uncritical for plants. The dehydration of plant cells is mainly regulated by the permeability of the cell walls with respect to water, which is in turn decisively determined by a structural property of the plant, the porosity of its cell walls.

Since there is an interest in a theory that is potentially transferable to various porous media and addresses the involved phenomena at the macroscale, the (plant) model is based on the Theory of Porous Media, a continuum-mechanical theory of superimposed partial continua, which are mutually interacting. The Theory of Porous Media has originally been proposed for investigations in the field of soil mechanics, however, in the meantime it has successfully been applied to problems in several fields of science and technology that are dealing with porous media. Although its application to problems in human biomechanics is emphasised, in plant biomechanics, the theory has not been utilised frequently. However, the Theory of Porous Media is of great use when it comes to multiphase flow through a deforming solid skeleton. Exactly this is the case here, as plants are porous materials, which are composed of a solid skeleton, which is itself a multiphase material. The solid skeleton may contain lignified elements, which assure via local anisotropies a load-bearing capacity, as well as tissue cells that are filled with water, which may also contribute to a load-bearing capacity. Furthermore, the pore space at the macroscopic scale, in plant-biomechanics terminology usually referred to as intercellular space, is filled with gaseous air and liquid water, which may potentially freeze. Therefore, the planttissue model proceeds from four constituents, which are the multiphasic solid skeleton as well as a pore space at the macroscopic scale that is filled with air and water, the latter in a liquid and a solid state of physical aggregation.

Thus, a substantial part of this doctoral thesis is concerned with the establishment of a

macroscopic theory for plants with the mentioned properties including the introduction of the constitutive equations with a proof of thermodynamic consistency. Especially the consideration of the phase transition of water from liquid to solid within the intercellular space of the porous plants and the consequential dehydration of their cells with particular attention on internal interfaces is of great interest. The formulation of the phase transition of water is conceptionally based on the introduction of singular surfaces, such that the set of balance equations (for mass, linear momentum, angular momentum, energy and entropy) is extended by so-called jump conditions across these singular surfaces. The phase transition of water as well as the dehydration of the tissue cells are included into the set of governing balance equations via mass-production terms. As already mentioned, the material at hand is a porous material with double porosity, since there is in addition to the macro-pore space, also a micro-pore space due to the porous cell wall, which is permeable with respect to water, however, not with respect to the gas. In this way, the water management at the microscopic scale is facilitated by a mass-production term between the solid skeleton and the (macro-) pore water. At the macroscopic scale, the water management is described by an extended Darcy law. It needs to be mentioned in this context, that the governing equations of the model are coupled via volume-specific quantities, however, mass-production terms are generally surface-specific quantities, such that these surface-specific quantities need to be homogenised via volume-specific averaging processes.

The coupled partial differential equations of the model are solved monolithically by applying the Finite-Element Method. In particular, the governing equations are implemented into the research code PANDAS utilising mixed Taylor-Hood elements. By discussing two numerical examples, distinction is made between dispersed ice formation in the whole cross section of a plant and rather localised ice formation at internal cavities of a plant. In the latter case, the application of a reduced (ternary) model is reasonable, where the ice is not included as an individual constituent. Instead, the impact of ice formation at the internal cavities on the plant tissue is included by appropriate boundary conditions. These are particularly Dirichlet boundary conditions of the water pressure, which are based on experimental investigations. The focus of this numerical example is the relation between the water management at the microscopic scale and the macroscopic scale as well as the location of the maximum ice formation. For the case of dispersed ice formation in the whole cross section, the consideration of the full (quaternary) model is necessary. Here, it has been observed that the ice formation leads to a change in water pressure, which also dehydrates the plant tissue. Hence, the focus of this numerical example is the phase transition as well as its impact on the water management of the plant. Finally, similarities and differences of the models are discussed and an outlook is given, how the results can be interpreted in the light of the questions that stood in the beginning of this research.

Thus, this monograph is structured as follows: In Chapter 1, the topic of this dissertation is introduced including a discussion concerning relevant approaches in this field. In Chapter 2, the biological foundations of frost-resistant plants are discussed with a focus on the structural properties of plants. In Chapter 3, the plant-tissue model is introduced, which is based on the Theory of Porous Media. The kinematics of the individual constituents is introduced along with stress measures and the coupled balance relations, also for the special case of singular surfaces in the domain. In Chapter 4, the assumptions of the plant-tissue model are introduced and the constitutive equations are derived based on the evaluation of the entropy inequality, which leads a priori to thermodynamically consistent equations. Also, the reduced (ternary) model is introduced and discussed. As the Finite-Element Method is utilised for the solution of the coupled governing equations, Chapter 5 is concerned with the derivation of the weak formulation of the governing equations as well as the spatial and temporal discretisation. In Chapter 6, two numerical examples are shown, where the quaternary model is applied to dispersed ice formation in the whole cross section of a plant, the ternary model is applied to localised ice formation at internal cavities of the cross section of a plant. Chapter 7 summarises this doctoral thesis and gives an outlook, what a follow-up project should consider. This monograph closes with the proof of thermodynamic consistency of the reduced model in Appendix A.

# Nomenclature

The notation used throughout this monograph is as far as possible in accordance with the modern tensor-calculus notation of de Boer [20] and Ehlers [50].

## Conventions

$(\cdot)$			placeholder for arbitrary quantities	
$\delta(\cdot)$			test functions of primary variables	
$\Delta(\cdot)$			difference of a quantity	
$d(\cdot)$	or	$\partial(\cdot)$	differential or partial derivative operator	
$a, b, \ldots$	or	$\phi, \psi, \ldots$	scalars (zero-order tensors)	
$\mathbf{a},\mathbf{b},\dots$	or	$\boldsymbol{\phi}, \boldsymbol{\psi}, \dots$	vectors (first-order tensors)	
$\mathbf{A},\mathbf{B},\ldots$	or	$\Phi, \Psi, \ldots$	second-order tensors	
$\overset{3}{\mathbf{A}},\overset{3}{\mathbf{B}},\ldots$	or	$\overset{3}{\Phi}, \overset{3}{\Psi}, \ldots$	third-order tensors	

#### General conventions

$i, j, k, n, \ldots$	indices
$(\cdot)_{lpha}$	subscripts for kinematic quantities of a constituent $\varphi^{\alpha}$ within the Theory of Porous Media
$(\cdot)^{lpha}$	superscripts for non-kinematic quantities of a constituent $\varphi^\alpha$ within the Theory of Porous Media
$(\cdot)_{0\alpha}^{(\cdot)}, (\cdot)_{0}^{(\cdot)}$	initial values of quantities referring to the reference configuration of constituent $\varphi^{\alpha}$ and $\varphi^{S}$
· (·)	total time derivatives with respect to the motion of the overall aggregate $\varphi$
$(\cdot)'_{lpha}$	material time derivatives with respect to the motion of constituent $\varphi^{\alpha}$
$(\overline{\cdot})$	value at the <i>Dirichlet</i> boundary
·	norm of a vector
$\llbracket \cdot \rrbracket$	jump operator for quantities across the singular surface $\Gamma$
$(\cdot)^+, \ (\cdot)^-$	quantities referring to one side of the singular surface $\Gamma$
$(\cdot)^h$	discretised quantities
$(\cdot)^j$	nodal values
$(\cdot)_{n+1}, \ (\cdot)_n$	quantity at current and previous time step

$(\cdot)^{lpha}_E$	extra term of a physical quantity of $\varphi^{\alpha}$
$(\cdot)^{lpha}_{E\mathrm{mech}}, \ (\cdot)^{lpha}_{E\mathrm{dis}}$	mechanical and dissipative extra quantity of $\varphi^{\alpha}$
$(\cdot)^{\alpha}_{\mathrm{iso}}, \ (\cdot)^{\alpha}_{\mathrm{aniso}}$	isotropic and anisotropic contribution of $\varphi^{\alpha}$
$(\cdot)^{-1}$	inverse of a tensor
$(\cdot)^T$	transpose of a tensor
$(\cdot)^{\Gamma},  (\cdot)_{\Gamma}$	quantities referring to the singular surface $\Gamma$
$(\cdot)^F,  (\cdot)_F$	quantities referring to the fluid constituents
$(\cdot)^W, (\cdot)_W$	quantities referring to the water

# Symbols

### Greek letters

Symbol	Unit	Description
α		identifier of q constituents, here: $\alpha = \{S, I, L, G\}$
$\alpha^S, \ \alpha^{IR}$	[1/K]	linear thermal expansion coefficient of $\varphi^S$ and $\varphi^I$
$\alpha_{S1}$	$[N/m^2]$	stiffness in the preferred direction of $\varphi^S$
$\alpha_{S2}$	[-]	exponent with respect to the preferred direction of $\varphi^S$
$\beta$		fluid constituent identifier, here: $\beta = \{L, G\}$
$\gamma$		identifier of $q-1$ constituents
$\gamma_0^S, \ \gamma_0^{IR}$	[-]	exponent in $U^S$ and $U^I$ of $\varphi^S$ and $\varphi^I$
δ		solid constituent identifier, here: $\delta = \{S, I\}$
$\epsilon_{ m tol}$		tolerance for the residuum
$\varepsilon, \ \varepsilon^{\alpha}$	[J/kg]	mass-specific internal energy of $\varphi$ and $\varphi^{\alpha}$
$\hat{\varepsilon}^{lpha}$	$[J/m^3 s]$	volume-specific production of internal energy of $\varphi^{\alpha}$
$\zeta^{lpha}$	[J/kg]	mass-specific enthalpy of $\varphi^{\alpha}$
$\Delta \zeta_{\rm fus}$	[J/kg]	mass-specific enthalpy of fusion
$\hat{\zeta}^{lpha}$	$[J/K m^3 s]$	volume-specific entropy production of $\varphi^{\alpha}$
$\eta, \; \eta^{lpha}$	[J/K kg]	mass-specific entropy of $\varphi$ and $\varphi^{\alpha}$
$\hat{\eta},~\hat{\eta}^{lpha}$	$[J/K m^3 s]$	volume-specific entropy production of $\varphi$ and $\varphi^{\alpha}$
$ heta, \  heta^{lpha}$	[K]	absolute temperature of $\varphi$ and $\varphi^{\alpha}$
$\theta_D$	[K]	prescribed temperature
$ heta_{ m diff}$	[K]	prescribed temperature difference
$ ilde{ heta}$	$[^{\circ}C]$	relative temperature
$\vartheta$	[rad]	contact angle of the fluid interface with the solid
$\kappa$	[-]	exponent accounting for actual available pore space
$\kappa_r^{eta}$	[-]	relative permeability factor of $\varphi^{\beta}$
$\kappa_0^{SL},\ \kappa^{SL}$	[-]	(reference) effective permeability coefficient

$\lambda, \ \lambda_L$	[-]	axial and lateral stretch
$\lambda_c$	[-]	pore size distribution index
$\Lambda^S, \ \Lambda^{IR}$	$[N/m^2]$	first $Lam\acute{e}$ constant of $\varphi^S$ and $\varphi^I$
$\mu^{eta R}$	$[N s/m^2]$	dynamic shear viscosity of $\varphi^{\beta}$
$\mu^S, \ \mu^{IR}$	$[N/m^2]$	second $Lam\acute{e}$ constant of $\varphi^S$ and $\varphi^I$
$\nu^S$	[-]	Poisson ratio of $\varphi^S$
ρ	$[kg/m^3]$	density of the overall aggregate $\varphi$
$ ho^lpha,\  ho^{lpha R}$	$[kg/m^3]$	partial and effective density of constituent $\varphi^{\alpha}$
$\hat{ ho}^{lpha}$	$[kg/m^3 s]$	volume-specific mass production of $\varphi^{\alpha}$
$\hat{\varrho}^{lpha}_{\Gamma}$	$[kg/m^2 s]$	surface-specific mass production at $\Gamma$ of $\varphi^{\alpha}$
$\sigma, \sigma^{\alpha}$		supply of a scalar-valued quantity
$\sigma_\eta, \ \sigma_\eta^{lpha}$	$[J/K m^3 s]$	volume-specific entropy supply of $\varphi$ and $\varphi^{\alpha}$
$\sigma_s$	[N/m]	surface tension of the fluid-fluid interface
Υ		scalar-valued field function
$\phi_{(\cdot)}^j$		global basis functions for scalar primary variables
$\varphi, \varphi^{\alpha}$		overall aggregate and specific constituent
$\varphi^F$		overall fluid aggregate
$arphi^W$		overall water component
$\psi^{lpha}$	[J/kg]	mass-specific $Helmholtz$ free energy of $\varphi^{\alpha}$
$\psi^G_{ heta}, \ \psi^G_{ ho^{GR}}$	[J/kg]	thermal and density-part of $Helmholtz$ free energy of $\varphi^G$
$\psi^L_{\theta}, \; \psi^L_{s^L}$	[J/kg]	thermal and saturation-part of $Helmholtz$ free energy of $\varphi^L$
$\Psi, \Psi^{lpha}$		arbitrary volume-specific scalar-valued quantity
$\hat{\Psi}, \ \hat{\Psi}^{lpha}$		volume-specific production of a scalar-valued quantity
$\Psi_{w,p,s,m,g}$	$[N/m^2]$	contributions to the water potential
ω	[1/m]	volume-specific surface of cell dehydration
$\Omega, \ \partial \Omega$		spatial domain and boundary of spatial domain
$\partial \Omega_D^{(\cdot)}, \ \partial \Omega_N^{(\cdot)}$		Dirichlet and Neumann boundary
$\Omega^e,~\Omega^h$		finite elements and discretised domain
$\boldsymbol{\sigma}, \ \boldsymbol{\sigma}^{lpha}$		supply of a vector-valued quantity
Υ		vector-/tensor-valued field function
$oldsymbol{\phi}, \ oldsymbol{\phi}^lpha$		vector-valued efflux of a physical quantity
$oldsymbol{\phi}_\eta, \; oldsymbol{\phi}_\eta^lpha$	$[J/K m^3 s]$	efflux of entropy of $\varphi$ and $\varphi^{\alpha}$
$oldsymbol{\phi}^{j}_{\mathbf{u}_{S}}$		global basis function for $\mathbf{u}_S$
$oldsymbol{\chi}_{lpha}, \ oldsymbol{\chi}_{lpha}^{-1}$		motion and inverse motion function of $\varphi^{\alpha}$
$\chi_{\Gamma}$		motion function of $\Gamma$
${f \Psi}, \ {f \Psi}^lpha$		arbitrary volume-specific vector-valued quantity
$\hat{oldsymbol{\Psi}},\;\hat{oldsymbol{\Psi}}^{lpha}$		production of a vector-valued quantity

$oldsymbol{ au}^lpha$	$[N/m^2]$	Kirchhoff stress tensor of $\varphi^{\alpha}$
${f \Phi}, \ {f \Phi}^lpha$		tensor-valued efflux of a physical quantity

### Latin letters

Symbol	$\mathbf{Unit}$	Description
$a_{1,2,4}$	$[^{\circ}C]$	fitting parameter for density of $\varphi^L$
$a_3$	$[^{\circ}C^{2}]$	fitting parameter for density of $\varphi^L$
$a_5$	$[\mathrm{kg/m^3}]$	fitting parameter for density of $\varphi^L$
$a_{\Gamma}$	[1/m]	volume-specific interfacial area
$\mathrm{d}a$	$[m^2]$	area element in the current configuration
$A_{\rm ice}$	$[m^2]$	ice covered area of cross section of representative pore
$A_{\mathrm{IL}}$	$[m^2]$	interfacial area of representative pore
$\mathrm{d}A_{\alpha}$	$[m^2]$	area element in the reference configuration of $\varphi^{\alpha}$
$c_v^S, c_v^{IR}, c_v^{eta R}$	[J/kg K]	specific heat capacity at constant volume of $\varphi^{\alpha}$
d		dimension of a physical problem
$\hat{e}^{lpha}$	$[J/m^3 s]$	volume-specific total energy production of $\varphi^{\alpha}$
$E_{\rm fus}$	$[N/K m^2]$	entropy of fusion of water
$E^S$	$[N/m^2]$	modulus of elasticity of $\varphi^S$
g	$[\mathrm{m/s^2}]$	norm of the gravitational acceleration
h	[m]	pressure head
$h_n$	$[\mathbf{s}]$	time step
$ ilde{h}$	[m]	height of cross section of representative pore
$h_W$	$[N/m^2]$	water potential
$H^{\alpha R}$	[W/K m]	isotropic effective thermal conductivity of $\varphi^{\alpha}$
$I_{\delta 1}, I_{\delta 2}, I_{\delta 3}$	[-]	principal invariants of deformation tensors of $\varphi^{\delta}$
$J, J_{\alpha}$	[-]	Jacobian determinant of $\varphi$ and $\varphi^{\alpha}$
$J_{S4}, J_{S5}$	[-]	mixed invariants of $\mathbf{C}_S$ and $\mathcal{M}_a^S$
$J_v$	[m/s]	surface-specific volume flow of water
$\widetilde{J}_{\delta}$	[-]	compaction point
$k^F$	[m/s]	isotropic hydraulic conductivity
$k^S, \ k^{IR}$	$[N/m^2]$	bulk modulus of $\varphi^S$ and $\varphi^I$
$l_1, l_2$	[m]	(water-filled part of) length of a representative pore
$\tilde{L}_p, \ L_p$	$[m^3/N s]$	hydraulic conductivity
$m_{ heta}^S$	$[N/K m^2]$	stress-temperature modulus of $\varphi^S$
$m_{d,g,w}$	[kg]	mass of dry wood, green wood and water in a specimen
$\mathrm{d}m^{\alpha}$	[kg]	mass element of $\varphi^{\alpha}$
$M_C$	[-]	moisture content

$ ilde{m}^{eta}$	$[kg/m^2 s]$	mass efflux through the <i>Neumann</i> boundary $\partial \Omega_N^{\tilde{m}^{\beta}}$
$n^{lpha}$	[-]	volume fraction of a constituent $\varphi^{\alpha}$
$n^F$	[-]	porosity
$n_{\rm res}^F,  n_{\rm res}^S$	[-]	residual porosity and solidity
$n_W^I, n_W^L$	[-]	ice and liquid fraction of the water
$n^W$	[-]	volume fraction of water
N		total number of nodes
$p_0$	$[N/m^2]$	ambient pressure
$p^{\beta R}$	$[N/m^2]$	pressures of $\varphi^{\beta}$
$p^C$	$[N/m^2]$	capillary pressure
$p_d$	$[N/m^2]$	bubbling or entry pressure
$p_{ m diff}$	$[N/m^2]$	pressure difference
$p^{FR}$	$[N/m^2]$	pore pressure or turgor pressure (of $\varphi^S$ )
$p^{IR}$	$[N/m^2]$	pressure of $\varphi^I$
$p_{\theta}^{IR}$	$[N/m^2]$	thermal part of the pressure of $\varphi^I$
$p_D^{LR}$	$[N/m^2]$	prescribed pressure of $\varphi^L$
$P^{j}$		nodal points
q		number of constituents
$\widetilde{q}$	$[J/m^2 s]$	heat flux through the Neumann boundary $\partial \Omega_N^{\tilde{q}}$
$r, r^{\alpha}$	$[J/kg \ s]$	mass-specific radiation of $\varphi$ and $\varphi^{\alpha}$
$\widetilde{r}$	[m]	radius of representative pore
$\bar{R}^G$	$[{\rm Nm/kgK}]$	gas constant of $\varphi^G$
$s^{eta}$	[-]	saturation of $\varphi^{\beta}$
$s_{ m res}^{eta}$	[-]	residual saturation of $\varphi^{\beta}$
$s^L_{ ext{eff}}$	[-]	effective saturation of $\varphi^L$
$\widetilde{s}$	[m]	chord length of cross section of representative pore
t	$[\mathbf{s}]$	time
$t_{ m diff}$	$[\mathbf{s}]$	time difference
$t_i$	$[N/m^2]$	coefficients of the surface traction $\tilde{\mathbf{t}}$
$U_{g,\hat{ ho}^S,\hat{ ho}^I}$	$[N/m^2]$	water potential due to gravitation and mass interactions of $\varphi^S$ and $\varphi^I$
$u_i$	[m]	coefficients of the displacement vector of $\varphi^S$
$U^S, \ U^I$	$[J/m^3]$	volumetric extension of the strain energy of $\varphi^S$ and $\varphi^I$
$V, V^{\alpha}$	$[m^3]$	volume of the overall body $\mathcal B$ and of the partial body $\mathcal B^{lpha}$
$V^P$	$[m^3]$	volume of representative pore
$\mathrm{d}v, \ \mathrm{d}v^{\alpha}$	$[m^3]$	current volume element of $\varphi$ and $\varphi^{\alpha}$
$\mathrm{d}V_{lpha}$	$[m^3]$	volume element in the reference configuration of $\varphi^{\alpha}$
$\tilde{v}^{\delta}$	[m/s]	volume flux through the Neumann boundary $\partial \Omega_N^{\tilde{v}^{\delta}}$

w		water constituent identifier, here: $w = \{I, L\}$
$W^S, W^I$	$[J/m^3]$	strain energy per reference volume element of $\varphi^S$ and $\varphi^I$
$W^I_{n^I}$	$[J/m^3]$	strain energy contribution from the volume fraction of $\varphi^I$
x	[m]	coordinate
$\mathbf{a}_0^S, \ \mathbf{a}^S$	[-]	unit vector of transversal isotropy in reference and current configuration of $\varphi^S$
$\mathrm{d}\mathbf{a}$	$[m^2]$	oriented area element in the current configuration
$\mathrm{d}ar{\mathbf{a}}_{lpha}$	$[m^2]$	weighted area element of $\varphi^{\alpha}$
$\mathrm{d}\mathbf{A}_{lpha}$	$[m^2]$	oriented area element in the reference configuration of $\varphi^{\alpha}$
$\mathbf{b},\mathbf{b}^{lpha}$	$[\mathrm{m/s^2}]$	mass-specific body force of $\varphi$ and $\varphi^{\alpha}$
$\mathbf{d}_{lpha}$	[m/s]	diffusion velocity of $\varphi^{\alpha}$
$\mathbf{e}_i$		basis vector
$\mathbf{f}^{lpha}$	$[N/m^3]$	volume-specific force of $\varphi^{\alpha}$
f		vector of external forces
g	$[\mathrm{m/s^2}]$	gravitation vector
$\hat{\mathbf{h}}^{lpha}$	$[N/m^2]$	volume-specific total angular momentum production of $\varphi^{\alpha}$
$\mathbf{k}^{lpha}$	[N]	total force of $\varphi^{\alpha}$
$\mathbf{k}^{lpha}_O$	[N]	contact force of $\varphi^{\alpha}$
$\mathbf{k}_V^{lpha}$	[N]	volume force of $\varphi^{\alpha}$
$\boldsymbol{k}$		generalised stiffness vector
$\hat{\mathbf{m}}^{lpha}$	$[N/m^2]$	volume-specific direct angular momentum production of $\varphi^{\alpha}$
n	[-]	outward-oriented unit surface vector
$\hat{\mathbf{p}}^{lpha}$	$[N/m^3]$	volume-specific direct momentum production of $\varphi^{\alpha}$
$\mathbf{q}, \; \mathbf{q}^{lpha}$	$[J/m^2 s]$	heat influx vector of $\varphi$ and $\varphi^{\alpha}$
$\hat{\mathbf{s}}^{lpha}$	$[N/m^3]$	volume-specific total momentum production of $\varphi^{\alpha}$
$\mathbf{t}^{lpha}$	$[N/m^2]$	surface traction of $\varphi^{\alpha}$
$\tilde{\mathbf{t}}$	$[N/m^2]$	surface traction at Neumann boundary $\partial \Omega_N^{\tilde{\mathbf{t}}}$
$oldsymbol{u}_1, \ oldsymbol{u}_2$		sets of primary variables for Model I and Model II
$\mathbf{u}_S$	[m]	displacement of $\varphi^S$
$\mathbf{w}_{lpha\Gamma}$	[m/s]	relative velocity of $\varphi^{\alpha}$ with respect to $\Gamma$
$\mathbf{w}_{eta}$	[m/s]	seepage velocity of $\varphi^{\beta}$
$\mathbf{w}_F$	[m/s]	seepage velocity of a fluid
x	[m]	position vector in the current configuration
$\mathbf{x}_{\Gamma}$	[m]	position vector of $\Gamma$
$\mathrm{d}\mathbf{x}$	[m]	line element in the current configuration
$\mathbf{X}_{lpha}$	[m]	position vector in the reference configuration of $\varphi^{\alpha}$
$\mathrm{d}\mathbf{X}_{lpha}$	[m]	line element in the reference configuration of $\varphi^{\alpha}$
$\hat{\mathbf{X}}_{lpha}$	[m]	position vector in the intermediate configuration of $\varphi^{\alpha}$

$\dot{\mathbf{x}}, \ \dot{\mathbf{x}}_{lpha}$	[m/s]	velocity of $\varphi$ and $\varphi^{\alpha}$
$\mathbf{x}_{\Gamma}'$	[m/s]	velocity of $\Gamma$
$\ddot{\mathbf{x}}, \ \overset{\prime\prime}{\mathbf{x}}_{lpha}$	$[\mathrm{m/s^2}]$	acceleration of $\varphi$ and $\varphi^{\alpha}$
$oldsymbol{y}, \ oldsymbol{y}'$		vector containing all degrees of freedom and derivatives
$\Delta oldsymbol{y}$		stage increment
$\mathbf{A}_{lpha}$	[-]	Almansi strain tensor of $\varphi^{\alpha}$
$\mathbf{B}_{lpha}$	[-]	left Cauchy-Green deformation tensor of $\varphi^{\alpha}$
$\mathbf{C}_{lpha}$	[-]	right Cauchy-Green deformation tensor of $\varphi^{\alpha}$
$\mathbf{D}_{lpha}$	[1/s]	rate of deformation tensor of $\varphi^{\alpha}$
D		generalised damping matrix
$\mathbf{E}_{lpha}$	[-]	Greenean strain tensor of $\varphi^{\alpha}$
$\mathbf{F}_{lpha}$	[-]	material deformation gradient of $\varphi^{\alpha}$
$\mathbf{F}_{\delta M}, \ \mathbf{F}_{\delta  heta}$	[-]	mechanical part and thermal part of $\mathbf{F}_{\delta}$ of $\varphi^{\delta}$
$\mathbf{F}_{S0}$	[-]	initial deformation of $\varphi^S$ until the intermediate configuration
$\mathbf{H}^{lpha},\mathbf{H}^{lpha R}$	[W/K m]	partial and effective thermal conductivity tensor of $\varphi^{\alpha}$
Ι	[-]	identity tensor of second order
$\mathbf{L}, \ \mathbf{L}_{\alpha}$	[1/s]	spatial velocity gradient of $\varphi$ and $\varphi^{\alpha}$
$\stackrel{R}{\mathbf{K}}_{lpha}, \ \mathbf{K}_{lpha}$	[-]	referential and spatial Karni-Reiner tensor of $\varphi^{\alpha}$
$\mathbf{K}^{eta}$	[m/s]	hydraulic conductivity tensor of $\varphi^{\beta}$
$\mathbf{K}_r^eta$	[m/s]	relative permeability tensor of $\varphi^{\beta}$
$\mathbf{K}^{S}$	$[m^2]$	intrinsic permeability tensor of $\varphi^S$
$\mathbf{P}^{lpha}$	$[N/m^2]$	first <i>Piola-Kirchhoff</i> stress tensor of $\varphi^{\alpha}$
$\mathbf{S}^{lpha}$	$[N/m^2]$	second <i>Piola-Kirchhoff</i> stress tensor of $\varphi^{\alpha}$
$\mathbf{T}, \ \mathbf{T}^{lpha}$	$[N/m^2]$	Cauchy stress of $\varphi$ and $\varphi^{\alpha}$
$\mathbf{W}_{lpha}$	[1/s]	spin tensor of $\varphi^{\alpha}$

### Calligraphic letters

Symbol	Unit	Description
$\mathcal{O}$		origin of a coordinate system
$\mathcal{A}^{(\cdot)}$		ansatz spaces
$\mathcal{B}, \; \mathcal{B}^{lpha}$		aggregate body of $\varphi$ and $\varphi^{\alpha}$
${\cal D}$		internal dissipation
$\mathcal{D}_{\hat{ ho}^I}$		internal dissipation with regard to $\hat{\rho}^{I}$
${\cal F}$		semi discretised functional
$\mathrm{D} oldsymbol{\mathcal{F}}$		global residual tangent
$\mathcal{G}_{(\cdot)}$		weak formulation of a governing equation
$\mathcal{H}^1$		Sobolev space

$\mathcal{M}^S$		structural tensor referring to $\varphi^S$
$\mathcal{M}_a^S$	[-]	structural tensor of transversal isotropy referring to $\varphi^S$
${\cal P}$	$[N/m^2]$	Lagrangean multiplier
$\mathcal{P}^{lpha}$		material point of $\varphi^{\alpha}$
$\mathcal{R}$		set of response functions
${\cal S},\;{\cal S}^{lpha}$		surface of $\mathcal{B}$ and $\mathcal{B}^{\alpha}$
$\mathcal{T}^{(\cdot)}$		test spaces
$\mathcal{V}$		set of independent process variables

# Selected acronyms

Description
anti-freeze protein
Civil Engineering
central processing unit
Collaborative Research Center
differential-algebraic equation
Deutsche Forschungsgemeinschaft
degree of freedom
Finite-Element
Finite-Element Method
Ladyzhenskaya-Babuška-Brezzi
Porous media adaptive nonlinear finite element solver based on differential algebraic systems
partial differential equation
representative elementary volume
Theory of Mixtures
Theory of Porous Media

## Chapter 1: Introduction

#### 1.1 Motivation

The topic of this doctoral thesis is inspired by the research association Transregional Collaborative Research Center (CRC) 141: Biological Design and Integrative Structures - Analysis, Simulation and Implementation in Architecture, which was dealing with and applying the biomimetic approach meaning that from the analysis of biological organisms new insights for the development of building constructions and/or materials were expected. In this framework, the research that is presented in this thesis aims to examine, model and simulate the strategies and properties of plants that lead to their frost resistance. The motivation for this particular question results from the observation that the exposure of conventional construction materials to freeze-thaw cycles often leads to frost damage. For the case of contruction materials, the damage is associated with two effects that are related to the ice formation in the pore space, which are in particular the increase in specific volume of water during the phase-transition process and the suction of water to the locations of ice formation. This imposes a pressure on the solid structure, which may lead to stresses that exceed the tensile strength of the material. This leads to the questions that have been posed in the abstract of this thesis: Which properties and strategies of plants lead to their frost resistance? How can these strategies be captured by a biologically motivated model? And how can simulations contribute to a better understanding of the involved thermo-hydro-mechanical processes and couplings - in plant tissues, but also with regard to construction materials?

With regard to frost resistance of plants, there are several factors involved, which can be categorised by the terms freezing tolerance and freezing avoidance. The first term refers to physiological processes, whereas the latter refers to physical mechanisms. One of those physical mechanisms is based on the blueprints of plants, which is particularly of interest with regard to construction materials. In this case, the formation of extracellular ice at species-specific and tissue-specific locations leads to a dehydration of plant cells. In this way, intracellular ice formation, which is lethal for plant cells, can be avoided. In contrast, extracellular ice formation is uncritical for plants. The dehydration of plant cells is mainly regulated by the permeability of the cells with respect to water, which is in turn decisively determined by the porosity of the cell wall. This is a purely structural property.

Having these notions in mind, the interest is in a macroscopic theory that is capable of addressing the mentioned properties and strategies of plants, where the focus is on the structural property that is based on the multiscale porosity feature of the plant. The interest is also in a theory that describes the processes and strategies in a way that is generic enough, such that it is transferable to a variety of porous media, for example in the future also to construction materials. It is expected that such a theoretical model would enable numerical simulations that lead to a better understanding of the freezing process in porous plants and the associated availability of water at different scales.

#### 1.2 State of the art, scope and aims

As already outlined, there are two kinds of strategies that are essential for the frost resistance of plants. Apart from physiological processes, there is also a process that is based on the structural properties of the plant, which is the dehydration of plant cells. In this way, intracellular ice formation, which is a critical process for plants, can be avoided as discussed in Beck *et al.* [12], Gusta & Wisniewski [87], Konrad *et al.* [107], Schott *et al.* [167] as well as Lenné *et al.* [115]. The revelation of this strategy of cell dehydration by extracellular ice formation dates back to the work of Prillieux [143] more than 150 years ago. In the light of these articles, plants are considered as porous material, which is composed of a solid skeleton, which is itself a multiphase material. The solid skeleton may contain lignified elements as well as tissue cells that are filled with water and represent, therefore, hard and soft tissue. Furthermore, these plant cells may dehydrate through microscopic pores in the cell wall, which has been recognised as a crucial mechanism of frost resistance. The pore space at the macroscopic scale, in plant-biomechanics terminology usually referred to as intercellular (or extracellular) space, is filled with gaseous air and liquid water, which may freeze at subzero temperatures.

In order to embed the research that is needed to address the basic questions that have been raised in the previous section, several important contributions from highly diverse fields have to be considered. On the one hand, there are experimental, theoretical and/or numerical studies describing the fluid dynamics (or the water status in biology-inspired terminology), and phase transitions in plant tissues. On the other hand, there are modelling approaches describing multiphase flow in porous media with double porosity and/or phase transitions in a more general sense or even applied to a different scientific discipline, for example soil mechanics. Those concepts from related fields can be utilised in order to derive a modelling approach for plant tissues.

In the field of plant biomechanics, the fluid dynamics in terms of a macro (bulk) flow in plants has been addressed many times, as for example in Boyer [31], Canny [34], Kramer [110], Molz [128], Rockwell *et al.* [152, 153, 154], also with regard to the micro-porosity-based flow such as cell dehydration, as addressed in Cosgrove [38], Kramer & Boyer [111], Mc Cully *et al.* [124], Nonami & Boyer [139], Roden *et al.* [155], Steudle [177], Steudle & Boyer [178], Taiz & Zeiger [179]. In these works, a water potential is usually introduced to describe the flow of water in the plants. Also, phase transitions have been addressed, compare Ashworth & Abeles [5], Graf *et al.* [82], Rajashekar & Burke [145], however, not with a holistic, meaning coupled macroscopic approach. Though, poroelastic approaches have been applied to plants, compare Bader *et al.* [8], Leyton [116], Rockwell *et al.* [153], Roth *et al.* [157, 158], considering them as multiphasic material in the sense of a simple binary poroelastic model of solid and liquid according to Biot's theory [14]. As the composition of the plants and the processes involved require a more sophisticated model with multiple constituents, the Theory of Porous Media (TPM) is applied, as it is

particularly suited to derive thermodynamically consistent constitutive models. Thus, the strategy for this monograph is to derive a model that connects the somehow fundamental concept of the water potential from biology to the continuum-mechanical TPM. For the theoretical foundations of the TPM, the interested reader is referred to the work of Bluhm *et al.* [18], de Boer [24], Ehlers [45, 46] and citations therein. The TPM has been applied and proven suitable not only for a variety of different engineering problems, such as Ehlers & Häberle [58], Leichsenring *et al.* [114], Specht *et al.* [173], but also for continuum-biomechanical applications in the field of human biology, compare, for example, Ehlers *et al.* [59], Ehlers & Wagner [61], Fink *et al.* [77], Ricken *et al.* [150].

In the given context of plants, the TPM allows to address the mechanical, hydraulic and thermal effects in the framework of finite deformations in a coupled manner. Moreover, it allows to address the dehydration of their cells via micro pores in the cell wall, which is a crucial property of their frost resistance. This microstructurally based process represents a double-porosity feature, where porosity is at the tissue scale and at the cell scale as well. Note that there are various engineering materials with double porosity. Therefore, there is already a sound continuum-mechanical framework given by Borja & Choo [26], Borja & Koliji [27], Choo & Borja [36], Choo *et al.* [37], Dykhuizen [42], Gerke & van Genuchten [80], Zhang *et al.* [194] as well as Khalili & Selvadurai [103].

In addition to microstructurally based processes, the focus of this monograph is the phase transition of the pore water. In general, phase transition phenomena, such as freezing of water, have been investigated in the framework of porous media, for instance by Gray & Miller [84], Gray *et al.* [85], Joekar-Niasar & Hassanizadeh [100], Niessner & Hassanizadeh [134], Coussy [39], Kowalski [109], de Boer [21], Bluhm *et al.* [16, 18], Morland & Gray [131], Morland & Sellers [132] and Ehlers & Häberle [58], where especially the latter one is also the basis for this investigation. Therein, the liquid-gas phase transition of carbon dioxide in porous media is addressed. In doing so, singular surfaces have to be introduced, where carbon dioxide is on one side liquid and on the other side gaseous. This singular surface introduces the so-called jump conditions into the balance relations, which have been utilised to determine the surface-specific mass-interaction term. Further homogeni-sations are then necessary, in order to determine the volume-specific mass-interaction term, where the approach of Graf [83] has been utilised.

In the context of this monograph, the introduced modelling approach allows to differentiate between localised and dispersed ice formation in plants. Thus, for the case of dispersed (intercellular) ice formation within large partitions or the whole cross section of a plant, as for example in *Betula nana* (dwarf birch) [166], the modelling approach includes the ice as an individual model constituent. This model requires an explicit inclusion of the phase transition of water. For the case of local ice accumulation within more extensive intercellular spaces, as for example in *Equisetum hyemale* (winter scouring rush) [167], the impact of ice formation onto the porous tissue aggregate can be modelled by imposing appropriate boundary conditions at the locations of ice formation. These are specifically *Dirichlet* water pressure boundary conditions that are based on experimental investigations. In this way, the concept of water potential from biology has been adapted and utilised to address the water management of plant tissues.

Note that the numerical results presented in this monograph have been computed with

the Finite-Element code PANDAS<sup>1</sup>. This tool has been developed at the Institute of Applied Mechanics (CE) at the University of Stuttgart under the supervision of Professor Wolfgang Ehlers. Back then, the tool has especially been set up by Ammann [3], Eipper [63], Ellsiepen [65] and utilised as well as extended since then in application to a variety of topics, as indicated by the list of monographs within this series of publications.

#### **1.3** Outline of the thesis

In **Chapter 1**, the topic of this dissertation is introduced and motivated by including a discussion concerning relevant approaches from a variety of scientific disciplines.

In **Chapter 2**, the biological foundations of frost-resistant plants are discussed with a focus on the structural properties of plants. Emphasis is also on the water status of plants that will be utilised in the modelling approach of this thesis, specifically in terms of a water potential.

In Chapter 3, the plant-tissue model is introduced, which is based on the TPM. Already at this point, distinction is made between dispersed ice and localised ice in plants and the consequences regarding the modelling equations. Furthermore, the kinematics of the individual constituents is introduced including the relevant kinematic coupling of the ice to the solid skeleton. Moreover, stress measures and the coupled balance relations are introduced, also for the special case of singular surfaces in the domain. With the introduction of singular surfaces, phase transitions of single substances can be described.

In **Chapter 4**, the assumptions of the plant-tissue models are introduced and the constitutive equations are derived based on the evaluation of the entropy inequality for the overall aggregate, which leads a priori to thermodynamically consistent equations. In particular, in terms of the solid skeleton, a new strain-energy function is proposed, which is chosen according to the required properties like finite deformations, thermoelasticity, the compaction point for the case of a closed or frozen pore space, mass interaction describing the double porosity and anisotropy. In a similar way, there is also a new strain-energy function for the ice proposed to account for the properties of finite deformations, thermoelasticity, the compaction point for the case of a closed pore space, mass interaction describing the formation of ice and the influence of the enthalpy of fusion (or similarly the entropy of fusion) that is related to the phase transition. For the description of the fluids in the macro-pore space, the focus is on the anisotropy of the pores as well as on the action of capillarity. Further attention is on the derivation of the mass-interaction terms, which are the phase transition of water based on the concept of singular surfaces and the cell dehydration, which is conceptually understood as a quasi double-porosity feature.

As the Finite-Element Method is utilised for the solution of the coupled governing equations, **Chapter 5** is concerned with the derivation of the weak formulations of the governing equations, the introduction of primary variables and boundary conditions as well as the spatial and temporal discretisation.

In Chapter 6, two numerical examples are shown, one for each ice-formation pattern.

<sup>&</sup>lt;sup>1</sup>Porous media adaptive nonlinear finite element solver based on differential algebraic systems (http://www.get-pandas.com).

In particular, the quaternary model is applied to dispersed ice formation in the whole cross section of a plant, the ternary model is applied to localised ice formation at internal cavities of the cross section of another plant.

**Chapter 7** summarises this doctoral thesis and gives an outlook, what a follow-up project should consider.

This monograph closes with the proof of thermodynamic consistency of the reduced model in **Appendix A**.

#### 1.4 List of publications

The research presented in this thesis has already been published in parts in the following articles.

Eurich, L.; Schott, R.; Shahmoradi, S.; Wagner, A.; Borja, R. I.; Roth-Nebelsick, A. & Ehlers, W.: A thermodynamically consistent quasi double-porosity thermo-hydro-mechanical model for cell dehydration of plant tissues at subzero temperatures. *Archive of Applied Mechanics* (2021), accepted.

Eurich, L.; Wagner, A. & Ehlers, W.: Water management of frost-resistant plant tissues as a consequence of extracellular ice formation. *Proceedings in Applied Mathematics and Mechanics* **20** (2021), e202000095.

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## Chapter 2: Biological background

In this chapter, the biological foundations of plants and their main mechanisms of frost resistance are concisely introduced. Attention is on the structural properties of plants, which greatly contribute to their frost resistance. In this context, the concept of water potential is introduced with an explanation, how it is utilised to address the fluid mechanics of plant tissues and how it relates to their frost resistance. Furthermore, plant-specific issues in relation to their material parameters are introduced. In particular, the value of these parameters or even the qualitative behaviour of the whole plant may depend on its water content.

### 2.1 Basic structure and frost resistance of plants

Among plants, there is a great variety with regard to morphology, function as well as specific properties. But there are also a couple of properties they have in common. As for example outlined in Taiz & Zeiger [179] or Eurich *et al.* [69], plants exhibit a cellular structure. In contrast to animal tissue, plant-tissue cells are surrounded by a rigid cell wall. Due to this cellular structure of the plants, where the arrangement of the cells defines an intracellular space and an intercellular (or extracellular) space, plants can be regarded as porous materials. The intracellular space contains large amounts of water, up to 90%, as given in Taiz & Zeiger [179]. The plant cells are on the one hand rigid, and on the other hand also elastic enough, that it allows to build up a considerable hydrostatic pressure, the so-called turgor pressure. This turgor pressure is important for many processes in plants, specifically it may contribute to a load-bearing capacity, particularly for plants without lignified plant cells, such as xylem (wood), compare Mc Cully *et al.* [124]. As the water content of the cells as well as the turgor pressure may vary, there is another porosity scale at the cell level. Therefore, there are two porosity scales involved when dealing with plants.

The behaviour of plants with regard to frost events differs completely depending on their natural habitat and their exposure to cold temperatures during their life span. The factors that contribute to the property of frost resistance are of quite diverse nature. However, they can be categorised by the terms freezing tolerance and freezing avoidance, as discussed in Gusta & Wisniewski [87], Mc Cully *et al.* [124], Pearce [142], Schott *et al.* [167], Taiz & Zeiger [179]. While freezing tolerance describes physiological processes, such as a change in membrane composition or even a complete rearrangement of cell metabolism [123], freezing avoidance includes physical mechanisms to prevent intracellular ice formation [167]. Note that the term freezing avoidance may be confusing, as one of the most crucial mechanisms is actually the formation of extracellular ice, thus, the term refers to intracellular ice formation, which is lethal for plant cells. This indicates that the location of ice within the plants is of crucial importance. Other factors that hinder ice

formation are, for example, certain anti-freeze proteins (AFPs) [86, 142], which mainly control the location of ice formation, but do not change the ice-nucleation temperature considerably, and also deep supercooling to decrease the ice nucleation temperature down to  $-40^{\circ}$ C, compare Srivastava [176].

A crucial and actually the most interesting mechanism of frost resistance, considering the research questions that have been posed, is the formation of extracellular ice, as this mechanism is based on a structural property of the plant, as it is mainly determined by the porosity of the cell wall. In fact, the ice nucleation starts to initiate within plants in regions with the lowest content of solutes and proteins, which is the extracellular space, specifically in the xylem. Note that the location of ice formation is of importance also regarding extracellular ice formation, as suggested by Griffith & Antikainen [86], Pearce [142]. In general, extracellular ice formation occurs either on the surface of the cells, or at external boundaries, as discussed in Guy [88]. To this extent, the ice-formation pattern is also addressed in this monograph, where dispersed ice and localised ice are distinguished. In both cases, the presence of ice in the extracellular space causes a drop in water potential, which dehydrates the tissue cells, as addressed inter alia in Guy [88], Mc Cully et al. [124], Schott et al. [167], Taiz & Zeiger [179]. Thus, the extracellular ice body is increasing, the cells are further dehydrating. But there are two problems related to cell dehydration. It is required that the temperature drop is not too fast and the formation of extracellular ice occurs just to a moderate extent. Sudden exposure to very cold temperatures is lethal for plant cells, as intracellular ice formation is very likely in that particular case, compare Taiz & Zeiger [179]. Therein, the other problem has been described as excessive cell dehydration, when the exposure to frost is for too long. However, when none of this is the case, the cells rehydrate the extracellular ice after thawing, compare for example Mc Cully et al. [124], Schott et al. [167]. From a biological perspective, this process of cell dehydration and rehydration is reversible, meaning repeatable without tissue damage, however, it is not reversible from a thermodynamical point of view, as discussed later within this monograph.

### 2.2 Water potential

According to Rand [146] and Kundu & Cohen [113], the transport of mass, especially of water, may occur at three levels. First of all, individual cells may take up or release water. Secondly, at the tissue level, water can be transported from cell to cell on a short distance. Thirdly, for the long distance transport at the level of the whole plant, water can be transported within the vascular system. However, one could argue that the first two mentioned transport mechanisms are similar, as they are both based on the transport through the porous cell wall. The physical driving force for the transport of water at all of these levels is in most biology-based articles introduced as water potential, compare for the fluid dynamics of the vascular flow in plants in Boyer [31], Canny [34], Kramer [110], Molz [128], Rockwell *et al.* [152, 153, 154] as well as for the micro-porosity-based flow at the cell scale addressed in Cosgrove [38], Kramer & Boyer [111], Mc Cully *et al.* [124], Nonami & Boyer [139], Roden *et al.* [155], Steudle [177], Steudle & Boyer [178], Taiz & Zeiger [179]. In general, the water potential  $\Psi_w$  may have several components depending on the investigation the authors had in mind. In Kramer & Boyer [111], a rather general form of the water potential is given as

$$\Psi_w = \Psi_p + \Psi_s + \Psi_m + \Psi_q. \tag{2.1}$$

Therein,  $\Psi_p$  refers to the effect of pressure,  $\Psi_s$  to the effect of solutes,  $\Psi_m$  is the matric potential describing the interaction of the fluids and the biological tissue and  $\Psi_g$  is the gravitational potential. Note that the pressure driven flow of water is the predominant mechanism for the long-distance transport in the xylem, but also with regard to the cellwall perfusion, compare Taiz & Zeiger [179]. It is to be mentioned that this definition of the water potential does not specifically address the issue of ice formation. However, (2.1) can be either extended by additional components, or the impact of ice formation may be included in the pressure component, which is utilised within this monograph. The direction of the transport is generally oriented towards the lower potential, where the hydraulic conductivity of the material determines how fast the water flows. Hence, with this definition, a drop in water potential due to ice formation leads to a flow of water through the cell wall and as a consequence, the cells will dehydrate.

For the transport specifically at the cell scale, as for example addressed in Cosgrove [38], Kramer & Boyer [111], Nonami & Boyer [139], a simple transport equation is proposed, which is based on the water potential difference between the intracellular space and the extracellular space, which results in

$$J_v = \hat{L}_p \,\Delta \Psi_w. \tag{2.2}$$

Therein,  $J_v$  represents the flow of water per surface area,  $L_p$  the hydraulic conductivity of the cell walls and  $\Delta \Psi_w$  the difference of water potential across the cell wall. Note that this simple transport equation is in most biology-based articles usually also applied to the long-distance transport, although with an adapted hydraulic conductivity, especially as the pore space at the macroscopic scale may be anisotropic.

#### 2.3 The influence of moisture

In general, in a thermo-hydro-mechanical setting, material parameters may depend on several process variables, such as temperature or also on pressure. When plant tissues are treated, there is another property that needs to be taken into account, which is of crucial importance: moisture [156]. It describes essentially the water status of the plant, or specifically of the tissue cells. It may determine, whether a plant is frost-resistant or not. But also apart from the frost resistance of plants, the status of the water content of tissue cells is important with regard to many processes occurring in plant tissues, inter alia photosynthesis, protein synthesis and other physiological processes, as outlined in Taiz & Zeiger [179]. The water status of plants is usually addressed by the moisture content  $M_C$ , as introduced in Ross [156]. It is defined via

$$M_C = \frac{m_w}{m_d} (\times 100\%) = \frac{m_g - m_d}{m_d} (\times 100\%),$$
(2.3)

where  $m_w$  is the mass of water in a (plant/wood) specimen,  $m_d$  is the mass of ovendry wood and  $m_g$  is the mass of green wood with a certain moisture content  $M_C$ . The term ovendry wood refers to the state of the wood (or plant) without any water, sometimes it is also referred to as dry weight. Note that the value for  $M_C$  defined in (2.3) may exceed unity, or 100 % in case the percentage is addressed.

Generally, plants are hygroscopic meaning that they are capable of taking moisture from the surrounding environment [156]. Furthermore, they can also take water from the soil by the roots [111]. Depending on the moisture content, the physical and mechanical properties of plants may change as a function of the moisture content, at least below a threshold value, above which, the depedency is rather low. However, a functional relationship of a certain material parameter to the moisture content is usually not known, therefore, standard values are utilised, which refer to a reference state of a moisture content of (usually) 12%, as discussed in Ross [156].

There is another property that needs to be discussed, that is closely related to the moisture content, namely the stability or structural rigidity of the plant. At this point, it is sensible to differentiate the plants between woody plants that contain lignified elements [133, 166, 167], and those plants that do not contain any lignified elements [124]. For example, herbaceous plants maintain their structural rigidity through the water uptake of their cells. This in turn creates the mentioned turgor pressure, a pressure in the cells, which allows these plants to keep upright, compare Mc Cully *et al.* [124], Taiz & Zeiger [179]. As the mechanism of frost resistance that is based on structural properties of the plant by the formation of extracellular ice applies to both types of plants, this monograph is focussed on woody plants in order to avoid issues in relation to a loss of rigidity. Furthermore, note that the material parameters introduced in this monograph will be constant values referring to the reference state discussed in Ross [156].

## Chapter 3: Fundamentals of multiphasic and multicomponent materials

This chapter provides an overview of the theoretical fundamentals for the description of the mechanics and thermodynamics of multiphasic and multicomponent materials with special attention on plants. However, within the scope of this monograph, the focus is solely on a continuum-mechanical and macroscopic description in the framework of the TPM. Therefore, the TPM is introduced with basic notions regarding the kinematics of superimposed and mutually interacting constituents including a kinematic coupling of the solid constituents. Furthermore, the stress concept for multiphasic continua is addressed, as are the specific balance relations based on the concept of master balances. Finally, the implications of the phase transition of water from a liquid state to a solid state, and vice versa, are discussed in terms of the conceptional basis. In particular, the phase transition is treated by introducing a singular surface.

#### 3.1 The Theory of Porous Media

The issue of ice formation and the related dehydration of the plant cells as a consequence of the involved thermo-hydro-mechanical processes requires a holistic approach that combines the well established classical theories from solid and fluid mechanics that accounts for the multiple interactions within the considered plant-tissue system. The first crucial question is how to treat the material under consideration with the mutual interactions in terms of homogenisation, as discussed, inter alia, in de Boer [22], Ehlers [44] or Wagner [187]. Therein, two possibilities are outlined: Either the parts of a certain multiphasic material are treated by the classical singlephasic theories by separating them from each other with *Euler*'s cut principle, where each part is considered in its own volume of the domain with appropriate transition conditions with the other parts, which requires the knowledge of the microstructure and the corresponding transition conditions. This can be regarded as the exact solution. However, this is not feasible for the current investigation, particularly as this geometric and physical data is not available. Moreover, within the scope of this investigation such a precise knowledge, a microstructural resolution, is not necessary and, therefore, not in the author's interest. This leads to the second possibility, where instead an a-priori statistical average of the on the microstructure involved parts of the multiphasic material is used. In this approach, "smeared" substitute continua emerge, which fill the entire control space simultaneously. For this description, the standard models from continuum mechanics apply, in which all geometrical and physical properties as well as parameters are defined anywhere in the domain in an average sense, in particular also the interactions and couplings among the different parts. This modern concept of the Theory of Porous Media traces back to the Theory of Mixtures (TM), compare Bowen [28].
Here, his pioneering work needs to be mentioned for the description of incompressible, cf. [29], and compressible, cf. [30], mixtures as well as the work of Truesdell & Toupin [184]. However, in the modern formulation of the TPM, the TM is extended by the concept of volume fractions. The concept of volume fractions has been introduced to have a measure of the local composition of the material. As pointed out by Ehlers [48], this measure has already been used by Woltmann [192]. Also Biot [14] addressed in his classical works the composition of a medium. The historical development of theories describing porous media with a focus on macroscopic theories is discussed in Bluhm & de Boer [17], de Boer [22], Ehlers [48, 51], Schanz & Diebels [160]. The current comprehension of the TPM is given, for example, in de Boer [23], Ehlers [47], Ehlers & Bluhm [54].

Both possibilities, i. e. the local singlephasic description as well as macroscopic descriptions, are extensively used in dealing with porous-media problems, where hereinafter of this monograph several ideas and applications will be reviewed in terms of their potential to describe the introduced processes at subzero temperatures in frost-resistant plant tissues.

Note that for the sake of accuracy, the nomenclature regarding the "parts" of a multiphasic material is as follows. The plant tissue is composed of several components, i. e. water, air and biological tissue material. Each of these components can, in general, exist in different phases, i. e. solid, liquid and gas, hence, the notion phase addresses the state of physical aggregation. The term constituent is used in the context of a modelling approach, where all constituents add up to the overall plant-tissue aggregate, cf. e. g. [187].

# 3.2 Modelling approach

In this section, the basic considerations of the applied TPM models are given including a statement regarding the involved components, phases and constituents. Already at this stage, the ice-formation pattern is addressed and its consequence on the modelling approach.

# 3.2.1 Basic considerations

For the in **Chapter 2** introduced plants, the composition in a natural (unfrozen) state is very similar with regard to the basic macroscopic components, i. e. biological (hard and soft) tissue material, water and air. In particular, the solid skeleton is assumed to be composed of lignified (hard) tissue material, i. e. the xylem, as well as (soft) tissue cells that contain predominantly water. Within the macro-pore space there are two immiscible fluids, namely water and air.

Since intracellular freezing needs to be avoided, the tissue cells may release (and in general also gain) water through the micro pores of the cell wall to the macro pore space. Therefore, the plants under consideration are materials that exhibit a double-porosity feature. Note that within the macro-pore space there are two immiscible fluids, i. e. water and air, whereas in the micro-pore space there is just water, as there is no significant air transport through the micro pores. For the intracellular water, there is no independent state of motion assumed, in fact, it is part of the solid aggregate. The relative motion of water within the micro pores is, therefore, neglected or, more precisely, considered in terms of mass exchange of water through the cell wall.

The difference between the two suggested plants is mainly in the location and pattern of ice formation, which motivates the introduction of two different modelling approaches. For the example of the *Betula nana*, ice formation occurs in a dispersed way within the intercellular (macro-pore) space of the plant tissue. Thus, it is reasonable to include the phase transition of water explicitly in the modelling approach. Instead, for the example of Equisetum hyemale, the ice predominantly forms localised at internal surfaces within the vallecular canals and the pith cavity. Hence, one can argue, that the ice formation actually occurs at the boundary of the material. Therefore, for Equisetum hyemale a ternary modelling approach (without the ice) has been chosen, where the impact of ice formation on the tissue material is modelled by imposing appropriate boundary conditions that are caused by the formation of ice at the internal surfaces. Consequently, two different modelling approaches are described below, the quaternary Model I for the description of dispersed ice formation in the intercellular space, and the reduced ternary Model II for the description of the impact of localised, extracellular ice formation at the plant's surface onto the plant tissue. Note that throughout Chapter 3 and Chapter 4, the quaternary Model I is addressed, unless stated differently.

# 3.2.2 Quasi double-porosity model with ice formation

The quaternary modelling approach for dispersed ice formation is based on the TPM and proceeds from a solid skeleton  $\varphi^S$  as introduced in **Subsection 3.2.1** representing biological hard and soft tissue material. The hard tissue is typically lignified biological material, the soft tissue is constituted by cells with trapped water, which can leave and enter the cells due to their micro porosity. The cells may contain a significant amount of water, namely up to 90%, compare Taiz & Zeiger [179]. In addition to the micro porosity at the cell scale, there is also the porosity at the tissue scale. This macro-pore space is filled with two immiscible fluids, namely, gaseous air  $\varphi^G$  and liquid water  $\varphi^L$ , where the latter is subjected to a phase transition and may turn into solid ice  $\varphi^I$ , as depicted in Figure 3.1 according to Eurich *et al.* [72], such that there are four constituents, viz.:

$$\varphi = \bigcup_{\alpha} \varphi^{\alpha} = \varphi^{S} \cup \varphi^{I} \cup \varphi^{L} \cup \varphi^{G}.$$
(3.1)

Their real microstructural properties have been volumetrically homogenised over the representative elementary volume (REV). Consequently, all physical quantities at the macroscale are defined anywhere in the considered domain, cf. e. g. Ehlers & Kubik [60].

## 3.2.3 Basic quantities of the TPM models

In general, a porous medium is comprised of a solid skeleton and one or more fluids in the pore space. Within the pore space there might be a mixture of miscible or immiscible liquids and/or gases. However, within this monograph, the mixture of miscible fluids can



concept of volume fractions

**Figure 3.1:** Representative elementary volume (REV) with schematically shown microstructure and resulting macroscopic quaternary TPM model specifying the volume fractions.

be omitted. Regarding miscible constituents, the interested reader is referred to the works of Ehlers [46] and Wagner [187]. The mixture of immiscible constituents, as discussed in Ehlers [44, 49], can be understood as "smeared" and superimposed continua, obtained after a virtual homogenisation. The volume of the overall aggregate  $\varphi$  is composed of the partial volumes via

$$V = \int_{\mathcal{B}} \mathrm{d}v = \sum_{\alpha} V^{\alpha}, \quad \text{with} \quad V^{\alpha} = \int_{\mathcal{B}} \mathrm{d}v^{\alpha} =: \int_{\mathcal{B}} n^{\alpha} \mathrm{d}v, \quad (3.2)$$

where the fundamental variable to address the amount of a constituent at a certain location has been introduced by the volume fraction  $n^{\alpha} = n^{\alpha}(\mathbf{x}, t)$ , viz.:

$$n^{\alpha} = \frac{\mathrm{d}v^{\alpha}}{\mathrm{d}v},\tag{3.3}$$

which is the ratio of the partial volume  $dv^{\alpha}$  to the bulk volume dv. As there is no vacant space within the porous domain, the saturation condition

$$\sum_{\alpha} n^{\alpha} = n^{S} + n^{I} + n^{L} + n^{G} = 1$$
(3.4)

holds at any time. In case there is more than one immiscible fluid in the pore space, it is common to introduce a further measure, the saturation, to address the amount of a pore fluid  $\varphi^{\beta}$  in reference to the pore space  $\varphi^{F}$ . Therein,  $\beta = \{L, G\}$  addresses a certain pore fluid of the overall pore space  $\varphi^{F} = \varphi^{L} \cup \varphi^{G}$ . Within this monograph the concept of saturation is only utilised for macro-pore fluids. In the particular case of the present modelling approaches, the saturations  $s^{\beta}$  are defined via

$$s^{\beta} = \frac{n^{\beta}}{n^{F}}, \quad \text{where} \quad n^{F} = \sum_{\beta} n^{\beta} = n^{L} + n^{G}.$$
 (3.5)

There is also a constraint for the sum of the saturations, which follows from (3.4), viz.:

$$\sum_{\beta} s^{\beta} = s^{L} + s^{G} = 1.$$
 (3.6)

Moreover, it is convenient to introduce also a relative volumetric measure regarding the water component, which might occur in a solid state  $\varphi^I$  and a liquid state  $\varphi^L$  within the chosen modelling approach. Thus, the relative amount of ice and liquid water, respectively, with respect to the volume fraction of water (ice and liquid), can be addressed via

$$n_W^I = \frac{n^I}{n^W}, \quad n_W^L = \frac{n^L}{n^W}, \quad \text{where} \quad n^W = n^I + n^L.$$
 (3.7)

The relative measures add also up to unity, viz.:

$$n_W^I + n_W^L = 1. (3.8)$$

As a result of the actual or virtual averaging process of the microstructure, two densities can be introduced, the partial density  $\rho^{\alpha}$  and the effective (realistic) density  $\rho^{\alpha R}$ , respectively, via

$$\rho^{\alpha} = \frac{\mathrm{d}m^{\alpha}}{\mathrm{d}v} \quad \text{and} \quad \rho^{\alpha R} = \frac{\mathrm{d}m^{\alpha}}{\mathrm{d}v^{\alpha}}, \quad \text{where} \quad \rho^{\alpha} = n^{\alpha}\rho^{\alpha R}.$$
(3.9)

Therein,  $dm^{\alpha}$  is the mass element of  $\varphi^{\alpha}$ . The summation over all partial densities  $\rho^{\alpha}$  yields the bulk density  $\rho$  of the overall aggregate via

$$\rho = \sum_{\alpha} \rho^{\alpha}. \tag{3.10}$$

# **3.3** Kinematics

This section is mainly based on fundamental works regarding the motion of superimposed constituents, as for example treated in de Boer [24], Ehlers & Bluhm [54] or in concise form in Häberle [89], Wagner [187]. Basic concepts with regard to the state of motion of a multicomponent and multiphasic aggregate are given including deformation measures, rate of deformation measures as well as concerning a kinematical coupling of two constituents, as in Bluhm *et al.* [18], Eurich *et al.* [72], Ricken & Bluhm [147]. Further details with respect to the deformation tensors within a thermomechanical framework are given in **Section 4.2**.

## 3.3.1 Motion of superimposed continua

A crucial postulation within the continuum-mechanical framework of the TPM is that the mutually interacting constituents are spatially superimposed. This idea of superposition requires that all constituents are present at any location with a certain amount that is characterised in this context by the volume fraction  $n^{\alpha}$ . More accurately stating, the

body  $\mathcal{B}$  consists of a collection of spatially superimposed material points  $\mathcal{P}^{\alpha}$ , where the set of material points at the boundary determines the surface  $\mathcal{S}$  of the body  $\mathcal{B}$ . Since the motion of the constituents is, in general, independent from each other, different reference configurations have to be introduced, as shown in Figure 3.2 according to Eurich *et al.* [72]. Therefore, for Model II, the reference configuration is given at time  $t_0$  with the constituents as indicated in Figure 3.2, the current configuration at time t with the superimposed material points  $\mathcal{P}^S, \mathcal{P}^L$  and  $\mathcal{P}^G$ . For Model I, however, there exists additionally to the in Figure 3.2 depicted reference configuration, an intermediate configuration at time  $t_{0I}$ , when ice formation starts, which can be understood as the reference configuration for the ice. The ice is then, for subsequent time steps, attached to the solid skeleton and, therefore, kinematically coupled, which is an a priori constitutive assumption, as introduced in Eurich *et al.* [72] for plant tissues. The kinematic coupling is discussed in **Subsection 3.3.4**. The current configuration at time t is given by superimposed material points  $\mathcal{P}^S, \mathcal{P}^G, \mathcal{P}^L$  and  $\mathcal{P}^I$ .



Figure 3.2: Motion and kinematic coupling of the quarternary TPM model.

In order to assure the independence of the motion of the respective constituents, one has to introduce formally individual motion functions  $\chi_{\alpha}$  that map for each constituent the reference configuration  $\mathbf{X}_{\alpha}$  to the current configuration  $\mathbf{x}$  via

$$\mathbf{x} = \boldsymbol{\chi}_{\alpha}(\mathbf{X}_{\alpha}, t). \tag{3.11}$$

Since the motion is unique and uniquely invertible, there is a corresponding reference configuration

$$\mathbf{X}_{\alpha} = \boldsymbol{\chi}_{\alpha}^{-1}(\mathbf{x}, t) \tag{3.12}$$

assigned to each current configuration via the inverse motion function  $\chi_{\alpha}^{-1}$ , in case a non-singular *Jacobian* determinant  $J_{\alpha}$  exists, viz.:

$$J_{\alpha} := \det\left(\frac{\partial \boldsymbol{\chi}_{\alpha}(\mathbf{X}_{\alpha}, t)}{\partial \mathbf{X}_{\alpha}}\right) \neq 0.$$
(3.13)

Based on (3.11) and (3.12), individual velocities and accelerations can be derived in the *Lagrange*an description via

$$\mathbf{\dot{x}}_{\alpha} = \frac{\partial \boldsymbol{\chi}_{\alpha}(\mathbf{X}_{\alpha}, t)}{\partial t} \quad \text{and} \quad \mathbf{\ddot{x}}_{\alpha} = \frac{\partial^2 \boldsymbol{\chi}_{\alpha}(\mathbf{X}_{\alpha}, t)}{\partial t^2},$$
 (3.14)

or in an *Euler*ian description by using the inverse motion resulting in

$$\mathbf{\dot{x}}_{\alpha} = \mathbf{\dot{x}}_{\alpha} \left[ \mathbf{\chi}_{\alpha}^{-1}(\mathbf{x}, t), t \right] = \mathbf{\dot{x}}_{\alpha} \left( \mathbf{x}, t \right) \quad \text{and} \quad \mathbf{\ddot{x}}_{\alpha} = \mathbf{\ddot{x}}_{\alpha} \left[ \mathbf{\chi}_{\alpha}^{-1}(\mathbf{x}, t), t \right] = \mathbf{\ddot{x}}_{\alpha} \left( \mathbf{x}, t \right). \tag{3.15}$$

In (3.14) and (3.15), the material time derivative  $(\cdot)'_{\alpha}$  of an arbitrary quantity following the motion of the constituent  $\varphi^{\alpha}$  has been utilised. The calculation of this derivative in a *Lagrange*an description is straightforward. However, in an *Euler*ian setting the implicit time dependency of **x** has to be considered for arbitrary scalar-valued field functions  $\Upsilon$ and vector-/tensor-valued field functions  $\Upsilon$ , respectively, via

$$(\Upsilon)'_{\alpha} = \frac{\mathrm{d}_{\alpha}}{\mathrm{d}t}\Upsilon(\mathbf{x},t) = \frac{\partial\Upsilon}{\partial t} + \operatorname{grad}\Upsilon\cdot\mathbf{\dot{x}}_{\alpha}, (\Upsilon)'_{\alpha} = \frac{\mathrm{d}_{\alpha}}{\mathrm{d}t}\Upsilon(\mathbf{x},t) = \frac{\partial\Upsilon}{\partial t} + (\operatorname{grad}\Upsilon)\mathbf{\dot{x}}_{\alpha}.$$
(3.16)

Similarly, the material time derivative with respect to the motion of the overall aggregate  $\varphi$  can be defined via

$$\dot{\Upsilon} = \frac{\mathrm{d}}{\mathrm{d}t}\Upsilon(\mathbf{x},t) = \frac{\partial\Upsilon}{\partial t} + \operatorname{grad}\Upsilon\cdot\dot{\mathbf{x}}, 
\dot{\Upsilon} = \frac{\mathrm{d}}{\mathrm{d}t}\Upsilon(\mathbf{x},t) = \frac{\partial\Upsilon}{\partial t} + (\operatorname{grad}\Upsilon)\dot{\mathbf{x}}.$$
(3.17)

Therein, the velocity of the overall aggregate has to be understood as barycentric velocity  $\dot{\mathbf{x}}$  that can be derived from the equality of the linear momentum of the overall aggregate to the sum of the linear momentum of the respective constituents via

$$\dot{\mathbf{x}} = \frac{1}{\rho} \sum_{\alpha} \rho^{\alpha} \, \dot{\mathbf{x}}_{\alpha} \,. \tag{3.18}$$

The difference between the velocity of a constituent to the velocity of the overall aggregate is defined as the diffusion velocity of  $\varphi^{\alpha}$ 

$$\mathbf{d}_{\alpha} := \mathbf{x}_{\alpha} - \dot{\mathbf{x}} \,. \tag{3.19}$$

Within the framework of the TPM it is customary to address the motion of the solid skeleton in a *Lagrange* setting by the solid displacement field, which is defined via

$$\mathbf{u}_S = \mathbf{x} - \mathbf{X}_S. \tag{3.20}$$

The velocity of the pore fluids is commonly described within a modified *Euler* ian description by the seepage velocity

$$\mathbf{w}_{\beta} = \mathbf{x}_{\beta} - \mathbf{x}_{S}, \tag{3.21}$$

where the velocity of the respective pore fluid is related to the velocity of the solid skeleton. Note in passing that the ice is kinematically coupled to the solid skeleton, the consequences will be discussed in **Subsection 3.3.4**.

Finally, in some case it is useful to switch the material time derivative of a quantity referring to the motion of the solid skeleton rather than to the motion of one of the fluids. This can be achieved by utilising  $(3.16)_1$  and (3.21), which leads to

$$(\cdot)'_{\beta} = (\cdot)'_{S} + \operatorname{grad}(\cdot) \cdot \mathbf{w}_{\beta}$$
(3.22)

for an arbitrary scalar-valued field function.

# **3.3.2** Deformation and strain measures

In continuum mechanics of single- and multiphasic materials, the basic quantity to characterise the motion and/or deformation is the material deformation gradient  $\mathbf{F}_{\alpha}$ , defined via

$$\mathbf{F}_{\alpha} = \frac{\partial \boldsymbol{\chi}_{\alpha}(\mathbf{X}_{\alpha}, t)}{\partial \mathbf{X}_{\alpha}} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}_{\alpha}} = \operatorname{Grad}_{\alpha} \mathbf{x}, 
\mathbf{F}_{\alpha}^{-1} = \frac{\partial \boldsymbol{\chi}_{\alpha}^{-1}(\mathbf{x}, t)}{\partial \mathbf{x}} = \frac{\partial \mathbf{X}_{\alpha}}{\partial \mathbf{x}} = \operatorname{grad} \mathbf{X}_{\alpha},$$
(3.23)

where  $\mathbf{F}_{\alpha}^{-1}$  is the inverse of the material deformation gradient. It is alternatively defined via

$$\mathbf{F}_{\alpha}^{-1} = \frac{(\operatorname{cof} \mathbf{F}_{\alpha})^{T}}{\det \mathbf{F}_{\alpha}}, \qquad (3.24)$$

where  $\operatorname{cof}(\cdot)$  is the cofactor of a tensor, cf. Ehlers [50]. It is evident that the inverse deformation gradient  $\mathbf{F}_{\alpha}^{-1}$  exists just for the case of det  $\mathbf{F}_{\alpha} \neq 0$ .

The physical interpretation of the deformation gradient is actually the transport of a line element from the reference configuration  $\mathbf{X}_{\alpha}$  to the current configuration  $\mathbf{x}$  via

$$\mathrm{d}\mathbf{x} = \mathbf{F}_{\alpha} \,\mathrm{d}\mathbf{X}_{\alpha}.\tag{3.25}$$

The corresponding transport theorems for the area element and the volume element are stated for the sake of completeness without proof, the interested reader is referred to the in the introductory remarks of this section mentioned works. The transport theorems are defined as

$$d\mathbf{a} = (\operatorname{cof} \mathbf{F}_{\alpha}) d\mathbf{A}_{\alpha} \quad \text{and} \quad dv = (\det \mathbf{F}_{\alpha}) dV_{\alpha}. \tag{3.26}$$

However, the deformation gradient may contain not only deformation, but also superimposed rigid body motion. Therefore, real deformation measures have to be derived that characterise the stretch of a line element and not its rotation. These are introduced based on the squares of line elements in the current and in the reference configuration, respectively,

$$d\mathbf{x} \cdot d\mathbf{x} = d\mathbf{X}_{\alpha} \cdot (\mathbf{F}_{\alpha}^{T} \mathbf{F}_{\alpha}) d\mathbf{X}_{\alpha} =: d\mathbf{X}_{\alpha} \cdot \mathbf{C}_{\alpha} d\mathbf{X}_{\alpha}, d\mathbf{X}_{\alpha} \cdot d\mathbf{X}_{\alpha} = d\mathbf{x} \cdot (\mathbf{F}_{\alpha}^{T-1} \mathbf{F}_{\alpha}^{-1}) d\mathbf{x} =: d\mathbf{x} \cdot \mathbf{B}_{\alpha}^{-1} d\mathbf{x},$$
(3.27)

where  $\mathbf{C}_{\alpha}$  is the right *Cauchy-Green* deformation tensor and  $\mathbf{B}_{\alpha}$  the left *Cauchy-Green* deformation tensor. It follows for the difference of the squares of line elements

$$d\mathbf{x} \cdot d\mathbf{x} - d\mathbf{X}_{\alpha} \cdot d\mathbf{X}_{\alpha} = \begin{cases} d\mathbf{X}_{\alpha} \cdot 2 \, \mathbf{E}_{\alpha} \, d\mathbf{X}_{\alpha}, \\ d\mathbf{x} \cdot 2 \, \mathbf{A}_{\alpha} \, d\mathbf{x}, \end{cases}$$
(3.28)

where the *Green*ean strain tensor  $\mathbf{E}_{\alpha}$  and the *Almansi* strain tensor  $\mathbf{A}_{\alpha}$  are defined as in (3.28) via

$$\mathbf{E}_{\alpha} = \frac{1}{2} (\mathbf{C}_{\alpha} - \mathbf{I}), \quad \mathbf{A}_{\alpha} = \frac{1}{2} (\mathbf{I} - \mathbf{B}_{\alpha}^{-1}). \tag{3.29}$$

Finally, in order to address both configurations (and variances, cf. e. g. Markert [121]), the *Karni-Reiner* tensors are defined as

$$\mathbf{K}_{\alpha} = \frac{1}{2} \left( \mathbf{I} - \mathbf{C}_{\alpha}^{-1} \right) : \text{ referential Karni-Reiner tensor,}$$

$$\mathbf{K}_{\alpha} = \frac{1}{2} \left( \mathbf{B}_{\alpha} - \mathbf{I} \right) : \text{ spatial Karni-Reiner tensor.}$$
(3.30)

# 3.3.3 Rates of deformation

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Although time-dependent effects are not considered in the chosen modelling approach, a proper definition of the rate of deformation measures is still of importance, since they are necessary to apply the entropy principle. Therefore, the material derivative of the deformation gradient is given via

$$(\mathbf{F}_{\alpha})'_{\alpha} = \frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \mathbf{F}_{\alpha} = \frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \left( \frac{\partial \mathbf{x}(\mathbf{X}_{\alpha}, t)}{\partial \mathbf{X}_{\alpha}} \right) = \frac{\partial \mathbf{x}_{\alpha}(\mathbf{X}_{\alpha}, t)}{\partial \mathbf{X}_{\alpha}} = \operatorname{Grad}_{\alpha} \mathbf{x}_{\alpha}$$

$$= \frac{\partial \mathbf{x}_{\alpha}(\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \mathbf{X}_{\alpha}} =: \mathbf{L}_{\alpha} \mathbf{F}_{\alpha},$$

$$(3.31)$$

where the spatial velocity gradient  $\mathbf{L}_{\alpha}$  has already been introduced, it is defined as

$$\mathbf{L}_{\alpha} = (\mathbf{F}_{\alpha})_{\alpha}' \mathbf{F}_{\alpha}^{-1} = \operatorname{grad} \mathbf{x}_{\alpha}'.$$
(3.32)

The spatial velocity gradient can be decomposed into a symmetric part  $\mathbf{D}_{\alpha}$  and a skew-symmetric part  $\mathbf{W}_{\alpha}$ , such that

$$\mathbf{L}_{\alpha} := \mathbf{D}_{\alpha} + \mathbf{W}_{\alpha}, \quad \text{where} \quad \begin{cases} \mathbf{D}_{\alpha} &= \frac{1}{2} \left( \mathbf{L}_{\alpha} + \mathbf{L}_{\alpha}^{T} \right) \quad \text{and} \quad \mathbf{D}_{\alpha} = \mathbf{D}_{\alpha}^{T}, \\ \mathbf{W}_{\alpha} &= \frac{1}{2} \left( \mathbf{L}_{\alpha} - \mathbf{L}_{\alpha}^{T} \right) \quad \text{and} \quad \mathbf{W}_{\alpha} = -\mathbf{W}_{\alpha}^{T}, \end{cases}$$
(3.33)

where  $\mathbf{D}_{\alpha}$  is the rate of deformation tensor and  $\mathbf{W}_{\alpha}$  the spin-tensor. The following property of these tensors will be used later in this monograph

$$\mathbf{L}_{\alpha} \cdot \mathbf{I} = \mathbf{D}_{\alpha} \cdot \mathbf{I} = (\operatorname{grad} \mathbf{x}_{\alpha}') \cdot \mathbf{I} = \operatorname{div} \mathbf{x}_{\alpha}' .$$
(3.34)

Here, use is made of a generic property of the scalar product of two tensors of second order. The scalar product of a symmetric tensor, here  $\mathbf{I}$ , with a skew symmetric tensor,

here  $\mathbf{W}_{\alpha}$ , vanishes, therefore, (3.34) holds. Finally, the derivative of the right *Cauchy-Green* deformation tensor will be needed in the evaluation of the entropy inequality, which is given via

$$(\mathbf{C}_{\alpha})_{\alpha}' = (\mathbf{F}_{\alpha}^{T}\mathbf{F}_{\alpha})_{\alpha}' = (\mathbf{F}_{\alpha}^{T})_{\alpha}' \mathbf{F}_{\alpha} + \mathbf{F}_{\alpha}^{T} (\mathbf{F}_{\alpha})_{\alpha}' = (\mathbf{L}_{\alpha}\mathbf{F}_{\alpha})^{T} \mathbf{F}_{\alpha} + \mathbf{F}_{\alpha}^{T} (\mathbf{L}_{\alpha}\mathbf{F}_{\alpha}) = \mathbf{F}_{\alpha}^{T} (\mathbf{L}_{\alpha}^{T} + \mathbf{L}_{\alpha}) \mathbf{F}_{\alpha}$$

$$= 2 \mathbf{F}_{\alpha}^{T} \mathbf{D}_{\alpha} \mathbf{F}_{\alpha}.$$

$$(3.35)$$

# 3.3.4 Kinematic coupling

The usual assumption within the TPM of an independent state of motion is maintained for the solid skleton and the two fluids in the macro-pore space. However, it should be noted that the solid skeleton is itself already a multicomponent material, as it is composed of hard and soft tissue material as well as enclosed cell water. The water within the cells including their micro pores is part of the solid skeleton and, therefore, addressed by the state of motion of the solid skeleton. Furthermore, in case of the ice, the assumption is made that the ice is also kinematically coupled to the solid skeleton. This assumption is justified by the fact that the ice nucleous forms most likely at the surface of the solid skeleton, compare Pearce [142]. Since ice is not necessarily present in the reference configuration, but it is rather the result of an evolving freezing process, an intermediate configuration is introduced, which is at the same time the reference configuration  $\hat{\mathbf{X}}_{I} = \hat{\mathbf{X}}_{I}(t)$  of the ice in the motion chart, when ice is initially formed. In particular, before the onset of ice formation, the pore water is present as liquid and is mobile within the macro-pore space. It is emphasized that only mobile pore water within the macro-pore space may freeze. After initial ice formation at time  $t = t_{0I}$ , cf. Figure 3.2, the ice is kinematically coupled to the solid skeleton indicating that they have the same motion function and the same velocity. This kind of kinematic coupling is comprehensively described in Bluhm et al. [18], Ricken & Bluhm [147] and in application to plant tissues given in Eurich *et al.* [72], viz.:

$$\boldsymbol{\chi}_{I}(\hat{\mathbf{X}}_{I},t) = \boldsymbol{\chi}_{S}(\mathbf{X}_{S},t) \longrightarrow \mathbf{x}_{I} = \mathbf{x}_{S}^{\prime}.$$
 (3.36)

This indicates also for the material time derivatives (3.22) that

$$(\cdot)_I' = (\cdot)_S'. \tag{3.37}$$

The deformation measures of the ice have been derived by using the intermediate configuration at time  $t = t_{0I}$ , together with the equality of the motion functions, cf.  $(3.36)_1$ , where the derivatives are interpreted as follows, viz.:

$$\underbrace{\frac{\partial \boldsymbol{\chi}_{S}(\mathbf{X}_{S},t)}{\partial \mathbf{X}_{S}}}_{\mathbf{F}_{S}} = \frac{\partial \boldsymbol{\chi}_{I}(\mathbf{\hat{X}}_{I},t)}{\partial \mathbf{X}_{S}} = \underbrace{\frac{\partial \boldsymbol{\chi}_{I}(\mathbf{\hat{X}}_{I},t)}{\partial \mathbf{\hat{X}}_{I}}}_{\mathbf{F}_{I}}\underbrace{\frac{\partial \mathbf{\hat{X}}_{I}}{\partial \mathbf{X}_{S}}}_{\mathbf{F}_{S0}}.$$
(3.38)

The left side of (3.38) is defined as the deformation gradient  $\mathbf{F}_S$  of the solid skeleton, the right side of the same equation defines the deformation gradient  $\mathbf{F}_I$  of the ice with respect

to its reference configuration  $\hat{\mathbf{X}}_{I}$ , which is the intermediate configuration, applied to the initial deformation of the solid skeleton  $\mathbf{F}_{S0}$  until the ice forms initially in the intermediate configuration, relating the solid line element in the intermediate configuration  $\hat{\mathbf{X}}_{I}$  to the reference configuration  $\mathbf{X}_{S}$  of the solid skeleton. Consequently, the deformation gradient  $\mathbf{F}_{I}$  is given via

$$\mathbf{F}_S = \mathbf{F}_I \mathbf{F}_{S0} \longrightarrow \mathbf{F}_I = \mathbf{F}_S \mathbf{F}_{S0}^{-1}. \tag{3.39}$$

With the deformation gradient  $\mathbf{F}_{I}$  of the ice as the basic deformation quantity, all other deformation measures, as generally discussed in **Subsection 3.3.2**, can be derived.

Concerning the rate of deformation measures, one can easily show with the definitions (3.32) and (3.36) that the spatial velocity gradient  $\mathbf{L}_I$  of the ice and the spatial velocity gradient  $\mathbf{L}_S$  of the solid skeleton coincide. This can be used to define also the material deformation gradient  $(\mathbf{F}_I)'_I$  of the ice via

$$(\mathbf{F}_{I})_{I}^{\prime} = \frac{\mathrm{d}_{I}}{\mathrm{d}t} \mathbf{F}_{I} = \frac{\mathrm{d}_{I}}{\mathrm{d}t} \left( \frac{\partial \mathbf{x}(\hat{\mathbf{X}}_{I}, t)}{\partial \hat{\mathbf{X}}_{I}} \right) = \frac{\partial \overset{\prime}{\mathbf{x}}_{I} (\hat{\mathbf{X}}_{I}, t)}{\partial \hat{\mathbf{X}}_{I}} = \operatorname{Grad}_{I} \overset{\prime}{\mathbf{x}}_{I}$$

$$= \frac{\partial \overset{\prime}{\mathbf{x}}_{I} (\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \hat{\mathbf{X}}_{I}} = \frac{\partial \overset{\prime}{\mathbf{x}}_{S} (\mathbf{x}, t)}{\partial \mathbf{x}} \frac{\partial \mathbf{x}}{\partial \hat{\mathbf{X}}_{I}}$$

$$= \mathbf{L}_{S} \mathbf{F}_{I} = \mathbf{L}_{S} \mathbf{F}_{S} \mathbf{F}_{S0}^{-1}, \qquad (3.40)$$

expressed in terms of the solid motion, which is customary, since the solid displacement  $\mathbf{u}_S$  will be primary variable in a numerical campaign. Remaining deformation measures for the ice can be derived as introduced in **Subsection 3.3.3**.

# **3.4** State of stress

Since the in the preceding sections introduced finite deformations are caused by stresses in the body  $\mathcal{B}$  (or vice versa), the acting foces on the volume of body  $\mathcal{B}$  and its surface  $\mathcal{S}$  need to be introduced, cf. Figure 3.2. Furthermore, they need to be related to the respective volume and surface elements on which they are acting. This motivates the introduction of several stress measures in this section, as discussed in Ehlers [45], Häberle [89].

## **3.4.1** Surface and volume forces

In general, there are forces that act from a distance on the body  $\mathcal{B}$  and contact forces that act at the surface  $\mathcal{S}$ . In this regard, on each material point  $\mathcal{P}^{\alpha}$  of constituent  $\varphi^{\alpha}$  there might act an external body force  $\mathbf{f}^{\alpha}$  per volume element dv leading to the total volume force per constituent

$$\mathbf{k}_{V}^{\alpha} = \int_{\mathcal{B}} \mathbf{f}^{\alpha} \mathrm{d}v, \quad \text{where} \quad \mathbf{f}^{\alpha} = \rho^{\alpha} \, \mathbf{b}^{\alpha}. \tag{3.41}$$

Here, the a priori assumption has been made that within the framework of thermo-hydromechanical modelling, gravitation is the only body force. In addition, there are also forces acting on material points  $\mathcal{P}^{\alpha}$  at the surface  $\mathcal{S}$  of body  $\mathcal{B}$ . These forces are contact forces that act on the oriented area element d**a** and are defined accordingly via

$$\mathbf{k}_{O}^{\alpha} = \int_{\mathcal{S}} \mathbf{t}^{\alpha} \mathrm{d}a, \qquad (3.42)$$

where  $\mathbf{t}^{\alpha} = \mathbf{t}^{\alpha}(\mathbf{x}, t, \mathbf{n})$  is the surface traction when  $\mathbf{n}$  is the outward-oriented unit surface normal. The summation of the volume and surface forces define the overall constituentspecific force vector

$$\mathbf{k}^{\alpha} = \mathbf{k}^{\alpha}_{V} + \mathbf{k}^{\alpha}_{O} = \int_{\mathcal{B}} \mathbf{f}^{\alpha} \mathrm{d}v + \int_{\mathcal{S}} \mathbf{t}^{\alpha} \mathrm{d}a.$$
(3.43)

## 3.4.2 Stress measures

As for the deformation measures, there are also for the stresses corresponding measures that act in the reference configuration and some that act in the current configuration. These are stated for the sake of completeness in this subsection without engaging in a detailed discussion regarding the variance of these tensors.

First of all, for the surface traction  $\mathbf{t}^{\alpha}$ , *Cauchy*'s Lemma holds, which can be understood as a direct consequence of *Newton*'s third law, i. e. actio est reactio, viz.:

$$\mathbf{t}^{\alpha}(\mathbf{x},t,\mathbf{n}) = -\mathbf{t}^{\alpha}(\mathbf{x},t,-\mathbf{n}), \qquad (3.44)$$

when the resulting surface forces at a cut and uncut body are compared. As stated in (3.44), the traction vector depends on the direction  $\mathbf{n}$  of the area element on which it acts. A more general notion of the stress acting at a specific point is given in the current configuration by the *Cauchy* stress  $\mathbf{T}^{\alpha}$ , which is related to the traction vector  $\mathbf{t}^{\alpha}$  via *Cauchy*'s theorem

$$\mathbf{t}^{\alpha}(\mathbf{x},t,\mathbf{n}) = \mathbf{T}^{\alpha}(\mathbf{x},t)\,\mathbf{n},\tag{3.45}$$

where the *Cauchy* stress  $\mathbf{T}^{\alpha}(\mathbf{x}, t)$ , also referred to as true stress, is independent from the orientation  $\mathbf{n}$  of the surface element. Therefore, the force increment  $d\mathbf{k}_{O}^{\alpha}$  at the surface element da and  $d\mathbf{a}$ , respectively, is given in the current configuration via

$$\mathrm{d}\mathbf{k}_{O}^{\alpha} = \mathbf{t}^{\alpha}\mathrm{d}a = \mathbf{T}^{\alpha}\mathrm{d}\mathbf{a}. \tag{3.46}$$

The *Cauchy* stress  $\mathbf{T}^{\alpha}$  relates the actual force to the cross section area d**a** in the current configuration. For the area elements, the following holds

$$d\mathbf{a} = \mathbf{n} da \quad \text{where} \quad da = |d\mathbf{a}|, d\mathbf{A}_{\alpha} = \mathbf{n}_{0\alpha} dA_{\alpha} \quad \text{where} \quad dA_{\alpha} = |d\mathbf{A}_{\alpha}|,$$
(3.47)

where the area element in the reference configuration is indicated by  $dA_{\alpha}$  and  $d\mathbf{A}_{\alpha}$ , respectively. An alternative representation of (3.46) is given via

$$\mathrm{d}\mathbf{k}_{O}^{\alpha} = \mathbf{t}^{\alpha}\mathrm{d}a = \boldsymbol{\tau}^{\alpha}\mathrm{d}\bar{\mathbf{a}}_{\alpha}, \qquad (3.48)$$

with the *Kirchhoff* tensor  $\tau^{\alpha} = \det \mathbf{F}_{\alpha} \mathbf{T}^{\alpha}$ , the weighted surface element is given via  $d\bar{\mathbf{a}}_{\alpha} = \det \mathbf{F}_{\alpha}^{-1} d\mathbf{a}$ . When the stress in the current configuration is referred to the area element in the reference configuration, viz.:

$$d\mathbf{k}_{O}^{\alpha} = \mathbf{T}^{\alpha} \det \mathbf{F}_{\alpha} \mathbf{F}_{\alpha}^{T-1} d\mathbf{A}_{\alpha} = \mathbf{P}^{\alpha} d\mathbf{A}_{\alpha}, \qquad (3.49)$$

the first *Piola-Kirchhoff* tensor  $\mathbf{P}^{\alpha} = \det \mathbf{F}_{\alpha} \mathbf{T}^{\alpha} \mathbf{F}_{\alpha}^{T-1}$  is the so-called nominal stress that refers the actual force to the area element in the reference configuration. When the force is mapped back to the reference configuration, it follows

$$\mathbf{F}_{\alpha}^{-1} \mathrm{d} \mathbf{k}_{O}^{\alpha} = \mathbf{F}_{\alpha}^{-1} \mathbf{P}^{\alpha} \mathrm{d} \mathbf{A}_{\alpha} = \mathbf{S}^{\alpha} \mathrm{d} \mathbf{A}_{\alpha}, \qquad (3.50)$$

where the second *Piola-Kirchhoff* tensor  $\mathbf{S}^{\alpha} = \mathbf{F}_{\alpha}^{-1} \mathbf{P}^{\alpha}$  relates the image of the force in the reference configuration to the area element in the reference configuration.

# **3.5** Balance relations

Within the framework of continuum-(thermo-) mechanics there are material-independent relations, the so-called conservation laws of physical quantities, and material-specific relations accounting for the physical character of the specific thermo-mechanical process. In this section, the conservation laws for multiphasic continua will be introduced, which have axiomatic character as they are founded on physical observations. Based on the master-balance concept that can be used for the balancing of any physical quantity, the respective balance relations in terms of the mechanical quantities mass, linear momentum and angular momentum as well as of the thermodynamical quantities energy and entropy. These will be discussed for the overall aggregate and for the specific constituents of a multiphasic aggregate and, in particular, their relation. This section is particularly based on de Boer [23], Ehlers [45, 47], Graf [83], Häberle [89], Karajan [102], Markert [121], Wagner [187] and traces back to the pioneering works of Bowen [28, 29, 30], Truesdell [182] and Truesdell & Toupin [184].

# 3.5.1 Preliminary remarks

In general, the balance relations are based on physical observations and can be stated within the framework of the classical singlephasic approach via the following axioms.

#### Basic axioms regarding the conservation of the physical quantities

- Mass: The mass of a body remains constant in a closed system.
- Linear momentum: The temporal change of linear momentum equals the sum of the externally applied forces.
- Angular momentum: The temporal change of angular momentum equals the sum of the externally applied moments of all forces when the same reference point is chosen.

- Energy: The temporal change of sum of internal and kinetic energy equals the sum of the externally applied mechanical and non-mechanical power (also referred to as the first law of thermodynamics).
- Entropy: (i) The temporal change of entropy equals the sum of the externally applied entropy and the internal entropy production. (ii) The entropy production is never negative (also referred to as the second law of thermodynamics).

The sense of these basic axioms is still valid for multiphasic materials, however, they need to be extended to account for multiple constituents and their mutual interaction. This extension is primarily based on the work of Truesdell [182, 183] and is well-known as the metaphysical principles, which are stated in the following.

## Truesdells's metaphysical principles [183, p. 221] according to [45]

- 1. All properties of the mixture must be mathematical consequences of properties of the constituents.
- 2. So as to describe the motion of a constituent, we may in imagination isolate it from the rest of the mixture, provided we allow properly for the actions of the other constituents upon it.
- 3. The motion of the mixture is governed by the same equations as is a single body.

According to Ehlers [45], these principles indicate that each constituent is governed by its own motion function and set of balance equations provided the mutual interaction is properly accounted for. Furthermore, the structure of the equations describing the mixture, i. e. the overall aggregate, is the same as for a singlephasic material, hence the mixture does not know whether it is a mixture. This indicates that the summation of the respective balance equations of the constituents yields the equations for the overall aggregate with the structure of a singlephasic material. Therefore, the balance equations for the overall aggregate are introduced as well as the balance equations for the individual constituents based on the master-balance principle.

## 3.5.2 Balance relations of the overall aggregate

According to the well-established theories for singlephasic materials, the balance relation for an arbitrary volume-specific physical quantity  $\Psi$  (scalar-valued) or  $\Psi$  (vector-valued) is stated as a master balance, viz.:

scalar-valued: 
$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi \,\mathrm{d}v = \int_{\mathcal{S}} (\boldsymbol{\phi} \cdot \mathbf{n}) \,\mathrm{d}a + \int_{\mathcal{B}} \boldsymbol{\sigma} \,\mathrm{d}v + \int_{\mathcal{B}} \hat{\Psi} \,\mathrm{d}v,$$
  
vector-valued: 
$$\frac{\mathrm{d}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi \,\mathrm{d}v = \int_{\mathcal{S}} (\boldsymbol{\Phi} \,\mathbf{n}) \,\mathrm{d}a + \int_{\mathcal{B}} \boldsymbol{\sigma} \,\mathrm{d}v + \int_{\mathcal{B}} \hat{\Psi} \,\mathrm{d}v,$$
(3.51)

where  $\phi$  and  $\Phi$  are the efflux of the physical quantity over the surface as an action at the vicinity,  $\sigma$  and  $\sigma$  is the supply of the physical quantity from a distance and  $\hat{\Psi}$  and  $\hat{\Psi}$ represents the production of the physical quantity. The latter term is zero, except for the entropy according to the second law of thermodynamics, as introduced in **Subsection 3.5.1**. This general representation in a global form, cf. (3.51), can be brought into a local representation in case the integrands are steady and steadily differentiable. This leads to the local master-balance formulation via

$$\dot{\Psi} + \Psi \operatorname{div} \dot{\mathbf{x}} = \operatorname{div} \boldsymbol{\phi} + \boldsymbol{\sigma} + \hat{\Psi}, 
\dot{\Psi} + \Psi \operatorname{div} \dot{\mathbf{x}} = \operatorname{div} \boldsymbol{\Phi} + \boldsymbol{\sigma} + \hat{\Psi}.$$
(3.52)

When the five physical quantities, i. e. mass, linear momentum, angular momentum, energy and entropy, are considered, the placeholder from (3.52) can be replaced with real physical quantities, which is shown in Table 3.1.

balance	$\Psi,  {oldsymbol \Psi}$	$oldsymbol{\phi},oldsymbol{\Phi}$	$\sigma,  \sigma$	$\hat{\Psi},\hat{\Psi}$
mass	ρ	0	0	0
momentum	$ ho \dot{\mathbf{x}}$	$\mathbf{T}$	$ ho{f b}$	0
m.o.m.	$\mathbf{x} \times (\rho  \dot{\mathbf{x}})$	$\mathbf{x}\times\mathbf{T}$	$\mathbf{x}  imes  ho  \mathbf{b}$	0
energy	$\rho\left(\varepsilon + \frac{1}{2}\dot{\mathbf{x}}\cdot\dot{\mathbf{x}}\right)$	$\mathbf{T}^T \dot{\mathbf{x}} - \mathbf{q}$	$\rho\left(\mathbf{b}\cdot\dot{\mathbf{x}}+r\right)$	0
entropy	$ ho\eta$	- $oldsymbol{\phi}_\eta$	$\sigma_\eta$	$\hat{\eta} \geq 0$

Table 3.1: Specific quantities of the respective balances of the overall aggregate

Therein,  $\rho \dot{\mathbf{x}}$  stands for the linear momentum of the overall aggregate,  $\mathbf{T}$  is the overall *Cauchy* stress and  $\rho \mathbf{b}$  the volume force on the body. Note that within a thermo-hydromechanical framework, this is given by the impact of gravity. Furthermore, the angular momentum  $\mathbf{x} \times (\rho \dot{\mathbf{x}})$  is the local moment of the linear momentum (m.o.m.) using the lever arm  $\mathbf{x}$ ,  $\mathbf{x} \times \mathbf{T}$  and  $\mathbf{x} \times \rho \mathbf{b}$  the respective externally applied moments referring to the same reference point. In the energy balance,  $\varepsilon$  is the internal energy and  $\frac{1}{2}\dot{\mathbf{x}} \cdot \dot{\mathbf{x}}$  the kinetic energy, both per unit mass,  $\mathbf{q}$  is the heat influx and r the radiation, i. e. the action from the distance. Finally, the entropy of the overall aggregate is denoted by  $\eta$ ,  $\phi_{\eta}$  is the influx of entropy and  $\sigma_{\eta}$  the external entropy supply. It is important to note that the entropy production  $\hat{\eta}$  of the overall aggregate is only zero in case of a thermodynamically reversible process, for irreversible processes, it is larger than zero. Putting the scheme in Table 3.1 into the local formulation (3.52) yields the classical balance relations for a singlephasic material or, equivalently, with the metaphysical principles of *Truesdell*, the balance relations of the overall aggregate, viz.:

$$\begin{array}{rcl} \text{mass} & : & \dot{\rho} + \rho \operatorname{div} \dot{\mathbf{x}} & = & 0, \\ \text{momentum} & : & \rho \ddot{\mathbf{x}} & = & \operatorname{div} \mathbf{T} + \rho \mathbf{b}, \\ \text{m.o.m.} & : & \mathbf{0} & = & \mathbf{I} \times \mathbf{T} \implies \mathbf{T} = \mathbf{T}^T, \\ \text{energy} & : & \rho \dot{\varepsilon} & = & \mathbf{T} \cdot \mathbf{L} - \operatorname{div} \mathbf{q} + \rho r, \\ \text{entropy} & : & \rho \dot{\eta} \geq & \operatorname{div} \phi_{\eta} + \sigma_{\eta}. \end{array}$$
(3.53)

## **3.5.3** Balance relations of the individual constituents

Since *Truesdell*'s metaphysical principles state that the same equations as for singlephasic materials apply also for multiphasic aggregates provided the interaction is properly accounted for, the general set of balance equations for the individual constituents is given via the same set of master-balance equations, viz.:

scalar-valued: 
$$\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi^{\alpha} \,\mathrm{d}v = \int_{\mathcal{S}} (\boldsymbol{\phi}^{\alpha} \cdot \mathbf{n}) \,\mathrm{d}a + \int_{\mathcal{B}} \sigma^{\alpha} \,\mathrm{d}v + \int_{\mathcal{B}} \hat{\Psi}^{\alpha} \,\mathrm{d}v,$$
  
vector-valued: 
$$\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi^{\alpha} \,\mathrm{d}v = \int_{\mathcal{S}} (\boldsymbol{\Phi}^{\alpha} \,\mathbf{n}) \,\mathrm{d}a + \int_{\mathcal{B}} \sigma^{\alpha} \,\mathrm{d}v + \int_{\mathcal{B}} \hat{\Psi}^{\alpha} \,\mathrm{d}v.$$
(3.54)

The interpretation of the specific terms in (3.54) is similar to the ones in **Subsection 3.5.2**, however, in reference to the individual constituents  $(\cdot)^{\alpha}$  instead of the quantities for the overall aggregate (·). Consequently, after applying the same procedure, the local formulation of the constituent-specific relations is given via

$$(\Psi^{\alpha})'_{\alpha} + \Psi^{\alpha} \operatorname{div} \mathbf{\dot{x}}_{\alpha} = \operatorname{div} \phi^{\alpha} + \sigma^{\alpha} + \hat{\Psi}^{\alpha},$$

$$(\Psi^{\alpha})'_{\alpha} + \Psi^{\alpha} \operatorname{div} \mathbf{\dot{x}}_{\alpha} = \operatorname{div} \Phi^{\alpha} + \sigma^{\alpha} + \hat{\Psi}^{\alpha}.$$

$$(3.55)$$

This scheme is used to evaluate the axioms regarding the physical quantities mass, linear momentum, angular momentum, energy and entropy, as indicated in Table 3.2. Therein, there are additional quantities describing the mutual interactions of the constituents. In detail, there is the mass production  $\hat{\rho}^{\alpha}$  describing, for example, phase transitions or, as in this monograph, the cell dehydration, the total momentum production  $\hat{\mathbf{s}}^{\alpha}$ , the total angular momentum production  $\hat{\mathbf{h}}^{\alpha}$ , the total energy production  $\hat{e}^{\alpha}$  and, finally, the total entropy production  $\hat{\eta}^{\alpha}$  of the respective constituents  $\varphi^{\alpha}$ .

Since the metaphysical principles state also that the mixture is the sum of its parts, there is a relation between the partial quantities  $(\cdot)^{\alpha}$  of the individual constituents  $\varphi^{\alpha}$  and the quantities  $(\cdot)$  of the overall aggregate  $\varphi$ . These are given via

$$\Psi = \sum_{\alpha} \Psi^{\alpha}, \quad \phi = \sum_{\alpha} (\phi^{\alpha} - \Psi^{\alpha} \mathbf{d}_{\alpha}), \qquad \sigma = \sum_{\alpha} \sigma^{\alpha}, \quad \hat{\Psi} = \sum_{\alpha} \hat{\Psi}^{\alpha}, \\ \Psi = \sum_{\alpha} \Psi^{\alpha}, \quad \Phi = \sum_{\alpha} (\Phi^{\alpha} - \Psi^{\alpha} \otimes \mathbf{d}_{\alpha}), \quad \sigma = \sum_{\alpha} \sigma^{\alpha}, \quad \hat{\Psi} = \sum_{\alpha} \hat{\Psi}^{\alpha}.$$
(3.56)

Balance	$\Psi^{lpha}, {oldsymbol \Psi}^{lpha}$	$oldsymbol{\phi}^{lpha},oldsymbol{\Phi}^{lpha}$	$\sigma^{lpha},oldsymbol{\sigma}^{lpha}$	$\hat{\Psi}^{lpha},\hat{\Psi}^{lpha}$
mass	$ ho^{lpha}$	0	0	$\hat{ ho}^{lpha}$
momentum	$ ho^{lpha}   {f x}_{lpha}$	$\mathbf{T}^{lpha}$	$ ho^{lpha}{f b}^{lpha}$	$\hat{\mathbf{s}}^{lpha}$
m.o.m.	$\mathbf{x}  imes ( ho^{lpha} \ \mathbf{x}_{lpha})$	$\mathbf{x}  imes \mathbf{T}^{lpha}$	$\mathbf{x} \times \rho^{\alpha} \mathbf{b}^{\alpha}$	$\hat{\mathbf{h}}^{lpha}$
energy	$\rho^{\alpha} \left( \varepsilon^{\alpha} + \frac{1}{2}  \mathbf{\dot{x}}_{\alpha} \cdot \mathbf{\dot{x}}_{\alpha} \right)$	$(\mathbf{T}^{lpha})^T \stackrel{\prime}{\mathbf{x}}_{lpha} - \mathbf{q}^{lpha}$	$\rho^{\alpha} \left( \mathbf{b}^{\alpha} \cdot \mathbf{\dot{x}}_{\alpha}' + r^{\alpha} \right)$	$\hat{e}^{\alpha}$
entropy	$ ho^lpha  \eta^lpha$	- $oldsymbol{\phi}^lpha_\eta$	$\sigma^lpha_\eta$	$\hat{\eta}^{lpha}$

Table 3.2: Specific quantities of the respective balances of the individual constituents

In particular, (3.56) is used to derive constraints for the mentioned interactions terms  $(\cdot)^{\alpha}$  in the very right column of Table 3.2, viz.:

$$\sum_{\alpha} \hat{\rho}^{\alpha} = 0, \qquad \sum_{\alpha} \hat{\mathbf{s}}^{\alpha} = \mathbf{0}, \qquad \sum_{\alpha} \hat{\mathbf{h}}^{\alpha} = \mathbf{0}, \qquad \sum_{\alpha} \hat{e}^{\alpha} = 0, \qquad \sum_{\alpha} \hat{\eta}^{\alpha} \ge 0.$$
(3.57)

Inserting the quantities from Table 3.2 into the local balance relations (3.55) yields the constituent-specific balance relations, viz.:

$$\begin{array}{rcl} \text{mass} & : & (\rho^{\alpha})'_{\alpha} + \rho^{\alpha} \operatorname{div} \mathbf{x}_{\alpha} & = & \hat{\rho}^{\alpha}, \\ \text{momentum} & : & \rho^{\alpha} \mathbf{x}_{\alpha}' & = & \operatorname{div} \mathbf{T}^{\alpha} + \rho^{\alpha} \mathbf{b}^{\alpha} + \hat{\mathbf{p}}^{\alpha}, \\ \text{m.o.m.} & : & \mathbf{0} & = & \mathbf{I} \times \mathbf{T}^{\alpha} + \hat{\mathbf{m}}^{\alpha}, \\ \text{energy} & : & \rho^{\alpha} \left( \varepsilon^{\alpha} \right)'_{\alpha} & = & \mathbf{T}^{\alpha} \cdot \mathbf{L}_{\alpha} - \operatorname{div} \mathbf{q}^{\alpha} + \rho^{\alpha} r^{\alpha} + \hat{\varepsilon}^{\alpha}, \\ \text{entropy} & : & \rho^{\alpha} \left( \eta^{\alpha} \right)'_{\alpha} & = & \operatorname{div} \left( -\frac{1}{\rho^{\alpha}} \mathbf{q}^{\alpha} \right) + \frac{1}{\rho^{\alpha}} \rho^{\alpha} r^{\alpha} + \hat{\zeta}^{\alpha}. \end{array}$$

$$(3.58)$$

Herein, the direct production terms are used. These are given as the direct momentum production  $\hat{\mathbf{p}}^{\alpha}$ , the direct angular momentum production  $\hat{\mathbf{m}}^{\alpha}$ , the direct energy production  $\hat{\varepsilon}^{\alpha}$  and the direct entropy production  $\hat{\zeta}^{\alpha}$ . Related to the direct production terms, the total production terms can be derived via

$$\hat{\mathbf{s}}^{\alpha} = \hat{\mathbf{p}}^{\alpha} + \hat{\rho}^{\alpha} \overset{\prime}{\mathbf{x}}_{\alpha}, \qquad \hat{\mathbf{h}}^{\alpha} = \hat{\mathbf{m}}^{\alpha} + \mathbf{x} \times \hat{\mathbf{s}}^{\alpha}, 
\hat{e}^{\alpha} = \hat{\varepsilon}^{\alpha} + \hat{\mathbf{p}}^{\alpha} \cdot \overset{\prime}{\mathbf{x}}_{\alpha} + \hat{\rho}^{\alpha} (\varepsilon^{\alpha} + \frac{1}{2} \overset{\prime}{\mathbf{x}}_{\alpha} \cdot \overset{\prime}{\mathbf{x}}_{\alpha}), \quad \hat{\eta}^{\alpha} = \hat{\zeta}^{\alpha} + \hat{\rho}^{\alpha} \eta^{\alpha}.$$
(3.59)

A special role plays in this context the balance of angular momentum  $(3.58)_3$ , since the assumption of non-polar *Cauchy-Boltzmann* continua is made, which indicates that the direct angular momentum production vanishes, i. e.  $\hat{\mathbf{m}}^{\alpha} = \mathbf{0}$ , and the partial stress is symmetric, i. e.  $\mathbf{T}^{\alpha} = (\mathbf{T}^{\alpha})^T$ . Regarding the micropolar theory for *Cosserat* continua as the more general micromorphic theory, the interested reader is referred to Ehlers [45], Scholz [161] or Ehlers & Bidier [52, 53].

Moreover, the general relations between the partial quantities and the quantities of the overall aggregate, cf. (3.56), are used to specify relations for the following quantities,

which are in accordance to Ehlers [45], viz.:

$$\rho = \sum_{\alpha} \rho^{\alpha}, \qquad \rho \mathbf{b} = \sum_{\alpha} \rho^{\alpha} \mathbf{b}^{\alpha},$$

$$\rho \dot{\mathbf{x}} = \sum_{\alpha} \rho^{\alpha} \dot{\mathbf{x}}_{\alpha}, \qquad \rho \ddot{\mathbf{x}} = \sum_{\alpha} [\rho^{\alpha} \overset{"}{\mathbf{x}}_{\alpha} - \operatorname{div} (\rho^{\alpha} \mathbf{d}_{\alpha} \otimes \mathbf{d}_{\alpha}) + \rho^{\alpha} \overset{'}{\mathbf{x}}_{\alpha}],$$

$$\mathbf{T} = \sum_{\alpha} (\mathbf{T}^{\alpha} - \rho^{\alpha} \mathbf{d}_{\alpha} \otimes \mathbf{d}_{\alpha}), \qquad \mathbf{q} = \sum_{\alpha} [\mathbf{q}^{\alpha} - (\mathbf{T}^{\alpha})^{T} \mathbf{d}_{\alpha} + \rho^{\alpha} \varepsilon^{\alpha} \mathbf{d}_{\alpha} + \frac{1}{2} \rho^{\alpha} (\mathbf{d}_{\alpha} \cdot \mathbf{d}_{\alpha}) \mathbf{d}_{\alpha}]$$

$$\rho r = \sum_{\alpha} \rho^{\alpha} (r^{\alpha} + \mathbf{b}^{\alpha} \cdot \mathbf{d}_{\alpha}), \qquad \rho \varepsilon = \sum_{\alpha} \rho^{\alpha} (\varepsilon^{\alpha} + \frac{1}{2} \mathbf{d}_{\alpha} \cdot \mathbf{d}_{\alpha}).$$

$$(3.60)$$

A special case in the set of balance relations (3.58), together with (3.57), plays the entropy relation, as the balance relations in terms of mass, linear momentum, angular momentum and energy are conservation laws. The entropy, however, is not conserved for a general thermo-hydro-mechanical process. In contrast, the entropy production of the overall process, i. e.  $(3.57)_5$ , is never negative, which will be used to derive restrictions for the material laws that will be introduced in **Chapter 4**. The proper form of the entropy production of the overall aggregate is based on two a priori constitutive assumptions from the thermodynamics of singlephasic materials, viz.:

$$\phi_{\eta}^{\alpha} = -\frac{1}{\theta^{\alpha}} \mathbf{q}^{\alpha} \quad \text{and} \quad \sigma_{\eta}^{\alpha} = \frac{1}{\theta^{\alpha}} \rho^{\alpha} r^{\alpha}.$$
 (3.61)

Therefore,  $(3.58)_5$  and  $(3.59)_4$  are used to derive the overall entropy production via

$$\hat{\eta} = \sum_{\alpha} \hat{\eta}^{\alpha} = \sum_{\alpha} \left[ \rho^{\alpha} (\eta^{\alpha})'_{\alpha} + \hat{\rho}^{\alpha} \eta^{\alpha} + \operatorname{div} \left( \frac{1}{\theta^{\alpha}} \mathbf{q}^{\alpha} \right) - \frac{1}{\theta^{\alpha}} \rho^{\alpha} r^{\alpha} \right] \ge 0.$$
(3.62)

This shows already that the entropy can never decrease in a closed system. But this form is not yet suitable to derive restrictions for the thermo-hydro-mechanical processes. Therefore, the partial energy balance  $(3.58)_4$  as well as the constraint for the overall energy production  $(3.59)_3$  will be used, where the internal energy is replaced by the *Helmholtz* free energy  $\psi^{\alpha}$  using a *Legendre* transformation of the internal energy  $\varepsilon^{\alpha}$  with respect to the conjugated pair entropy  $\eta^{\alpha}$  and temperature  $\theta^{\alpha}$ , viz.:

$$\psi^{\alpha} := \varepsilon^{\alpha} - \theta^{\alpha} \eta^{\alpha}. \tag{3.63}$$

This is an important step, as the internal energy is, in general, a function of the generalised deformation and the entropy, which is impossible to measure directly. The *Helmholtz* free energy, however, is a function of the generalised deformation and the temperature, which is clearly measurable. Finally, this leads to the *Clausius-Duhem* inequality for general thermo-mechanical processes

$$\sum_{\alpha} \frac{1}{\theta^{\alpha}} \{ -\rho^{\alpha} [(\psi^{\alpha})'_{\alpha} + (\theta^{\alpha})'_{\alpha} \eta^{\alpha}] - \mathbf{p}^{\alpha} \cdot \mathbf{\dot{x}}_{\alpha} - \\ -\hat{\rho}^{\alpha} (\psi^{\alpha} + \frac{1}{2} \mathbf{\dot{x}}_{\alpha} \cdot \mathbf{\dot{x}}_{\alpha}) + \mathbf{T}^{\alpha} \cdot \mathbf{L}_{\alpha} - \frac{1}{\theta^{\alpha}} \mathbf{q}^{\alpha} \cdot \operatorname{grad} \theta^{\alpha} + \hat{e}^{\alpha} \} \ge 0.$$
(3.64)

# **3.6** Singular surfaces

The idea of utilising an immaterial smooth surface within the framework of porous media is not new. Based on the works of Morland & Gray [131] and Morland & Sellers [132], contact surfaces between fluid-saturated porous media within the TPM have been described using a singular surface, cf. Markert *et al.* [122], or also fluid-fluid phase transitions of a single substance, cf. Ehlers & Häberle [58] and Häberle [89]. These two applications lead to very similar equations, when the intrinsic surface supply in [122] is neglected and the fluid flux over the interface is regarded as mass transfer (phase transition) of the single substance under consideration. The basic ideas of a sharp singular surface within the context of the TPM have been stated in detail in Mahnkopf [119] in application to shear-band localisation. Thus, for a comprehensive description of the concept, the notion of interface kinematics as well as the consequence of its very existence on the balance relations and associated jumps in the physical quantities mass, linear momentum and energy, the interested reader is referred to Mahnkopf [119], whose work traces back to Kosinski [108], Truesdell & Toupin [184].

Since the concept of singular surfaces is utilised within this monograph to describe solidliquid phase transitions, this section is mainly based on the work of Häberle [89] and Ehlers & Häberle [58]. Therefore, in order to avoid too much repitition, in this context only a short summary of the work done by Mahnkopf [119] and especially Häberle [89] as well as Ehlers & Häberle [58] is given for the sake of completeness.

# **3.6.1** Kinematics of the singular surface

The overall triphasic aggregate  $\mathcal{B} = \bigcup_{\alpha} \mathcal{B}^{\alpha}$ , where  $\alpha = \{S, I, L, G\}$ , is enclosed by its surface S and is separated by the singular surface  $\Gamma$  into two partitions  $\mathcal{B}^+$  and  $\mathcal{B}^-$ , where  $\mathcal{B} = \mathcal{B}^+ \cup \mathcal{B}^-$  and  $\mathcal{S} = \mathcal{S}^+ \cup \mathcal{S}^-$ . The partition  $\mathcal{B}^+$  is enclosed by the surface  $\mathcal{S}^+$ with unit normal vector  $\mathbf{n}^+$  and interface  $\Gamma$  with unit normal vector  $\mathbf{n}_{\Gamma}^+$ , the partition  $\mathcal{B}^$ correspondingly by the surface  $\mathcal{S}^-$  with unit normal vector  $\mathbf{n}^-$  and interface  $\Gamma$  with unit normal vector  $\mathbf{n}_{\Gamma}^-$ , as shown in Figure 3.3. Note that all field functions are steady in  $\mathcal{B}^+$ ,  $\mathcal{B}^-$  and on  $\Gamma$ , however, jumps in these field functions across the interface  $\Gamma$  are admissible.

The jump across the interface  $\Gamma$  of an arbitrary, but scalar-valued physical quantity can be denoted by the jump operator  $[\cdot]$ , viz.:

$$[\![\Psi]\!] := \Psi^+ - \Psi^-, \tag{3.65}$$

where  $\Psi(\mathbf{x}, t)$  is continuous in  $\mathcal{B}^+$  and  $\mathcal{B}^-$ . The limit value of  $\Psi$  at the interface in  $\mathcal{B}^+$ is denoted by  $\Psi^+$ , the corresponding limit value in the partition  $\mathcal{B}^-$  is denoted by  $\Psi^-$ . Since the interface  $\Gamma$  is allowed to move through the porous material, the position of the interface is expressed via  $\mathbf{x}_{\Gamma}$  and its velocity by  $\mathbf{x}_{\Gamma}$ . The relative velocity of a constituent  $\varphi^{\alpha}$  with regard to the interface  $\Gamma$  is defined via

$$\mathbf{w}_{\alpha\Gamma} = \mathbf{x}_{\alpha}' - \mathbf{x}_{\Gamma}' . \tag{3.66}$$



**Figure 3.3:** Body  $\mathcal{B}$  is separated by an immaterial singular surface  $\Gamma$  into the partitions  $\mathcal{B}^+$  and  $\mathcal{B}^-$ .

The introduced outward-oriented unit normal vector  $\mathbf{n}_{\Gamma}$  points from  $\mathcal{B}^+$  to  $\mathcal{B}^-$ , with the convention as follows, viz.:

$$\mathbf{n}_{\Gamma}^{+} = -\mathbf{n}_{\Gamma}^{-}, \text{ such that } \mathbf{n}_{\Gamma}^{+} =: \mathbf{n}_{\Gamma}, \quad \mathbf{n}_{\Gamma}^{-} =: -\mathbf{n}_{\Gamma}.$$
 (3.67)

# 3.6.2 Balance relations of continua with singular surface

Global master balance with singular surface: As a next step, the global balance relations will be derived for discontinuous field functions. Therefore, the global balance relations will be written down for both sides of the interface in analogy to (3.54) in case there is no further discontinuity in  $\mathcal{B}^+$  or  $\mathcal{B}^-$ . In particular, the scalar-valued fields  $\Psi^{\alpha}$ ,  $\phi^{\alpha}$  and  $\sigma^{\alpha}$  as well as the vector-valued field functions  $\Psi^{\alpha}$ ,  $\Phi^{\alpha}$ ,  $\sigma^{\alpha}$  and  $\dot{\mathbf{x}}_{\alpha}$  are continuous in  $\mathcal{B}^+$ ,  $\mathcal{B}^-$  and on  $\Gamma$ , but, in general, discontinuous across  $\Gamma$ . Under consideration of the singular surface, the global balance relations read for the partitions  $\mathcal{B}^+$  and  $\mathcal{B}^-$ , viz.:

$$\text{in } \mathcal{B}^{-} : \frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}^{+}} \Psi^{\alpha} \mathrm{d}v = \int_{\mathcal{S}^{+}} \phi^{\alpha} \cdot \mathbf{n}^{-} \mathrm{d}a + \int_{\mathcal{B}^{+}} (\sigma^{\alpha} + \hat{\Psi}^{\alpha}) \, \mathrm{d}v + \int_{\Gamma} (\phi^{\alpha})^{-} \cdot \mathbf{n}_{\Gamma}^{-} \, \mathrm{d}a,$$

$$\text{in } \mathcal{B}^{+} : \frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}^{+}} \Psi^{\alpha} \mathrm{d}v = \int_{\mathcal{S}^{+}} \phi^{\alpha} \cdot \mathbf{n}^{+} \mathrm{d}a + \int_{\mathcal{B}^{+}} (\sigma^{\alpha} + \hat{\Psi}^{\alpha}) \, \mathrm{d}v + \int_{\Gamma} (\phi^{\alpha})^{+} \cdot \mathbf{n}_{\Gamma}^{+} \, \mathrm{d}a.$$

$$(3.68)$$

Therein, the flux over the surface has been decomposed into a flux over external surfaces, i. e.  $S^+$  and  $S^-$ , and internal surfaces  $\Gamma$ . The sum of  $(3.68)_1$  and  $(3.68)_2$  is given via

The vectorial form is given via

$$\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}} \mathbf{\Psi}^{\alpha} \mathrm{d}v = \int_{\mathcal{S}} \mathbf{\Phi}^{\alpha} \mathbf{n} \, \mathrm{d}a + \int_{\mathcal{B}} (\boldsymbol{\sigma}^{\alpha} + \hat{\mathbf{\Psi}}^{\alpha}) \, \mathrm{d}v + \int_{\Gamma} \left[ \!\!\!\left[ \mathbf{\Phi}^{\alpha} \right] \!\!\!\right] \mathbf{n}_{\Gamma} \, \mathrm{d}a.$$
(3.70)

In order to derive the local form of the balance relations (3.69) and (3.70), the left-hand side needs to be determined for continua with discontinuities, which will be done with a modified form of the *Reynolds*' transport theorem.

Modified *Reynolds*' transport theorem: From classic continuum mechanics, for example Holzapfel [95], the general form of the transport theorem without internal interfaces is given in application to a constituent  $\varphi^{\alpha}$  via

$$\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi^{\alpha} \mathrm{d}v = \int_{\mathcal{B}} \frac{\partial \Psi^{\alpha}}{\partial t} \,\mathrm{d}v + \int_{\mathcal{S}} \Psi^{\alpha} \, \mathbf{\dot{x}}_{\alpha} \cdot \mathbf{n} \,\mathrm{d}a.$$
(3.71)

When this theorem is according to Mahnkopf [119] evaluated with regard to the motions  $\chi_{\alpha}$  and  $\chi_{\Gamma}$ , their difference is given via

$$\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi^{\alpha} \mathrm{d}v = \frac{\mathrm{d}_{\Gamma}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi^{\alpha} \mathrm{d}v + \int_{\mathcal{S}} \Psi^{\alpha} (\mathbf{\dot{x}}_{\alpha} - \mathbf{\dot{x}}_{\Gamma}) \cdot \mathbf{n} \, \mathrm{d}a.$$
(3.72)

Evaluating (3.72) for both partitions, i. e.  $\mathcal{B}^+$  and  $\mathcal{B}^-$ , yields

in 
$$\mathcal{B}^{-}$$
:  $\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}^{-}} \Psi^{\alpha} \mathrm{d}v = \frac{\mathrm{d}_{\Gamma}}{\mathrm{d}t} \int_{\mathcal{B}^{-}} \Psi^{\alpha} \mathrm{d}v + \int_{\mathcal{S}^{-}} \Psi^{\alpha} (\mathbf{x}_{\alpha} - \mathbf{x}_{\Gamma}) \cdot \mathbf{n}^{-} \mathrm{d}a + \int_{\Gamma} (\Psi^{\alpha})^{-} [(\mathbf{x}_{\alpha})^{-} - \mathbf{x}_{\Gamma}] \cdot \mathbf{n}_{\Gamma}^{-} \mathrm{d}a,$   
in  $\mathcal{B}^{+}$ :  $\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}^{+}} \Psi^{\alpha} \mathrm{d}v = \frac{\mathrm{d}_{\Gamma}}{\mathrm{d}t} \int_{\mathcal{B}^{+}} \Psi^{\alpha} \mathrm{d}v + \int_{\mathcal{S}^{+}} \Psi^{\alpha} (\mathbf{x}_{\alpha} - \mathbf{x}_{\Gamma}) \cdot \mathbf{n}^{+} \mathrm{d}a + \int_{\Gamma} (\Psi^{\alpha})^{+} [(\mathbf{x}_{\alpha})^{+} - \mathbf{x}_{\Gamma}] \cdot \mathbf{n}_{\Gamma}^{+} \mathrm{d}a.$ 

$$(3.73)$$

It follows for the sum of  $(3.73)_1$  and  $(3.73)_2$  with definitions (3.67), viz.:

Applying (3.66) and (3.71) for the interface term yields

$$\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}} \Psi^{\alpha} \mathrm{d}v = \int_{\mathcal{B}} \frac{\partial \Psi^{\alpha}}{\partial t} \,\mathrm{d}v + \int_{\mathcal{S}} \Psi^{\alpha} \,\mathbf{x}_{\alpha} \cdot \mathbf{n} \,\mathrm{d}a + \int_{\Gamma} \left[\!\!\left[ \Psi^{\alpha} \mathbf{w}_{\alpha\Gamma} \right]\!\!\right] \cdot \mathbf{n}_{\Gamma} \,\mathrm{d}a, \tag{3.75}$$

or for the vectorial case

$$\frac{\mathrm{d}_{\alpha}}{\mathrm{d}t} \int_{\mathcal{B}} \mathbf{\Psi}^{\alpha} \mathrm{d}v = \int_{\mathcal{B}} \frac{\partial \mathbf{\Psi}^{\alpha}}{\partial t} \,\mathrm{d}v + \int_{\mathcal{S}} (\mathbf{\Psi}^{\alpha} \otimes \mathbf{x}_{\alpha}') \,\mathbf{n} \,\mathrm{d}a + \int_{\Gamma} \left[\!\!\left[ \mathbf{\Psi}^{\alpha} \otimes \mathbf{w}_{\alpha\Gamma} \right]\!\!\right] \,\mathbf{n}_{\Gamma} \,\mathrm{d}a.$$
(3.76)

Local master balance for continua with singular surface: In order to derive the local form of the balance relations, the right-hand sides of (3.69) and (3.75) for the scalar-valued quantity  $\Psi^{\alpha}$ , and (3.70) and (3.76) for the vector-valued quantity  $\Psi^{\alpha}$  have been utilised, such that

$$\int_{\mathcal{B}} \frac{\partial \Psi^{\alpha}}{\partial t} dv + \int_{\mathcal{S}} \Psi^{\alpha} \mathbf{x}_{\alpha} \cdot \mathbf{n} da + \int_{\Gamma} \left[ \!\!\!\left[ \Psi^{\alpha} \mathbf{w}_{\alpha\Gamma} \right] \!\!\right] \cdot \mathbf{n}_{\Gamma} da =$$

$$= \int_{\mathcal{S}} \boldsymbol{\phi}^{\alpha} \cdot \mathbf{n} da + \int_{\mathcal{B}} (\boldsymbol{\sigma}^{\alpha} + \hat{\Psi}^{\alpha}) dv + \int_{\Gamma} \left[ \!\!\left[ \boldsymbol{\phi}^{\alpha} \right] \!\!\right] \cdot \mathbf{n}_{\Gamma} da,$$

$$\int_{\mathcal{B}} \frac{\partial \Psi^{\alpha}}{\partial t} dv + \int_{\mathcal{S}} (\Psi^{\alpha} \otimes \mathbf{x}_{\alpha}) \mathbf{n} da + \int_{\Gamma} \left[ \!\!\left[ \Psi^{\alpha} \otimes \mathbf{w}_{\alpha\Gamma} \right] \!\!\right] \mathbf{n}_{\Gamma} da =$$

$$= \int_{\mathcal{S}} \boldsymbol{\Phi}^{\alpha} \mathbf{n} da + \int_{\mathcal{B}} (\boldsymbol{\sigma}^{\alpha} + \hat{\Psi}^{\alpha}) dv + \int_{\Gamma} \left[ \!\!\left[ \boldsymbol{\Phi}^{\alpha} \right] \!\!\right] \mathbf{n}_{\Gamma} da.$$
(3.78)

The surface integral over S is converted into a volume integral within B using the divergence theorem, which results in

$$\int_{\mathcal{B}} [(\Psi^{\alpha})'_{\alpha} + \Psi^{\alpha} \operatorname{div} \mathbf{x}'_{\alpha}] \, \mathrm{d}v + \int_{\Gamma} [\![\Psi^{\alpha} \mathbf{w}_{\alpha\Gamma}]\!] \cdot \mathbf{n}_{\Gamma} \, \mathrm{d}a = 
= \int_{\mathcal{B}} [\operatorname{div} \phi^{\alpha} + \sigma^{\alpha} + \hat{\Psi}^{\alpha}] \, \mathrm{d}v + \int_{\Gamma} [\![\phi^{\alpha}]\!] \cdot \mathbf{n}_{\Gamma} \, \mathrm{d}a,$$

$$\int_{\mathcal{B}} [(\Psi^{\alpha})'_{\alpha} + \Psi^{\alpha} \operatorname{div} \mathbf{x}'_{\alpha}] \, \mathrm{d}v + \int_{\Gamma} [\![\Psi^{\alpha} \otimes \mathbf{w}_{\alpha\Gamma}]\!] \mathbf{n}_{\Gamma} \, \mathrm{d}a = 
= \int_{\mathcal{B}} [\operatorname{div} \Phi^{\alpha} + \sigma^{\alpha} + \hat{\Psi}^{\alpha}] \, \mathrm{d}v + \int_{\Gamma} [\![\Phi^{\alpha}]\!] \mathbf{n}_{\Gamma} \, \mathrm{d}a,$$
(3.79)
$$(3.80)$$

for the scalar case (3.79) as for the vectorial case (3.80). Since these equations have to be equally fulfilled as (3.54), two relations can be concluded each, in accordance to the integrands. In particular, these relations are given, for a scalar  $\Psi^{\alpha}$  as well as a vectorial  $\Psi^{\alpha}$ , respectively, viz.:

$$(\Psi^{\alpha})'_{\alpha} + \Psi^{\alpha} \operatorname{div} \, \stackrel{\prime}{\mathbf{x}}_{\alpha} = \operatorname{div} \, \boldsymbol{\phi}^{\alpha} + \sigma^{\alpha} + \hat{\Psi}^{\alpha} \quad \forall \, \mathbf{x} \in \mathcal{B},$$

$$[\![\Psi^{\alpha} \mathbf{w}_{\alpha\Gamma} - \boldsymbol{\phi}^{\alpha}]\!] \cdot \mathbf{n}_{\Gamma} = 0 \qquad \forall \, \mathbf{x} = \mathbf{x}_{\Gamma} \in \Gamma,$$

$$(\Psi^{\alpha})'_{\alpha} + \Psi^{\alpha} \operatorname{div} \, \stackrel{\prime}{\mathbf{x}}_{\alpha} = \operatorname{div} \Phi^{\alpha} + \boldsymbol{\sigma}^{\alpha} + \hat{\Psi}^{\alpha} \quad \forall \, \mathbf{x} \in \mathcal{B},$$

$$[\![\Psi^{\alpha} \otimes \mathbf{w}_{\alpha\Gamma} - \Phi^{\alpha}]\!] \mathbf{n}_{\Gamma} = \mathbf{0} \qquad \forall \, \mathbf{x} = \mathbf{x}_{\Gamma} \in \Gamma.$$

$$(3.81)$$

Finally, this results in the same local form of the balance relations as (3.55), however, additionally with corresponding jump conditions across the interface for the physical quantities mass, linear momentum and energy, as denoted below.

Mass balance of continua with singular surface:

$$(\rho^{\alpha})'_{\alpha} + \rho^{\alpha} \operatorname{div} \, \stackrel{\prime}{\mathbf{x}}_{\alpha} = \hat{\rho}^{\alpha} \quad \forall \, \mathbf{x} \in \mathcal{B},$$

$$[\![\rho^{\alpha} \mathbf{w}_{\alpha\Gamma}]\!] \cdot \mathbf{n}_{\Gamma} = 0 \qquad \forall \, \mathbf{x} = \mathbf{x}_{\Gamma} \in \Gamma,$$
(3.83)

Balance of linear momentum of continua with singular surface:

$$\rho^{\alpha} \overset{"}{\mathbf{x}}_{\alpha} = \operatorname{div} \mathbf{T}^{\alpha} + \rho^{\alpha} \mathbf{b}^{\alpha} + \hat{\mathbf{p}}^{\alpha} \quad \forall \, \mathbf{x} \in \mathcal{B},$$

$$[\![\rho^{\alpha} \overset{'}{\mathbf{x}}_{\alpha} \otimes \mathbf{w}_{\alpha\Gamma} - \mathbf{T}^{\alpha}]\!] \mathbf{n}_{\Gamma} = \mathbf{0} \quad \forall \, \mathbf{x} = \mathbf{x}_{\Gamma} \in \Gamma,$$
(3.84)

Energy balance of continua with singular surface:

$$\rho^{\alpha} (\varepsilon^{\alpha})'_{\alpha} = \mathbf{T}^{\alpha} \cdot \mathbf{L}_{\alpha} - \operatorname{div} \mathbf{q}^{\alpha} + \rho^{\alpha} r^{\alpha} + \hat{\varepsilon}^{\alpha} \qquad \forall \mathbf{x} \in \mathcal{B},$$

$$[\![\rho^{\alpha} (\varepsilon^{\alpha} + \frac{1}{2} \mathbf{x}'_{\alpha} \cdot \mathbf{x}'_{\alpha}) \mathbf{w}_{\alpha\Gamma} - (\mathbf{T}^{\alpha})^{T} \mathbf{x}'_{\alpha} + \mathbf{q}^{\alpha}]\!] \cdot \mathbf{n}_{\Gamma} = 0 \quad \forall \mathbf{x} = \mathbf{x}_{\Gamma} \in \Gamma,$$
(3.85)

These jump relations will be utilised in order to derive the phase transition of the water from liquid to ice, and vice versa, compare **Subsection 4.7.1**.

# Chapter 4: Constitutive setting

Thus far, material-independent relations have been introduced describing general concepts and notions of multicomponent and multiphasic continua at the macroscale including singular surface, which will be utilised to address the phase transition of water. This chapter is dedicated to introduce the material-specific relations to account for the biophysical characteristics of plant tissues.

Note that throughout this chapter, the quaternary model (Model I) is addressed unless stated differently, as it is more general. But due to the downward compatibility of the Model I, the equations for the reduced ternary model (Model II) are the ones as stated in this chapter for the quaternary model after neglecting the parts related to the ice. However, for the sake of completeness, the evaluation of the entropy inequality as well as a short summary of the ternary model in terms of the governing equations and the primary variables is included in **Appendix A** and **Section 4.9**, respectively.

# 4.1 Preliminary modelling assumptions

In order to reduce the complexity of the model to a reasonable degree, a number of preliminary modelling assumptions is introduced.

First of all, the heat and flow processes are assumed to be sufficiently slow, which is motivated from the necessary acclimatisation of the plant tissue in a subzero environment, cf. e. g. Schott [165], Schott *et al.* [167]. This leads to the assumption of a local thermodynamical equilibrium, which indicates particularly that a common temperature for all constituents can be postulated, viz.:

$$\theta^{\alpha} = \theta. \tag{4.1}$$

This assumption requires the consideration of the energy balance of the overall aggregate instead of the constituent-specific energy balances with their individual temperatures. However, it does not restrict a temporal or spatial change in temperature. The hypothesis of slow processes motivates also the assumption of quasi-static processes, which allows for the neglection of the inertia forces, such that

$$\mathbf{x}_{\alpha}^{\prime\prime} = \mathbf{0}. \tag{4.2}$$

Furthermore, it motivates another standard assumption from thermodynamics, that the thermal quantities dominate the processes, indicating that the internal energy is large in comparison to the kinetic energy, viz.:

$$\mathbf{x}_{\alpha} \cdot \mathbf{x}_{\alpha} \ll \varepsilon^{\alpha}. \tag{4.3}$$

Moreover, the gaseous component is assumed to be materially compressible, implying that within a thermomechanical framework, the density is a function of the local temperature and pressure, i. e.  $\rho^{GR} = \rho^{GR}(\theta, p^{GR})$ . The other constituents are assumed to be materially incompressible, meaning that the effective density is a function of temperature only, such that  $\rho^{SR} = \rho^{SR}(\theta)$ ,  $\rho^{IR} = \rho^{IR}(\theta)$  and  $\rho^{LR} = \rho^{LR}(\theta)$ . Thus, the respective material time derivative of the effective densities with respect to the motion of the solid skeleton are given via

$$(\rho^{SR})'_{S} = \frac{\partial \rho^{SR}}{\partial \theta} \theta'_{S}, \quad (\rho^{IR})'_{S} = \frac{\partial \rho^{IR}}{\partial \theta} \theta'_{S}, \quad (\rho^{LR})'_{S} = \frac{\partial \rho^{LR}}{\partial \theta} \theta'_{S}. \tag{4.4}$$

Within the chosen modelling approach, there are two types of mass interactions. There is cell dehydration, which is the flow of water from the intracellular space to the extracellular space through the porous cell wall, and the phase transformation of water within the macro-pore space, which is included by a mass-production term between solid ice  $\varphi^I$  and water  $\varphi^L$ . The cell dehydration is also addressed by a mass-production term, here between the solid skeleton  $\varphi^S$  and water  $\varphi^L$ . This is obviously a simplification, as the biological tissue material is not converted into water, however, it is still a valid assumption, as the cells consist predominantly of water, by up to 90%. Therefore, cell dehydration is characterised by a local decrease in solid volume fraction  $n^S$ . The amount of ice in the intercellular (macro-pore) space is naturally addressed by its local volume fraction  $n^I$ . The amount of mobile water within the macro-pore space, characterised by  $n^L$ , is the result of the two mentioned mass interactions. The gaseous phase is not assumed to exchange mass with the other constituents, which leads to

$$\hat{\rho}^G = 0. \tag{4.5}$$

Regarding external, volumetric supply, gravitation is generally considered to act as constant and homogeneous body force on all constituents

$$\mathbf{b}^{\alpha} = \mathbf{g},\tag{4.6}$$

however, its impact can be neglected for the in **Chapter 6** presented numerical examples, as the relevant processes are acting in-plane, while the gravitation naturally acts out-of-plane along the twig. Furthermore, radiation is neglected in the current modelling approach, as an interaction of the strategies in plants in a subzero-temperature environment with processes like photosynthesis is not within the scope of this monograph, as the strategies regarding frost resistance work also in the absence of radiation, thus

$$r^{\alpha} = 0. \tag{4.7}$$

The assumptions regarding kinematics have already been introduced in terms of the water in the micro-pore space, which is bounded to the solid skeleton and exhibits, therefore, the same motion, and in terms of the ice, which is also kinematically coupled to the solid skeleton, as stated in **Subsection 3.2.1** and **Subsection 3.3.4**, respectively.

# 4.2 Thermo-elastic solids with mass interaction

The discussion concerning the use of the mass balance of materially incompressible solids with mass interaction in the framework of thermoelastic plants is based on the corresponding notions regarding the solid skeleton that have been introduced in Eurich *et al.* [67]. Here, within the context of this monograph, these concepts are extended to account also for the behaviour of the solid ice, which results in slightly different equations in case of the ice. When possible, the placeholder  $\delta = \{S, I\}$  is utilised to address both solids.

## 4.2.1 Decomposition of the deformation

In the framework of thermoelasticity, the material deformation gradient  $\mathbf{F}_{\delta}$  is usually split into a thermal part  $\mathbf{F}_{\delta\theta}$  and a mechanical part  $\mathbf{F}_{\delta M}$ , compare [58, 67, 91, 118]. This indicates for the deformation gradient

$$\mathbf{F}_{\delta} = \frac{\partial \boldsymbol{\chi}_{\delta}(\mathbf{X}_{\delta}, t)}{\partial \mathbf{X}_{\delta}} = \mathbf{F}_{\delta M} \, \mathbf{F}_{\delta \theta}. \tag{4.8}$$

Note that the thermal part is defined by a fictive mechanical unloading, cf. Hartmann [91]. Therein, it has also been shown, that for the chosen setting of an isotropic thermal part of the deformation gradient, the order in (4.8) does not matter. Hence, according to Lu & Pister [118] or Ehlers & Häberle [58], the thermal deformation is given via

$$\mathbf{F}_{\delta\theta} = (\det \mathbf{F}_{\delta\theta})^{1/3} \mathbf{I},\tag{4.9}$$

where the respective determinant can be stated as follows, viz.:

det 
$$\mathbf{F}_{S\theta} = \exp\left[3\,\alpha^S(\theta - \theta_{0S}^S)\right]$$
 and det  $\mathbf{F}_{I\theta} = \exp\left[3\,\alpha^{IR}(\theta - \theta_{0I}^I)\right].$  (4.10)

Note that the material parameters of the solid skeleton refer always to the empty porous solid material and not to the bulk solid material. Thus, the parameters are understood as homogenised quantities, as for example  $\alpha^{S}$ . For all other constituents, as for the ice in this case, the material parameters have to be understood as effective quantities, as for example  $\alpha^{IR}$ , as they refer to the bulk material.

A further multiplicative split of the deformation gradient of the solid skeleton into a growth-dependent part and a deformation-dependent part, as introduced in Ambrosi & Mollica [2] for a singlephasic material or in Humphrey & Rajagopal [97] for a multiphase model, is omitted in this context, as the involved bio-physical phenomena are different; particularly there is no real growth in this case. Instead, the solid skeleton is shrinking or swelling via dehydration or rehydration of the cells, respectively. This effect is accounted for by the local decrease or increase of the solid volume fraction governed by the mass-production term  $\hat{\rho}^S$ , similar to the approaches of Ricken & Bluhm [148] and Ricken *et al.* [151]. This applies in the same way to the solid ice, where the growth or shrinkage of the ice body is solely addressed by an increase or decrease of the ice volume fraction via the mass-production term  $\hat{\rho}^I$ .

# 4.2.2 Materially incompressible thermo-elastic solids

Based on  $(3.58)_1$ , (4.9) and (4.10), an alternative version of the mass balance for a thermoelastic and materially incompressible solid constituent with mass interaction is derived. For solids, the mass balance is usually utilised in integrated form for the determination of its volume fraction. Thus, the mass balance  $(3.58)_1$  can be reformulated, as for example in Krause [112], obtaining

$$\frac{(\rho^{\delta})_{\delta}'}{\rho^{\delta}} + \frac{(\det \mathbf{F}_{\delta})_{\delta}'}{\det \mathbf{F}_{\delta}} = \frac{\hat{\rho}^{\delta}}{\rho^{\delta}}.$$
(4.11)

With the method of separation of variables, (4.11) yields

$$\int_{\rho_{0\delta}^{\delta}}^{\rho^{\delta}} \frac{1}{\tilde{\rho}^{\delta}} d_{\delta} \tilde{\rho}^{\delta} + \int_{\det \mathbf{I}}^{\det \mathbf{F}_{\delta}} \frac{1}{\det \mathbf{\tilde{F}}_{\delta}} d_{\delta} (\det \mathbf{\tilde{F}}_{\delta}) = \int_{t_0}^{t} \frac{\hat{\rho}^{\delta}}{\rho^{\delta}} dt.$$
(4.12)

The formal integration of (4.12) leads to

$$\ln(\rho^{\delta}) - \ln(\rho_{0\delta}^{\delta}) + \ln(\det \mathbf{F}_{\delta}) = \int_{t_0}^t \frac{\hat{\rho}^{\delta}}{\rho^{\delta}} dt, \qquad (4.13)$$

where the application of appropriate logarithm rules reveals

$$\rho^{\delta} = \rho_{0\delta}^{\delta} \, (\det \mathbf{F}_{\delta})^{-1} \, \exp\left(\int_{t_0}^t \frac{\hat{\rho}^{\delta}}{\rho^{\delta}} \, \mathrm{d}t\right). \tag{4.14}$$

Note that this formal procedure might cause problems, since the initial value  $\rho_{0\delta}^{\delta}$  might not differ from zero, particularly for the ice. Equation (4.14) is further elaborated by considering the split of deformation, compare (4.8), as well as the density definitions (3.9), which yields

$$n^{\delta} \rho^{\delta R} = n_{0\delta}^{\delta} \rho_{0\delta}^{\delta R} \left( \det \mathbf{F}_{\delta M} \right)^{-1} \left( \det \mathbf{F}_{\delta \theta} \right)^{-1} \exp \left( \int_{t_0}^t \frac{\hat{\rho}^{\delta}}{\rho^{\delta}} \, \mathrm{d}t \right).$$
(4.15)

From (4.15), it is seen that the partial density  $\rho^{\delta} = n^{\delta} \rho^{\delta R}$  may change due to a variety of reasons, due to mechanical deformation, thermal deformation or mass production, respectively. In order to recap, for the case of materially incompressible solids, the intrinsic density  $\rho^{\delta R}$  is constant under isothermal conditions and depends under non-isothermal conditions only on the thermal part det  $\mathbf{F}_{\delta\theta}$  of det  $\mathbf{F}_{\delta}$ . Thus,

$$\rho^{\delta R} = \rho_{0\delta}^{\delta R} \, (\det \mathbf{F}_{\delta\theta})^{-1}. \tag{4.16}$$

By use of this relation, (4.15) reduces to

$$n^{\delta} \rho^{\delta R} = n_{0\delta}^{\delta} \rho^{\delta R} \left( \det \mathbf{F}_{\delta M} \right)^{-1} \exp \left( \int_{t_0}^t \frac{\hat{n}^{\delta} \rho^{\delta R}}{n^{\delta} \rho^{\delta R}} \, \mathrm{d}t \right).$$
(4.17)

In (4.17), the mass production  $\hat{\rho}^{\delta}$  has been substituted by  $\hat{n}^{\delta}\rho^{\delta R}$ . Thus, the production of partial density actually means that the volume that is covered by  $\varphi^{\delta}$  with density  $\rho^{\delta R}$  is changing through  $\hat{n}^{\delta}$ , the effective density  $\rho^{\delta R}$  remains unchanged in terms of a production. Therefore, while  $\rho^{\delta R}$  is governed by (4.16), the solid volume fraction is governed by

$$n^{\delta} = n_{0\delta}^{\delta} \left(\det \mathbf{F}_{\delta M}\right)^{-1} \exp\left(\int_{t_0}^t \frac{\hat{n}^{\delta}}{n^{\delta}} \,\mathrm{d}t\right)$$
(4.18)

indicating that the volume fraction  $n^{\delta}$  may change due to mechanical deformation or mass production. Regarding (4.18), there are two important circumstances that are worth noting. Firstly, the initial volume fraction  $n_{0\delta}^{\delta}$  may not differ from zero, and, secondly, (4.18) is an implicit equation with respect to  $n^{\delta}$  due to the non-vanishing volume production  $\hat{n}^{\delta}$ . Therefore, the respective volume fraction  $n^{\delta}$  has to be solved by the respective weak form (5.6)<sub>3</sub> (or (5.9)<sub>3</sub> for the ternary model) and (5.6)<sub>4</sub> of the mass balances (4.158) (or (4.168) for the ternary model) and (4.159), for the solid skeleton and solid ice. Note in passing that for the case of a linear dependency of the volume production  $\hat{n}^{\delta}$  on the volume fraction  $n^{\delta}$ , relation (4.18) can be considered as explicit equation for the solution of the respective volume fraction  $n^{\delta}$ . However, such an approach is bio-physically not reasonable within this context.

Since the thermal part det  $\mathbf{F}_{\delta\theta}$  of det  $\mathbf{F}_{\delta}$  is given according to [58, 118], the respective functions of the effective density for the solid skeleton and the ice are given via

$$\rho^{SR} = \rho_{0S}^{SR} \exp\left[-3\,\alpha^{S}(\theta - \theta_{0S}^{S})\right] \quad \text{and} \quad \rho^{IR} = \rho_{0I}^{IR} \exp\left[-3\,\alpha^{IR}(\theta - \theta_{0I}^{I})\right]. \tag{4.19}$$

It needs to be kept in mind that the material parameters of the solid skeleton depend highly on the plant species or even on the status of the specimen, potentially also in terms of its water content, that is being tested. Therefore, the thermal dependence of the density remains rather inaccessible. However, for the ice, the chosen ansatz  $(4.19)_2$  can be compared to experimental data. This is done and shown together with the density of liquid water in Figure 4.4.

# 4.3 Thermodynamic consistency

In order to ensure thermodynamic consistency of the material-specific equations that have to be introduced, the basic principles of continuum thermodynamics need to be paid attention on. These principles are determinism, equipresence, local action, material frame indifference and dissipation. They are discussed in this section in application to the plant-tissue model. In particular, the dissipation principle needs to be evaluated using the entropy inequality of the overall aggregate in order to identify the direction of a certain process and also the couplings amongst these processes. Here, only the entropy inequality of the quaternary aggregate is evaluated, the one for the ternary model can be found in **Appendix A**. The saturation constraint and effective stress principle: The thermodynamic basis for the constitutive equations that need to be developed is given by the entropy inequality of the overall aggregate. It states the direction, in which a certain process has to occur and reads in the generic form

$$\sum_{\alpha} \{-\rho^{\alpha}[(\psi^{\alpha})'_{\alpha} + \theta'_{\alpha}\eta^{\alpha}] - \hat{\mathbf{p}}^{\alpha} \cdot \mathbf{\dot{x}}_{\alpha} - \hat{\rho}^{\alpha}(\psi^{\alpha} + \frac{1}{2} \mathbf{\dot{x}}_{\alpha} \cdot \mathbf{\dot{x}}_{\alpha}) + \mathbf{T}^{\alpha} \cdot \mathbf{L}_{\alpha} - \frac{1}{\theta} \mathbf{q}^{\alpha} \cdot \operatorname{grad} \theta - \mathcal{P}(n^{\alpha})'_{S}\} \ge 0,$$

$$(4.20)$$

where the side condition of fully saturation by means of the time derivative  $(\cdot)'_S$  of (3.4) multiplied with the *Lagrangean* multiplier  $\mathcal{P}$  has already been included. The mentioned saturation condition is an equation in excess that restricts the motion of the involved constituents, which causes the reaction force  $\mathcal{P}$ , as discussed in Bluhm *et al.* [19], Ricken & Bluhm [148]. Relation (3.4) is added by using (3.22), the respective mass balances  $(3.58)_1$  and the constraint for the density production  $(3.57)_1$ , which leads to

$$\sum_{\alpha} (n^{\alpha})'_{S} = (n^{S})'_{S} + (n^{I})'_{S} + (n^{L})'_{S} + (n^{G})'_{S} =$$

$$= (n^{S})'_{S} + (n^{I})'_{S} + (n^{L})'_{L} - \operatorname{grad} n^{L} \cdot \mathbf{w}_{L} + (n^{G})'_{G} - \operatorname{grad} n^{G} \cdot \mathbf{w}_{G} =$$

$$= \frac{\hat{\rho}^{S}}{\rho^{SR}} - n^{S} \mathbf{I} \cdot \mathbf{D}_{S} - \frac{n^{S}}{\rho^{SR}} \frac{\partial \rho^{SR}}{\partial \theta} \theta'_{S} +$$

$$+ \frac{\hat{\rho}^{I}}{\rho^{IR}} - n^{I} \mathbf{I} \cdot \mathbf{D}_{S} - \frac{n^{I}}{\rho^{IR}} \frac{\partial \rho^{IR}}{\partial \theta} \theta'_{S} -$$

$$- \frac{\hat{\rho}^{S}}{\rho^{LR}} - \frac{\hat{\rho}^{I}}{\rho^{LR}} - n^{L} \mathbf{I} \cdot \mathbf{D}_{L} - \frac{n^{L}}{\rho^{LR}} \frac{\partial \rho^{LR}}{\partial \theta} \theta'_{L} - \operatorname{grad} n^{L} \cdot \mathbf{w}_{L} -$$

$$- n^{G} \mathbf{I} \cdot \mathbf{D}_{G} - \frac{n^{G}}{\rho^{GR}} (\rho^{GR})'_{G} - \operatorname{grad} n^{G} \cdot \mathbf{w}_{G} = 0.$$

$$(4.21)$$

Therein, the material time derivative with respect to the motion of the ice has been included considering the kinematic coupling of the ice to the solid skeleton via (3.37). The saturation constraint will be included into the entropy inequality in *Clausius-Duhem* form (4.20), along with the constraint concerning momentum production, i. e.  $(3.57)_2$ ,

 $(3.59)_1$ , and (3.34), yielding

$$\begin{split} &(\underbrace{\mathbf{T}^{S} + n^{S}\mathcal{P}\mathbf{I}}_{\mathbf{T}_{E}^{S}}) \cdot \mathbf{D}_{S} - \rho^{S}(\psi^{S})_{S}' - \rho^{S}(\underbrace{\eta^{S} - \mathcal{P}\frac{1}{(\rho^{SR})^{2}}\frac{\partial\rho^{SR}}{\partial\theta}})\theta_{S}' + \\ &+ (\underbrace{\mathbf{T}^{I} + n^{I}\mathcal{P}\mathbf{I}}_{\mathbf{T}_{E}^{I}}) \cdot \mathbf{D}_{S} - \rho^{I}(\psi^{I})_{S}' - \rho^{I}(\underbrace{\eta^{I} - \mathcal{P}\frac{1}{(\rho^{IR})^{2}}\frac{\partial\rho^{IR}}{\partial\theta}})\theta_{S}' + \\ &+ (\underbrace{\mathbf{T}^{L} + n^{L}\mathcal{P}\mathbf{I}}_{\mathbf{T}_{E}^{L}}) \cdot \mathbf{D}_{L} - \rho^{L}(\psi^{L})_{L}' - \rho^{L}(\underbrace{\eta^{L} - \mathcal{P}\frac{1}{(\rho^{LR})^{2}}\frac{\partial\rho^{LR}}{\partial\theta}})\theta_{L}' + \\ &+ (\underbrace{\mathbf{T}^{G} + n^{G}\mathcal{P}\mathbf{I}}_{\mathbf{T}_{E}^{G}}) \cdot \mathbf{D}_{G} - \rho^{G}(\psi^{G})_{G}' - \rho^{G}\eta^{G}\theta_{G}' + \mathcal{P}\frac{n^{G}}{\rho^{GR}}(\rho^{GR})_{G}' - \\ &- (\underbrace{\hat{\mathbf{p}}^{L} - \mathcal{P}\operatorname{grad} n^{L}}_{\mathbf{p}_{E}^{L}}) \cdot \mathbf{w}_{L} - \widehat{\rho^{S}}\overset{'}{\mathbf{x}}_{S} \cdot \mathbf{w}_{L} - \widehat{\rho^{I}}\overset{'}{\mathbf{x}}_{S} \cdot \mathbf{w}_{L} - \\ &- (\underbrace{\hat{\mathbf{p}}^{G} - \mathcal{P}\operatorname{grad} n^{G}}_{\mathbf{p}_{E}^{G}}) \cdot \mathbf{w}_{G} - \frac{1}{\theta}(\mathbf{q}^{S} + \mathbf{q}^{I} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \operatorname{grad} \theta - \\ &- \widehat{\rho}^{S}(\psi^{S} + \frac{1}{2}\overset{'}{\mathbf{x}}_{S} \cdot \overset{'}{\mathbf{x}}_{S} - \psi^{L} - \frac{1}{2}\overset{'}{\mathbf{x}}_{L} \cdot \overset{'}{\mathbf{x}}_{L} + \frac{\mathcal{P}}{\rho^{SR}} - \frac{\mathcal{P}}{\rho^{LR}}) - \\ &- \widehat{\rho}^{I}(\psi^{I} + \frac{1}{2}\overset{'}{\mathbf{x}}_{S} \cdot \overset{'}{\mathbf{x}}_{S} - \psi^{L} - \frac{1}{2}\overset{'}{\mathbf{x}}_{L} \cdot \overset{'}{\mathbf{x}}_{L} + \frac{\mathcal{P}}{\rho^{IR}} - \frac{\mathcal{P}}{\rho^{LR}}) \geq 0. \end{split}$$

Therein, the extra quantities that are due to the saturation condition (3.4) have been identified. These extra quantities are defined via

$$\mathbf{T}_{E}^{S} = \mathbf{T}^{S} + n^{S} \mathcal{P} \mathbf{I}, \qquad \mathbf{T}_{E}^{I} = \mathbf{T}^{I} + n^{I} \mathcal{P} \mathbf{I}, \qquad \mathbf{T}_{E}^{L} = \mathbf{T}^{L} + n^{L} \mathcal{P} \mathbf{I},$$
$$\mathbf{T}_{E}^{G} = \mathbf{T}^{G} + n^{G} \mathcal{P} \mathbf{I}, \qquad \hat{\mathbf{p}}_{E}^{L} = \hat{\mathbf{p}}^{L} - \mathcal{P} \operatorname{grad} n^{L}, \qquad \hat{\mathbf{p}}_{E}^{G} = \hat{\mathbf{p}}^{G} - \mathcal{P} \operatorname{grad} n^{G},$$
$$\eta_{E}^{S} = \eta^{S} - \mathcal{P} \frac{1}{(\rho^{SR})^{2}} \frac{\partial \rho^{SR}}{\partial \theta}, \qquad \eta_{E}^{I} = \eta^{I} - \mathcal{P} \frac{1}{(\rho^{IR})^{2}} \frac{\partial \rho^{IR}}{\partial \theta}, \qquad \eta_{E}^{L} = \eta^{L} - \mathcal{P} \frac{1}{(\rho^{LR})^{2}} \frac{\partial \rho^{LR}}{\partial \theta}.$$
$$(4.23)$$

Hence, the entropy inequality (4.22) can be displayed with the introduced extra quantities (4.23), viz.:

$$\mathbf{T}_{E}^{S} \cdot \mathbf{D}_{S} - \rho^{S}(\psi^{S})_{S}^{\prime} - \rho^{S}\eta_{E}^{S}\theta_{S}^{\prime} + \mathbf{T}_{E}^{I} \cdot \mathbf{D}_{S} - \rho^{I}(\psi^{I})_{S}^{\prime} - \rho^{I}\eta_{E}^{I}\theta_{S}^{\prime} + \mathbf{T}_{E}^{L} \cdot \mathbf{D}_{L} - \rho^{L}(\psi^{L})_{L}^{\prime} - \rho^{L}\eta_{E}^{L}\theta_{L}^{\prime} + \mathbf{T}_{E}^{G} \cdot \mathbf{D}_{G} - \rho^{G}(\psi^{G})_{G}^{\prime} - \rho^{G}\eta^{G}\theta_{G}^{\prime} + \mathcal{P}\frac{n^{G}}{\rho^{GR}}(\rho^{GR})_{G}^{\prime} - \hat{\mathbf{p}}_{E}^{L} \cdot \mathbf{w}_{L} - \hat{\rho}^{S} \mathbf{x}_{S} \cdot \mathbf{w}_{L} - \hat{\rho}^{I} \mathbf{x}_{S} \cdot \mathbf{w}_{L} - \hat{\mathbf{p}}_{E}^{G} \cdot \mathbf{w}_{G} - \frac{1}{\theta}(\mathbf{q}^{S} + \mathbf{q}^{I} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \operatorname{grad} \theta - \hat{\rho}^{S}(\psi^{S} + \frac{1}{2}\mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2}\mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{\mathcal{P}}{\rho^{SR}} - \frac{\mathcal{P}}{\rho^{LR}}) - \hat{\rho}^{I}(\psi^{I} + \frac{1}{2}\mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2}\mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{\mathcal{P}}{\rho^{IR}} - \frac{\mathcal{P}}{\rho^{LR}}) \geq 0.$$

$$(4.24)$$

**Thermodynamical principles and process variables:** With the help of the entropy inequality, restrictions for those quantities, the so-called response functions  $\mathcal{R}$ , that cannot be determined with the knowledge of the initial state and the balance relations, need to derived. The set of response functions for the given TPM model is given via

$$\mathcal{R} = \{\psi^{\alpha}, \mathbf{T}_{E}^{\alpha}, \eta_{E}^{S}, \eta_{E}^{I}, \eta_{E}^{L}, \eta^{G}, \hat{\mathbf{p}}_{E}^{\beta}, \hat{\rho}^{\delta}, \mathbf{q}^{\alpha}\}.$$
(4.25)

These response functions depend on process variables that have to be included into (4.24) by proposing appropriate dependencies of the *Helmholtz* free energies  $\psi^{\alpha}$  considering the basic principles of continuum thermodynamics, such as determinism, equipresence, local action, material frame indifference and dissipation, cf. e. g. Ehlers [47, 49] and the fundamental investigation by Truesdell [182]. In particular, the set of process variables proceeds also from the principle of phase separation [43]. Thus, based on the work of Ehlers [45, 47], the basic set  $\mathcal{V}$  of process variables for homogeneous porous materials with a common temperature field is given via

$$\mathcal{V} = \{\theta, \operatorname{grad} \theta, n^{\gamma}, \operatorname{grad} n^{\gamma}, \rho^{\alpha R}, \operatorname{grad} \rho^{\alpha R}, \mathbf{F}_{\alpha}, \operatorname{Grad}_{\alpha} \mathbf{F}_{\alpha}, \mathbf{x}_{\alpha}, \operatorname{Grad}_{\alpha} \mathbf{x}_{\alpha}^{\prime}\}, \qquad (4.26)$$

where, as usual,  $\alpha = 1, ..., q$ , where q = 4 for the quaternary model, and additionally  $\gamma = 2, ..., q$ , due to (3.4). Recalling (4.26) and the principle of phase separation, the basic set of process variables for the underlying TPM model reads for the respective constituents

$$\psi^{S} = \psi^{S}(\theta, \operatorname{grad} \theta, \mathbf{C}_{S}, \operatorname{Grad}_{S} \mathbf{C}_{S}, \mathcal{M}^{S}),$$
  

$$\psi^{I} = \psi^{I}(\theta, \operatorname{grad} \theta, n^{I}, \operatorname{grad} n^{I}, \mathbf{C}_{I}, \operatorname{Grad}_{I} \mathbf{C}_{I}),$$
  

$$\psi^{L} = \psi^{L}(\theta, \operatorname{grad} \theta, s^{L}, \operatorname{grad} s^{L}, \mathbf{w}_{L}, \mathbf{D}_{L}),$$
  

$$\psi^{G} = \psi^{G}(\theta, \operatorname{grad} \theta, \rho^{GR}, \operatorname{grad} \rho^{GR}, \mathbf{w}_{G}, \mathbf{D}_{G}).$$
  
(4.27)

Therein, for the solid skeleton, the dependency of the *Helmholtz* free energy  $\psi^S$  on its volume fraction  $n^S$ , effective density  $\rho^{SR}$ , velocity  $\mathbf{\dot{x}}_S$  and their derivatives can be omitted

(4.28)

due to the assumptions of fully saturation, material incompressibility and elasticity, respectively. Instead of the deformation gradient  $\mathbf{F}_{S}$ , the right Cauchy-Green deformation tensor  $C_S$  is used, since the first-mentioned is lacking of frame indifference, cf. e. g. Ehlers [47]. Furthermore, biological materials may be anisotropic. In the present case, transversal isotropy can be assumed, where one preferred direction needs to be considered with a structural tensor  $\mathcal{M}^S$ , cf. Subsection 4.4.1. The heterogeneity of the tissue material may be accounted for with spatially varying material parameters rather than including explicitly the dependency on the reference position  $\mathbf{X}_{S}$ , cf. e. g. Wagner [187]. For the ice, following the work of Bluhm et al. [16, 18], a set of assumptions is proposed. The ice is assumed to behave like a materially incompressible elastic solid, therefore, the effective density  $\rho^{IR}$ , the velocity  $\mathbf{x}_{I}$  and their derivatives can be omitted as process variables. The liquid water in the macro-pore space is assumed to be materially incompressible, which leads to the deletion of the effective density  $\rho^{LR}$  and its derivative, the volume fraction  $n^{L}$  has been replaced with the saturation  $s^{L}$ . For the fluids at hand, the inclusion of the deformation gradient can be omitted, since the deformation is sufficiently described by the partial density or their replacement. Finally, the liquid velocity  $\mathbf{\dot{x}}_{L}$  and its derivative has been replaced by the seepage velocity  $\mathbf{w}_L$  and the rate of deformation  $\mathbf{D}_L$ , since the first-mentioned quantities lack of frame indifference cf. e. g. Ehlers [47]. The gaseous air has no mass exchange with the other constituents, hence, no measure accounting for its relative amount needs to be considered. However, the air is materially compressible and, consequently, the effective density  $\rho^{GR}$  needs to be considered as process variable. The comments on the liquid constituent regarding deformation and material frame indifference are also true for the gaseous constituent, therefore, the deformation gradient of the gas can be omitted, and the velocity  $\mathbf{\dot{x}}_{G}$  and its derivative are replaced by the objective functions  $\mathbf{w}_G$  and  $\mathbf{D}_G$ . Therefore, the derivatives of the *Helmholtz* free energies  $(\psi^{\alpha})'_{\alpha}$  are given via

$$\begin{split} (\psi^{S})'_{S} &= \frac{\partial \psi^{S}}{\partial \theta} \, \theta'_{S} + \frac{\partial \psi^{S}}{\partial \operatorname{grad} \theta} \cdot (\operatorname{grad} \theta)'_{S} + \frac{\partial \psi^{S}}{\partial \mathbf{C}_{S}} \cdot (\mathbf{C}_{S})'_{S} + \frac{\partial \psi^{S}}{\partial \operatorname{Grad}_{S} \mathbf{C}_{S}} \cdot (\operatorname{Grad}_{S} \mathbf{C}_{S})'_{S}, \\ (\psi^{I})'_{S} &= \frac{\partial \psi^{I}}{\partial \theta} \, \theta'_{S} + \frac{\partial \psi^{I}}{\partial \operatorname{grad} \theta} \cdot (\operatorname{grad} \theta)'_{S} + \frac{\partial \psi^{I}}{\partial n^{I}} (n^{I})'_{S} + \frac{\partial \psi^{I}}{\partial \operatorname{grad} n^{I}} \cdot (\operatorname{grad} n^{I})'_{S} + \\ &+ \frac{\partial \psi^{I}}{\partial \mathbf{C}_{I}} \cdot (\mathbf{C}_{I})'_{S} + \frac{\partial \psi^{I}}{\partial \operatorname{grad} \theta} \cdot (\operatorname{grad} \theta)'_{L} + \frac{\partial \psi^{L}}{\partial s^{L}} (s^{L})'_{L} + \frac{\partial \psi^{L}}{\partial \operatorname{grad} s^{L}} \cdot (\operatorname{grad} s^{L})'_{L} + \\ &+ \frac{\partial \psi^{L}}{\partial \mathbf{W}_{L}} \cdot (\mathbf{W}_{L})'_{L} + \frac{\partial \psi^{L}}{\partial \mathbf{D}_{L}} \cdot (\mathbf{D}_{L})'_{L}, \\ (\psi^{G})'_{G} &= \frac{\partial \psi^{G}}{\partial \theta} \, \theta'_{G} + \frac{\partial \psi^{G}}{\partial \operatorname{grad} \theta} \cdot (\operatorname{grad} \theta)'_{G} + \frac{\partial \psi^{G}}{\partial \rho^{GR}} (\rho^{GR})'_{G} + \frac{\partial \psi^{G}}{\partial \operatorname{grad} \rho^{GR}} \cdot (\operatorname{grad} \rho^{GR})'_{G} + \\ &+ \frac{\partial \psi^{G}}{\partial \mathbf{W}_{G}} \cdot (\mathbf{W}_{G})'_{G} + \frac{\partial \psi^{G}}{\partial \mathbf{D}_{G}} \cdot (\mathbf{D}_{G})'_{G}. \end{split}$$

**Thermodynamical restrictions:** The inclusion of the derivatives of the *Helmholtz* free energies  $(\psi^{\alpha})'_{\alpha}$  into the entropy inequality with the introduced extra quantities (4.24) yields

$$\begin{split} \mathbf{T}_{E}^{S} \cdot \mathbf{D}_{S} &- \rho^{S} \frac{\partial \psi^{S}}{\partial \theta} \, \theta_{S}^{\prime} - \rho^{S} \frac{\partial \psi^{S}}{\partial \operatorname{grad}} \cdot (\operatorname{grad} \theta)_{S}^{\prime} - \rho^{S} \frac{\partial \psi^{S}}{\partial \mathbf{C}_{S}} \cdot (\mathbf{C}_{S})_{S}^{\prime} - \\ &- \rho^{S} \frac{\partial \psi^{S}}{\partial \operatorname{Grad}_{S} \mathbf{C}_{S}} \cdot (\operatorname{Grad}_{S} \mathbf{C}_{S})_{S}^{\prime} - \rho^{S} \eta_{E}^{S} \theta_{S}^{\prime} + \\ &+ \mathbf{T}_{E}^{I} \cdot \mathbf{D}_{S} - \rho^{I} \frac{\partial \psi^{I}}{\partial \theta} \, \theta_{S}^{\prime} - \rho^{I} \frac{\partial \psi^{I}}{\partial \operatorname{grad}} \cdot (\operatorname{grad} \theta)_{S}^{\prime} - \rho^{I} \frac{\partial \psi^{I}}{\partial \operatorname{Grad}_{I} \mathbf{C}_{I}} \cdot (\operatorname{Grad}_{I} \mathbf{C}_{I})_{S}^{\prime} - \\ &- \rho^{I} \frac{\partial \psi^{I}}{\partial \operatorname{grad} n^{I}} \cdot (\operatorname{grad} n^{I})_{S}^{\prime} - \rho^{I} \frac{\partial \psi^{I}}{\partial \mathbf{C}_{I}} \cdot (\mathbf{C}_{I})_{S}^{\prime} - \rho^{I} \frac{\partial \psi^{I}}{\partial \operatorname{Grad}_{I} \mathbf{C}_{I}} \cdot (\operatorname{Grad}_{I} \mathbf{C}_{I})_{S}^{\prime} - \rho^{I} \eta_{E}^{I} \theta_{S}^{\prime} + \\ &+ \mathbf{T}_{E}^{I} \cdot \mathbf{D}_{L} - \rho^{L} \frac{\partial \psi^{L}}{\partial \theta} \, \theta_{L}^{\prime} - \rho^{L} \frac{\partial \psi^{L}}{\partial \operatorname{grad}} \cdot (\operatorname{grad} \theta)_{L}^{\prime} - \rho^{L} \frac{\partial \psi^{L}}{\partial \mathbf{D}_{L}} \cdot (\mathbf{D}_{L})_{L}^{\prime} - \rho^{L} \eta_{E}^{L} \theta_{L}^{\prime} + \\ &+ \mathbf{T}_{E}^{G} \cdot \mathbf{D}_{G} - \rho^{G} \frac{\partial \psi^{G}}{\partial \theta} \, \theta_{G}^{\prime} - \rho^{G} \frac{\partial \psi^{G}}{\partial \operatorname{grad}} \cdot (\operatorname{grad} \theta)_{G}^{\prime} - \rho^{G} \frac{\partial \psi^{G}}{\partial \mathbf{D}_{L}} \cdot (\mathbf{D}_{G})_{L}^{\prime} - \rho^{L} \eta_{E}^{L} \theta_{L}^{\prime} + \\ &+ \mathbf{T}_{E}^{G} \cdot \mathbf{D}_{G} - \rho^{G} \frac{\partial \psi^{G}}{\partial \theta} \, \theta_{G}^{\prime} - \rho^{G} \frac{\partial \psi^{G}}{\partial \operatorname{grad}} \theta \cdot (\operatorname{grad} \theta)_{G}^{\prime} - \rho^{G} \frac{\partial \psi^{G}}{\partial \mathbf{D}_{L}} \cdot (\mathbf{D}_{G})_{G}^{\prime} - \rho^{G} \eta_{E}^{G} \theta_{G}^{\prime} - \\ &- \rho^{G} \frac{\partial \psi^{G}}{\partial \operatorname{grad} \rho^{GR}} \cdot (\operatorname{grad} \rho^{GR})_{G}^{\prime} - \rho^{G} \frac{\partial \psi^{G}}{\partial \operatorname{wG}} \cdot (\operatorname{w}_{G})_{G}^{\prime} - \rho^{G} \frac{\partial \psi^{G}}{\partial \mathbf{D}_{G}} \cdot (\mathbf{D}_{G})_{G}^{\prime} - \rho^{G} \eta^{G} \theta_{G}^{\prime} - \\ &- \hat{p}_{E}^{L} \cdot \mathbf{w}_{L} - \hat{p}^{S} \, \mathbf{x}_{S} \cdot \mathbf{w}_{L} - \hat{p}^{I} \, \mathbf{x}_{S} \cdot \mathbf{w}_{L} - \hat{p}_{E}^{S} \cdot \mathbf{w}_{G} - \\ &- \hat{p}_{G}^{I} (\mathbf{q}^{S} + \mathbf{q}^{I} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \operatorname{grad} \theta + \mathcal{P} \frac{\eta^{G}}{\rho^{GR}} (\rho^{GR})_{G}^{\prime} - \\ &- \hat{\rho}_{S}^{I} (\psi^{S} + \frac{1}{2} \, \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2} \, \mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{\mathcal{P}}{\rho^{FR}} - \frac{\mathcal{P}}{\rho^{LR}} \right) - \\ &- \hat{\rho}^{I} (\psi^{I} + \frac{1}{2} \, \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2} \, \mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{\mathcal{P}}{\rho^{IR}} - \frac{\mathcal{P}}{\rho^{L}} \partial \mathbf{D}_{L} \right) = 0. \end{split}$$

The entropy inequality (4.29) has to be fulfilled according to the *Coleman-Noll* procedure for arbitrary and independent values of the process variables. In order to ensure their independence, each term in (4.29) is evaluated separately, compare Ehlers [46, 49]. In particular, the entropy inequality (4.29) is split into an equilibrium part and a nonequilibrium part, compare Ehlers [49], Eurich *et al.* [67]. The equilibrium part of (4.29), where the constitutive terms, for which thermodynamical restrictions are needed, do not depend on the rates of deformation and temperature, has to be zero corresponding to the case of no entropy production. Thus, the terms in front of the rates  $(\operatorname{grad} \theta)'_S$ ,  $(\operatorname{Grad}_S \mathbf{C}_S)'_S$ ,  $(\operatorname{grad} n^I)'_S$ ,  $(\operatorname{Grad}_I \mathbf{C}_I)'_S$ ,  $(\operatorname{grad} \theta)'_L$ ,  $(\operatorname{grad} s^L)'_L$ ,  $(\mathbf{D}_L)'_L$ ,  $(\operatorname{grad} \theta)'_G$ ,  $(\operatorname{grad} \rho^{GR})'_G$ ,  $(\mathbf{w}_G)'_G$  and  $(\mathbf{D}_G)'_G$  have to vanish, such that the equation is fulfilled for arbitrary rates. This procedure is exemplarily discussed in Ghadiani [81] for the biphasic model without mass interaction. For the current model, the following derivatives have to vanish, which indicates that the respective dependencies concerning the solids do not have to be maintained, viz.:

$$\frac{\partial \psi^{S}}{\partial \operatorname{grad} \theta} = \mathbf{0}, \qquad \frac{\partial \psi^{S}}{\partial \operatorname{Grad}_{S} \mathbf{C}_{S}} = \overset{3}{\mathbf{0}}, 
\frac{\partial \psi^{I}}{\partial \operatorname{grad} \theta} = \mathbf{0}, \qquad \frac{\partial \psi^{I}}{\partial \operatorname{grad} n^{I}} = \mathbf{0}, \qquad (4.30) 
\frac{\partial \psi^{I}}{\partial \operatorname{Grad}_{I} \mathbf{C}_{I}} = \overset{3}{\mathbf{0}}.$$

Furthermore, for the fluids the following derivatives have to vanish, such that the corresponding dependencies do not need to be considered in the following evaluation of the entropy inequality, viz.:

$$\frac{\partial \psi^{L}}{\partial \operatorname{grad} \theta} = \mathbf{0}, \qquad \frac{\partial \psi^{S}}{\partial \operatorname{grad} s^{L}} = \mathbf{0}, 
\frac{\partial \psi^{L}}{\partial \mathbf{w}_{L}} = \mathbf{0}, \qquad \frac{\partial \psi^{L}}{\partial \mathbf{D}_{L}} = \mathbf{0}, 
\frac{\partial \psi^{G}}{\partial \operatorname{grad} \theta} = \mathbf{0}, \qquad \frac{\partial \psi^{G}}{\partial \operatorname{grad} \rho^{GR}} = \mathbf{0}, 
\frac{\partial \psi^{G}}{\partial \mathbf{w}_{G}} = \mathbf{0}, \qquad \frac{\partial \psi^{G}}{\partial \mathbf{D}_{G}} = \mathbf{0}.$$
(4.31)

Consequently, this leads to the *Helmholtz* free energies  $\psi^{\alpha}$ , which depend on the following process variables that need to be considered when corresponding functions are proposed, viz.:

$$\psi^{S} = \psi^{S}(\theta, \mathbf{C}_{S}, \mathcal{M}^{S}), \qquad \psi^{I} = \psi^{I}(\theta, n^{I}, \mathbf{C}_{I}),$$
  

$$\psi^{L} = \psi^{L}(\theta, s^{L}), \qquad \psi^{G} = \psi^{G}(\theta, \rho^{GR}).$$
(4.32)

The fact, that the motion and, consequently, also the deformation of the ice, are given by the motion of the solid skeleton via (3.39), does not affect the required phase separation. With regard to  $(4.28)_3$ , the material time derivative of the liquid saturation is needed, which has to be derived based on the definition of the saturation itself (3.5), the quotient rule of calculus, relation (3.22) and the respective mass balances  $(3.58)_1$ , leading to

$$(s^{L})'_{L} = \frac{1}{n^{F}} [(n^{L})'_{L} - s^{L}(n^{F})'_{L}] =$$

$$= -\frac{\hat{\rho}^{S}}{n^{F} \rho^{LR}} - \frac{\hat{\rho}^{I}}{n^{F} \rho^{LR}} - s^{L} \mathbf{I} \cdot \mathbf{D}_{L} - \frac{s^{L}}{\rho^{LR}} \frac{\partial \rho^{LR}}{\partial \theta} \theta'_{L} +$$

$$+ \frac{s^{L} \hat{\rho}^{S}}{n^{F} \rho^{SR}} - \frac{s^{L} n^{S}}{n^{F}} \mathbf{I} \cdot \mathbf{D}_{S} - \frac{s^{L} n^{S}}{n^{F} \rho^{SR}} \frac{\partial \rho^{SR}}{\partial \theta} \theta'_{S} + \frac{s^{L}}{n^{F}} \operatorname{grad} n^{S} \cdot \mathbf{w}_{L} +$$

$$+ \frac{s^{L} \hat{\rho}^{I}}{n^{F} \rho^{IR}} - \frac{s^{L} n^{I}}{n^{F}} \mathbf{I} \cdot \mathbf{D}_{S} - \frac{s^{L} n^{I}}{n^{F} \rho^{IR}} \frac{\partial \rho^{IR}}{\partial \theta} \theta'_{S} + \frac{s^{L}}{n^{F}} \operatorname{grad} n^{I} \cdot \mathbf{w}_{L}.$$

$$(4.33)$$

This, in turn, is included into the entropy inequality to state its final form, from which the restrictions for the response functions (4.25) can be concluded, viz.:

$$\begin{split} \underbrace{(\mathbf{T}_{E}^{S}+n^{S}(s^{L})^{2}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\mathbf{I}}_{\mathbf{T}_{E}^{S}\operatorname{mech}} &= -\rho^{S}(\underline{\eta}_{E}^{S}-(s^{L})^{2}\frac{\rho^{LR}}{(\rho^{SR})^{2}}\frac{\partial\psi^{L}}{\partial s^{L}}\frac{\partial\rho^{SR}}{\partial \theta} + \frac{\partial\psi^{S}}{\partial \theta})\theta_{S}^{\prime} + \\ &+ \underbrace{(\mathbf{T}_{E}^{I}+n^{I}(s^{L})^{2}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\mathbf{I} + n^{I}\rho^{I}\frac{\partial\psi^{I}}{\partial n^{I}}\mathbf{I}}_{\eta_{E}^{E}\operatorname{mech}} - 2\rho^{I}\mathbf{F}_{I}\frac{\partial\psi^{I}}{\partial \mathbf{C}_{I}}\mathbf{F}_{I}^{T})\cdot\mathbf{D}_{S} - \\ &- \rho^{I}(\underline{\eta_{E}^{I}-(s^{L})^{2}\frac{\rho^{LR}}{(\rho^{IR})^{2}}\frac{\partial\psi^{L}}{\partial s^{L}}\frac{\partial\rho^{IR}}{\partial \theta} - \frac{n^{I}}{\rho^{IR}}\frac{\partial\psi^{I}}{\partial n^{I}}\frac{\partial\rho^{IR}}{\partial \theta}}{\partial \theta} + \frac{\partial\psi^{I}}{\partial \theta})\theta_{S}^{\prime} + \\ &+ \underbrace{(\mathbf{T}_{E}^{L}+n^{L}s^{L}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\mathbf{I})\cdot\mathbf{D}_{L}-\rho^{L}(\eta_{E}^{L}-s^{L}\frac{1}{\rho^{LR}}\frac{\partial\psi^{L}}{\partial s^{L}}\frac{\partial\rho^{LR}}{\partial \theta}}{\eta_{E}^{L}\operatorname{mech}} + \\ &+ \underbrace{(\mathbf{T}_{E}^{L}+n^{L}s^{L}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\mathbf{I})\cdot\mathbf{D}_{L}-\rho^{L}(\eta_{E}^{L}-s^{L}\frac{1}{\rho^{LR}}\frac{\partial\psi^{L}}{\partial s^{L}}\frac{\partial\rho^{LR}}{\partial \theta}} + \frac{\partial\psi^{L}}{\partial \theta})\theta_{L}^{\prime} + \\ &+ \underbrace{\mathbf{T}_{E}^{C}\cdot\mathbf{D}_{G}-\rho^{G}(\eta^{G}+\frac{\partial\psi^{G}}{\partial \theta})\theta_{G}^{\prime} + (\mathcal{P}\frac{n^{G}}{\rho^{GR}}-\rho^{G}\frac{\partial\psi^{G}}{\partial\rho^{GR}})(\rho^{GR})_{G}^{\prime} - \\ &- \underbrace{(\dot{\mathbf{p}}_{E}^{L}+(s^{L})^{2}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\operatorname{grad} n^{S}+(s^{L})^{2}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\operatorname{grad} n^{I}+\hat{\rho}^{S}\dot{\mathbf{x}}_{S}+\hat{\rho}^{I}\dot{\mathbf{x}}_{S})\cdot\mathbf{w}_{L} - \\ &- \underbrace{\dot{\mathbf{p}}_{E}^{C}\cdot\mathbf{w}_{G}-\frac{1}{\theta}(\mathbf{q}^{S}+\mathbf{q}^{I}+\mathbf{q}^{L}+\mathbf{q}^{G})\cdot\operatorname{grad} \theta - \\ &- \hat{\rho}^{S}(\psi^{S}+\frac{1}{2}\dot{\mathbf{x}}_{S}\cdot\dot{\mathbf{x}}_{S}-\psi^{L}-\frac{1}{2}\dot{\mathbf{x}}_{L}\cdot\dot{\mathbf{x}}_{L}+\mathcal{P}\frac{1}{\rho^{IR}}-\mathcal{P}\frac{1}{\rho^{LR}}+(s^{L})^{2}\frac{\rho^{LR}}{\rho^{SR}}\frac{\partial\psi^{L}}{\partial s^{L}}-s^{L}\frac{\partial\psi^{L}}{\partial s^{L}}) - \\ &- \hat{\rho}^{I}(\psi^{I}+\frac{1}{2}\dot{\mathbf{x}}_{S}\cdot\dot{\mathbf{x}}_{S}-\psi^{L}-\frac{1}{2}\dot{\mathbf{x}}_{L}\cdot\dot{\mathbf{x}}_{L}+\mathcal{P}\frac{1}{\rho^{IR}}-\mathcal{P}\frac{1}{\rho^{LR}}+(s^{L})^{2}\frac{\rho^{LR}}{\rho^{LR}}\frac{\partial\psi^{L}}{\partial s^{L}} - \\ &- s^{L}\frac{\partial\psi^{L}}{\partial s^{L}}+n^{I}\frac{\partial\psi^{I}}{\partial s^{L}} = 0. \end{split}$$

The first six lines of (4.34) are considered as equilibrium part of the entropy inequality. Therefore, the terms in front of the rates  $\mathbf{D}_S$ ,  $\mathbf{D}_L$ ,  $\mathbf{D}_G$ ,  $\theta'_S$ ,  $\theta'_L$ ,  $\theta'_G$  and  $(\rho^{GR})'_G$  have to be zero. Thus, the *Lagrange*an multiplier  $\mathcal{P}$  is determined via

$$\mathcal{P} = (\rho^{GR})^2 \frac{\partial \psi^G}{\partial \rho^{GR}} =: p^{GR}, \qquad (4.35)$$

and can be identified as the excess gas pressure. It is the standard form for compressible fluids, cf. Ehlers [49].

In general, the fluid stresses  $\mathbf{T}^{\beta}$  consist of equilibrium and non-equilibrium parts. However, for this investigation, only the equilibrium parts are considered, the frictional stresses in the fluids are neglected in comparison to the respective momentum productions by arguments of a dimensional analysis, cf. [56], such that

$$\mathbf{T}_E^G = \mathbf{0} \quad \text{and} \quad \mathbf{T}_{E\,\text{dis}}^L = \mathbf{0}. \tag{4.36}$$

The equilibrium fluid stresses read

$$\mathbf{T}^{G} = -n^{G} p^{GR} \mathbf{I},$$
  

$$\mathbf{T}^{L} = -n^{L} (p^{GR} + s^{L} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}}) \mathbf{I} =: -n^{L} p^{LR} \mathbf{I}.$$
(4.37)

Based on  $(4.37)_2$  and the definition of the gas pressure  $p^{GR}$ , the liquid pressure  $p^{LR}$  is given via

$$p^{LR} = p^{GR} + s^L \rho^{LR} \frac{\partial \psi^L}{\partial s^L}.$$
(4.38)

The evaluation of the stress of the solid skeleton is based on the first line of (4.34) yielding

$$\mathbf{T}_{E\,\mathrm{mech}}^{S} = \mathbf{T}_{E}^{S} + n^{S} (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} \mathbf{I}.$$
(4.39)

The partial stress  $\mathbf{T}^{S}$  is derived based on  $(4.23)_{1}$  and (4.39), and is given via

$$\mathbf{T}^{S} = -n^{S} [p^{GR} + (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}}] \mathbf{I} + \mathbf{T}^{S}_{E \,\mathrm{mech}} = -n^{S} p^{FR} \mathbf{I} + \mathbf{T}^{S}_{E \,\mathrm{mech}}, \qquad (4.40)$$

where

$$p^{FR} = p^{GR} + (s^L)^2 \rho^{LR} \frac{\partial \psi^L}{\partial s^L} =: s^L p^{LR} + s^G p^{GR},$$
  
$$\mathbf{T}^S_{E \,\mathrm{mech}} = 2\rho^S \mathbf{F}_S \frac{\partial \psi^S}{\partial \mathbf{C}_S} \mathbf{F}^T_S.$$
(4.41)

Note that (4.39) to (4.41) naturally recovers Dalton's law (4.41)<sub>1</sub>, compare Dalton [41]. Note, furthermore, that a vanishing pore pressure, i. e.  $p^{FR} = 0$ , does not necessarily indicate limp tissue cells, as only the excess pore pressure vanishes, the real pressure equals the ambient pressure. A hyperelastic material law, based on the introduction of the energy potential  $\psi^S$ , defines the stress  $\mathbf{T}^S_{E\,\mathrm{mech}}$  in (4.41)<sub>2</sub>, as discussed in **Subsection 4.4.1**.

Furthermore, the evaluation of the third line of (4.34) yields constraints for the ice via

$$\mathbf{T}_{E\,\mathrm{mech}}^{I} = \mathbf{T}_{E}^{I} + n^{I} (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} \mathbf{I} + n^{I} \rho^{I} \frac{\partial \psi^{I}}{\partial n^{I}} \mathbf{I}.$$
(4.42)

Thus, the partial stress of the ice reads

$$\mathbf{T}^{I} = -n^{I} [p^{GR} + (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} + \rho^{I} \frac{\partial \psi^{I}}{\partial n^{I}}] \mathbf{I} + \mathbf{T}^{I}_{E \,\mathrm{mech}} = -n^{I} [p^{FR} + \rho^{I} \frac{\partial \psi^{I}}{\partial n^{I}}] \mathbf{I} + \mathbf{T}^{I}_{E \,\mathrm{mech}},$$

$$(4.43)$$
where

$$p^{IR} := p^{FR} + \rho^{I} \frac{\partial \psi^{I}}{\partial n^{I}}$$

$$\mathbf{T}^{I}_{E \,\mathrm{mech}} = 2 \,\rho^{I} \, \mathbf{F}_{I} \frac{\partial \psi^{I}}{\partial \mathbf{C}_{I}} \mathbf{F}^{T}_{I}.$$
(4.44)

Therein, the ice pressure  $p^{IR}$  has an additional component in excess to the pore pressure  $p^{FR}$ , which is in accordance to the general understanding of freezing processes in porous media, cf. e. g. Bluhm *et al.* [16, 18] and Coussy [39]. The stress  $\mathbf{T}^{I}_{E\,\mathrm{mech}}$  is determined by a hyperelastic material law, as discussed in **Subsection 4.4.2**.

The entropy of the solid skeleton is derived from the second line of (4.34) yielding

$$\eta_{E\,\mathrm{mech}}^{S} = \eta_{E}^{S} - (s^{L})^{2} \frac{\rho^{LR}}{(\rho^{SR})^{2}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{SR}}{\partial \theta} =$$

$$= \eta^{S} - \frac{p^{GR}}{(\rho^{SR})^{2}} \frac{\partial \rho^{SR}}{\partial \theta} - (s^{L})^{2} \frac{\rho^{LR}}{(\rho^{SR})^{2}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{SR}}{\partial \theta} =$$

$$= \eta^{S} - \frac{p^{FR}}{(\rho^{SR})^{2}} \frac{\partial \rho^{SR}}{\partial \theta} =$$

$$= -\frac{\partial \psi^{S}}{\partial \theta}.$$
(4.45)

The entropy of the ice is given via the fourth line of (4.34), viz.:

$$\eta_{E \,\mathrm{mech}}^{I} = \eta_{E}^{I} - (s^{L})^{2} \frac{\rho^{LR}}{(\rho^{IR})^{2}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{IR}}{\partial \theta} - \frac{n^{I}}{\rho^{IR}} \frac{\partial \psi^{I}}{\partial n^{I}} \frac{\partial \rho^{IR}}{\partial \theta} =$$

$$= \eta^{I} - \frac{p^{GR}}{(\rho^{IR})^{2}} \frac{\partial \rho^{IR}}{\partial \theta} - (s^{L})^{2} \frac{\rho^{LR}}{(\rho^{IR})^{2}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{IR}}{\partial \theta} - \frac{n^{I}}{\rho^{IR}} \frac{\partial \psi^{I}}{\partial n^{I}} \frac{\partial \rho^{IR}}{\partial \theta} =$$

$$= \eta^{I} - \frac{p^{IR}}{(\rho^{IR})^{2}} \frac{\partial \rho^{IR}}{\partial \theta} =$$

$$= -\frac{\partial \psi^{I}}{\partial \theta}.$$
(4.46)

The entropy of the liquid is given by the fifth line of (4.34), such that

$$\eta_{E \,\mathrm{mech}}^{L} = \eta_{E}^{L} - s^{L} \frac{1}{\rho^{LR}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{LR}}{\partial \theta} =$$

$$= \eta^{L} - \frac{p^{GR}}{(\rho^{LR})^{2}} \frac{\partial \rho^{LR}}{\partial \theta} - s^{L} \frac{1}{\rho^{LR}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{LR}}{\partial \theta} =$$

$$= \eta^{L} - \frac{p^{LR}}{(\rho^{LR})^{2}} \frac{\partial \rho^{LR}}{\partial \theta} =$$

$$= -\frac{\partial \psi^{L}}{\partial \theta}.$$
(4.47)

Finally, the entropy of the gas is given in the sixth line of (4.34) and has the standard form for compressible fluids, viz.:

$$\eta^G = -\frac{\partial \psi^G}{\partial \theta}.\tag{4.48}$$

Moreover, the dissipative production of momentum of the liquid reads

$$\hat{\mathbf{p}}_{E\,\text{dis}}^{L} = \hat{\mathbf{p}}_{E}^{L} + (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} \left( \operatorname{grad} n^{S} + \operatorname{grad} n^{I} \right) + \hat{\rho}^{S} \, \overset{\prime}{\mathbf{x}}_{S} + \hat{\rho}^{I} \, \overset{\prime}{\mathbf{x}}_{S} = \\ = \hat{\mathbf{p}}^{L} - p^{GR} \operatorname{grad} n^{L} + (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} \left( \operatorname{grad} n^{S} + \operatorname{grad} n^{I} \right) + \hat{\rho}^{S} \, \overset{\prime}{\mathbf{x}}_{S} + \hat{\rho}^{I} \, \overset{\prime}{\mathbf{x}}_{S} \,.$$

$$\tag{4.49}$$

Thus, the non-equilibrium part of the entropy inequality (4.34) leads to internal dissipation, which is given via

$$\mathcal{D} = -\hat{\mathbf{p}}_{E\,\text{dis}}^{L} \cdot \mathbf{w}_{L} - \hat{\mathbf{p}}_{E}^{G} \cdot \mathbf{w}_{G} - \frac{1}{\theta} (\mathbf{q}^{S} + \mathbf{q}^{I} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \text{grad} \theta - - \hat{\rho}^{S} (\psi^{S} + \frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{p^{FR}}{\rho^{SR}} - \frac{p^{LR}}{\rho^{LR}}) - - \hat{\rho}^{I} (\psi^{I} + \frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{p^{IR}}{\rho^{IR}} - \frac{p^{LR}}{\rho^{LR}}) \geq 0.$$

$$(4.50)$$

In order to fulfil the dissipation inequality (4.50), the following proportionalities must hold

$$\hat{\mathbf{p}}_{E\,\mathrm{dis}}^{L} \propto -\mathbf{w}_{L}, \quad \hat{\mathbf{p}}_{E}^{G} \propto -\mathbf{w}_{G}, \quad \mathbf{q}^{\alpha} \propto -\mathrm{grad}\,\theta.$$
 (4.51)

Similarly, for the mass interactions the following proportionalities must hold for the (potentially) non-equilibrium processes at hand, viz.:

$$\hat{\rho}^{S} \propto -(\psi^{S} + \frac{1}{2} \, \mathbf{\dot{x}}_{S} \cdot \mathbf{\dot{x}}_{S} - \psi^{L} - \frac{1}{2} \, \mathbf{\dot{x}}_{L} \cdot \mathbf{\dot{x}}_{L} + \frac{p^{FR}}{\rho^{SR}} - \frac{p^{LR}}{\rho^{LR}}), 
\hat{\rho}^{I} \propto -(\psi^{I} + \frac{1}{2} \, \mathbf{\dot{x}}_{S} \cdot \mathbf{\dot{x}}_{S} - \psi^{L} - \frac{1}{2} \, \mathbf{\dot{x}}_{L} \cdot \mathbf{\dot{x}}_{L} + \frac{p^{IR}}{\rho^{IR}} - \frac{p^{LR}}{\rho^{LR}}).$$
(4.52)

### 4.4 The solid constituents

This section is dedicated to the introduction of the material laws for the solid constituents, which are the solid skeleton and the water in a solid state of aggregation. These constituents exhibit very different characteristics, but they have also a few properties in common, as for example the framework of hyperelasticity, compare  $(4.41)_2$  and  $(4.44)_2$ . Furthermore, porous media are generally described as a compressible material, even with materially incompressible solid constituents, as volumetric deformation is possible due to related changes in the involved volume fractions. These changes, originating from mechanical deformation or mass interactions, as indicated by (4.18), may lead to a vanishing of the pore space. This behaviour is described as point of compaction (compression of the porous aggregate until the pore space is closed), that needs to be considered in the respective material descriptions, compare Bluhm [15], Ehlers & Eipper [55], Eipper [63]. These and other solid-specific effects are addressed within this section.

Note that the constraints and considerations regarding the compaction point are discussed in detail for the solid skeleton. However, for the ice, the results are stated solely in order to avoid too much repetition.

### 4.4.1 Solid skeleton

#### **Basic considerations**

As introduced in **Chapter 2**, the solid skeleton of plant tissues is a highly complex material, which has to be considered as some sort of composite material. For the plants under consideration, the solid skeleton is comprised of lignified elements. Furthermore, there are also tissue cells, which generally also contribute to the load bearing capacity of the plant. These tissue cells contain a considerable amount of enclosed water, which causes a turgor pressure within the cells as a function of the water content of the cells. However, their contribution to the overall stiffness is considered as low in comparison, cf. [76, 156]. For the numerical simulations presented in **Chapter 6**, the mechanical properties are assumed to be constant, thermal dependencies as well as the dependency on moisture, i. e. the water content of the solid skeleton, are not taken into consideration, since there is to the best of the author's knowledge no comprehensive study regarding their influence on the mechanical properties in a freezing environment.

### Specific properties

**Elasticity:** The solid skeleton of plant tissues is assumed to behave as thermo-elastic solid material. Time effects, that have been reported by Speck *et al.* [174] for *Equisetum hyemale*, are assumed to be caused by the interaction of the solid skeleton with the pore fluids and not by an inherent material property of the solid skeleton itself. In fact, viscous parts are usually ignored in application to plant tissues, compare, for example McCoy [125], Ross [156].

**Compressibility:** Within this thesis, the notions regarding compressibility of the porous aggregate and the compaction point in application to plant tissues are based on Eurich *et al.* [72]. Therein, the importance of the development of an appropriate constitutive material description of the solid skeleton is emphasised in order to account for the property of material incompressibility  $(4.4)_1$  of the consituents. Note that volumetric deformation is generally possible when the porosity changes, which indicates according to  $(3.26)_2$  in terms of the solid *Jacobian*  $J_S = \det \mathbf{F}_S \neq 1$ . Thus, according to Ehlers & Eipper [55] and Bluhm [15], a compressible material law has to be considered for porous materials as long as the pore space can be compressed. However, the pore space may vanish, i. e.  $n^F = 0$ , as a consequence of ice formation. This indicates an incompressible characteristic and is described by the compaction point. It implies, moreover, that the volumetric deformation

mation of the solid skeleton, measured as differing values from unity in  $J_S$ , is constrained by a limiting value  $\tilde{J}_S$  accounting for the actual available pore space and thereby for the compaction point via

$$0 < J_S < J_S < \infty. \tag{4.53}$$

**Double porosity:** Tissue cells contain water and facilitate their dehydration via micro pores in the cell wall, which makes the solid skeleton itself a multicomponent material due to the enclosed water. Moreover, plants have to be considered as a material with a multiscale porosity feature, in particular, as a material with double porosity, compare Eurich *et al.* [67]. The double-porosity models, that have been introduced by Borja & Koliji [27], Choo & Borja [36], Choo *et al.* [37] or within the framework of a thermo-hydromechanical modelling by Khalili & Selvadurai [103], are characterised by individual fluid constituents at both porosity scales and, consequently, individual states of motion at these scales. In contrast, in the present context, such a sophisticated model with independent states of motion at two porosity scales is not necessary, since the water is either confined to the solid skeleton as cell water or it is mobile within the macro-pore space. Thus, a customised quasi double-porosity model is introduced, where the flow of water within the micro pores of the cell wall is considered by a homogenised mass-interaction term. Note, this double-porosity effect is reflected in the formulation of the stress of the solid skeleton, compare (4.72) and (4.77).

Anisotropy: Moreover, plant tissues are generally anisotropic. This anisotropic behaviour is mainly due to the lignified elements of the tissue, specifically by the xylem. Usually, one preferred direction is considered, which is the longitudinal direction of the branch, twig or petiole. For wood, there is additionally a distinction between lateral and radial stiffness, however, the difference between the lateral and the radial stiffness is mostly low in comparison to the longitudinal stiffness, compare Ross [156]. In case one preferred direction is considered, the material is transversely isotropic. In contrast to many other living tissues, plant tissues are not necessarily considered as soft tissue with a typical J-shape in the stress-strain diagram, where initial deformation is associated with small stresses but further deformation with rapidly increasing stresses, compare Fung [78], Holzapfel [96]. Many plant tissues are rather considered as biological hard tissue, which is mainly due to the lignified elements. In the particular case of the plant tissues under investigation, the stiffness has a rather low dependence on the deformation, compare Niklas [138], Speck *et al.* [174], Zajaczkowska *et al.* [193]. This basic observation will be utilised for the introduction of the anisotropic part of the related energy and stress.

#### Hyperelastic material law

Additive split: Based on the fundamental considerations regarding the solid skeleton so far, the *Helmholtz* free energy  $\psi^S$ , or similarly the strain energy  $W^S$ , is chosen according to the required properties like finite deformations, thermoelasticity, the compaction point for the case of a closed or frozen pore space, mass interaction describing the double porosity and anisotropy. In order to account for all the mentioned effects, a customised strain energy needs to be proposed.

Within solid mechanics, instead of the *Helmholtz* free energy  $\psi^S$ , the strain energy  $W^S$  per reference volume element is utilised, which is defined via

$$W^{S}(\theta, \mathbf{C}_{S}, \mathcal{M}^{S}) = \rho_{0S}^{S} \psi^{S}(\theta, \mathbf{C}_{S}, \mathcal{M}^{S}).$$
(4.54)

However, rather than the in (4.54) introduced dependencies, an invariant representation is utilised, which a priori satisfies the basic thermodynamical principles, such as frame indifference as well as the isotropy requirements. Further explanations regarding these principles are omitted in this context. The interested reader is referred to Ehlers *et al.* [59], Ehlers & Wagner [61], Ehret & Itskov [62], Schröder & Neff [168], which traces mainly back to Spencer [175] in this context.

In order to define these invariants, the structural tensor  $\mathcal{M}^S$  needs to be specified, which is based on the works of Karajan [102], Wagner [187]. For transversely isotropic materials,  $\mathcal{M}_a^S$  is defined by the dyadic product of the unit vector  $\mathbf{a}_0^S$  of the preferred direction, accounting for the fibre orientation in the reference configuration, such that

$$\mathcal{M}_a^S = \mathbf{a}_0^S \otimes \mathbf{a}_0^S, \tag{4.55}$$

where the following properties apply, viz.:

$$\mathcal{M}_{a}^{S} = (\mathcal{M}_{a}^{S})^{T}, \quad \mathcal{M}_{a}^{S} = \mathcal{M}_{a}^{S}\mathcal{M}_{a}^{S}, \quad \operatorname{tr} \mathcal{M}_{a}^{S} = 1.$$
 (4.56)

For the case of isotropy, the set of three principal invariants  $I_{S1}$ ,  $I_{S2}$ ,  $I_{S3}$  of  $\mathbf{C}_S$  (or equally for  $\mathbf{B}_S$ ) suffices to describe the deformation, these are given via

$$I_{S1} = \operatorname{tr} \mathbf{C}_S, \quad I_{S2} = \operatorname{tr} (\operatorname{cof} \mathbf{C}_S), \quad I_{S3} = \det \mathbf{C}_S, \tag{4.57}$$

compare Ehlers [50]. The Jacobian  $J_S$  relates via  $J_S = \det \mathbf{F}_S = (\det \mathbf{C}_S)^{\frac{1}{2}} = \sqrt{I_{S3}}$ . This leads to the introduction of the isotropic part of the strain-energy function via

$$W_{\rm iso}^S(\theta, \mathbf{C}_S) \longrightarrow W_{\rm iso}^S(\theta, I_{S1}, I_{S2}, J_S).$$
 (4.58)

In case of an transversely isotropic behaviour, the set of invariants (4.57) is accompanied by mixed invariants

$$J_{S4} = \operatorname{tr} \left( \mathcal{M}_a^S \mathbf{C}_S \right) = \mathbf{a}_0^S \cdot \mathbf{C}_S \, \mathbf{a}_0^S = \mathbf{F}_S \, \mathbf{a}_0^S \cdot \mathbf{F}_S \, \mathbf{a}_0^S = \mathbf{a}^S \cdot \mathbf{a}^S,$$
  

$$J_{S5} = \operatorname{tr} \left( \mathcal{M}_a^S \mathbf{C}_S^2 \right) = \mathbf{a}_0^S \cdot \mathbf{C}_S^2 \, \mathbf{a}_0^S = \mathbf{C}_S \, \mathbf{a}_0^S \cdot \mathbf{C}_S \, \mathbf{a}_0^S = \mathbf{F}_S^T \, \mathbf{a}^S \cdot \mathbf{F}_S^T \, \mathbf{a}^S.$$
(4.59)

Therein,  $J_{S4}$  represents the squared fibre stretch in direction  $\mathbf{a}^{S} = \mathbf{F}_{S} \mathbf{a}_{0}^{S}$ , which is the mapping of  $\mathbf{a}_{0}^{S}$  to the current configuration. There is according to Wagner [187] no direct physical interpretation for  $J_{S5}$ , yet, it enables the possibility to include the effect of matrix-fibre interaction.

Thus, the anisotropic part of the strain-energy function is in its generic form given via

$$W^{S}_{\text{aniso}}(\theta, \mathbf{C}_{S}, \mathcal{M}^{S}) \longrightarrow W^{S}_{\text{aniso}}(\theta, J_{S4}, J_{S5}).$$
 (4.60)

Note that it is common practice, compare [59, 61, 62, 168], to introduce an additive split of the strain energy  $W^S$  into an isotropic part and an anisotropic part as done within this monograph, viz.:

$$W^S = W^S_{\rm iso} + W^S_{\rm aniso}.$$
(4.61)

With the introduction of an additive split of the strain-energy function, an additive split for the stresses is implied. Thus, the total mechanical extra stress  $\mathbf{T}_{E\,\mathrm{mech}}^{S}$  is decomposed into an isotropic part  $\mathbf{T}_{\mathrm{iso}}^{S}$  and an anisotropic part  $\mathbf{T}_{\mathrm{aniso}}^{S}$  via

$$\mathbf{T}_{E\,\mathrm{mech}}^{S} = \mathbf{T}_{\mathrm{iso}}^{S} + \mathbf{T}_{\mathrm{aniso}}^{S},\tag{4.62}$$

where the respective parts are with  $(4.41)_2$  and (4.54) given by

$$\mathbf{T}_{iso}^{S} = 2 \frac{\rho^{S}}{\rho_{0S}^{S}} \mathbf{F}_{S} \frac{\partial W_{iso}^{S}}{\partial \mathbf{C}_{S}} \mathbf{F}_{S}^{T}, \quad \mathbf{T}_{aniso}^{S} = 2 \frac{\rho^{S}}{\rho_{0S}^{S}} \mathbf{F}_{S} \frac{\partial W_{aniso}^{S}}{\partial \mathbf{C}_{S}} \mathbf{F}_{S}^{T}.$$
(4.63)

**Isotropic contribution:** The isotropic part  $W_{iso}^S$  of the strain-energy function  $W^S$  is based on the work of Simo & Pister [171]. Their material model has been proposed for a single-component compressible material under isothermal conditions in the form

$$W_{\rm iso}^S(I_{S1}, J_S) = U^S(J_S) - \mu^S \ln J_S + \frac{\mu^S}{2}(I_{S1} - 3), \qquad (4.64)$$

where  $\mu^S$  is the second *Lamé* constant. For the specification of  $U^S(J_S)$ , several approaches have been proposed, depending on the application the authors had in mind. The most important ones are reviewed in Hartmann & Neff [92]. For the present case, the volumetric extension  $U^S(J_S)$  is introduced in Eurich *et al.* [72] including the considered test cases. They are conceptually based on Ehlers & Eipper [55], who described the compaction point under isothermal conditions and on Bluhm [15], who accounted also for thermal effects. In the latter work, the general form for  $W^S_{iso}$  is given via

$$W_{\rm iso}^{S}(\theta, I_{S1}, J_{S}) = U^{S}(J_{S}) - \mu^{S} \ln J_{S} + \frac{\mu^{S}}{2}(I_{S1} - 3) - 3\alpha^{S}k^{S} \ln J_{S}(\theta - \theta_{0S}^{S}) - \rho_{0S}^{S}c_{v}^{S}(\theta \ln \frac{\theta}{\theta_{0S}^{S}} - \theta + \theta_{0S}^{S}),$$

$$(4.65)$$

where  $k^S$  is the bulk modulus and  $c_v^S$  the specific heat capacity at constant volume. Note in passing that the stress-temperature modulus  $m_{\theta}^S = -3 \alpha^S k^S$  is frequently introduced, cf. [58].

The extension term  $U^{S}(J_{S})$  to the strain-energy function accounts for volumetric deformation and specifically also for the compaction point. Thus, according to the work of Ehlers & Eipper [55], a set of constraints and conditions has to be fulfilled. Note, that the first derivative with respect to  $J_{S}$  has to be considered, when there is a condition regarding the *Cauchy* stress.

• Undeformed configuration: It is required that the strain energy as well as the hydrostatic *Cauchy* stress vanish in the undeformed configuration, i. e.  $J_S = 1$ , viz.:

$$U^{S}(J_{S}=1) = 0$$
 and  $\frac{\partial U^{S}}{\partial J_{S}}(J_{S}=1) = 0.$  (4.66)

• Compaction point: When the volumetric deformation reaches the limiting deformation value, i. e.  $J_S \to \tilde{J}_S$ , the energy and the hydrostatic compressive stress have to be infinite

$$U^{S}(J_{S} \to \tilde{J}_{S}) \to +\infty \quad \text{and} \quad \frac{\partial U^{S}}{\partial J_{S}}(J_{S} \to \tilde{J}_{S}) \to -\infty.$$
 (4.67)

Specification (4.67) replaces the condition for non-porous, single-component and compressible materials, where the singularity is reached for infinite compression, i. e.  $J \rightarrow 0$ . Here, the transition from a compressible to an incompressible material behaviour replaces this singularity. Note that the limiting value  $\tilde{J}_S$  of volumetric deformation may change with time.

• Growth condition: When the local deformation approaches positive infinity, the energy and the (tensile) stress have to be infinite as well, viz.:

$$U^{S}(J_{S} \to +\infty) \to +\infty \text{ and } \frac{\partial U^{S}}{\partial J_{S}}(J_{S} \to +\infty) \to +\infty.$$
 (4.68)

This can be understood as the case when the local porosity reaches unity.

• Convexity condition: A detailed discussion regarding convexity is omitted in this context, more information is for example given in Markert [121]. For this purpose, it states, under the premise that the volumetric extension  $U^S$  is twice differentiable, that the second derivative with respect to  $J_S$  has to be positive semi-definite

$$\frac{\partial^2 U^S}{\partial J_S^2} \ge 0, \quad \forall J_S > \tilde{J}_S > 0. \tag{4.69}$$

• Compatibility assumption: As a linearisation of the proposed energy function is supposed to yield *Hooke*'s law, it can be shown that the first *Lamé* constant  $\Lambda^S$ is determined via

$$\Lambda^S := \frac{\partial^2 U^S}{\partial J_S^2} (J_S = 1). \tag{4.70}$$

The consideration of these conditions leads to a new strain-energy formulation, that meets the requirements of the current case and is given via

$$U^{S}(J_{S}) = \frac{\Lambda^{S}}{\gamma_{0}^{S}(\gamma_{0}^{S}-1) + \frac{2}{(\tilde{J}_{S}-1)^{2}}} [J_{S}^{\gamma_{0}^{S}} - (\gamma_{0}^{S} + \frac{2}{\tilde{J}_{S}-1})J_{S} + \gamma_{0}^{S} + \frac{2}{\tilde{J}_{S}-1} - 1 + \ln\left(\frac{(\tilde{J}_{S}-1)^{2}}{(\tilde{J}_{S}-J_{S})^{2}}\right)].$$

$$(4.71)$$

Therein,  $\gamma_0^S \ge 1$  describes the volumetric behaviour, compare Ogden [141].

With the establishment of this volumetric extension to the strain-energy function, the isotropic part of the *Cauchy* stress is given via

$$\mathbf{T}_{iso}^{S} = \frac{\rho^{S}}{\rho_{0S}^{S}} \left[ 2\mu^{S} \mathbf{K}_{S} - 3\,\alpha^{S} k^{S} (\theta - \theta_{0S}^{S}) \,\mathbf{I} + \frac{\Lambda^{S}}{\gamma_{0}^{S} (\gamma_{0}^{S} - 1) + \frac{2}{(\tilde{J}_{S} - 1)^{2}}} (\gamma_{0}^{S} J_{S}^{\gamma_{0}^{S}} - \gamma_{0}^{S} J_{S} - \frac{2J_{S}}{\tilde{J}_{S} - 1} + \frac{2J_{S}}{\tilde{J}_{S} - J_{S}}) \,\mathbf{I} \right].$$

$$(4.72)$$

In order to assess the introduced strain energy  $U^{S}(J_{S})$  in terms of the compaction point, the emerging stresses are compared for the case with and the case witout compaction point. Due to  $(4.63)_{1}$  and (4.65) it is sufficient to examine the derivative of  $U^{S}(J_{S})$ , which is given via

$$\frac{\partial U^S}{\partial J_S} = \frac{\Lambda^S}{\gamma_0^S(\gamma_0^S - 1) + \frac{2}{(\tilde{J}_S - 1)^2}} (\gamma_0^S J_S^{\gamma_0^S - 1} - \gamma_0^S - \frac{2}{\tilde{J}_S - 1} + \frac{2}{\tilde{J}_S - J_S}).$$
(4.73)

For the mentioned comparison,  $\gamma_0^S = 2$  was chosen. For the case without compaction point, i. e.  $\tilde{J}_S = 0$ , the material law according to Simo & Taylor [172] is revealed describing compressible solid constituents under isothermal conditions, as shown in Hartmann [90]. This compressible material law is compared to a case with compaction point, where as the limiting value  $\tilde{J}_S = 0.5$  was chosen. Figure 4.1 illustrates the compaction point indicating that the deformation state under compression is penalised when getting too close to the limiting volumetric deformation  $\tilde{J}_S = 0.5$ . The compressible material can be compressed until the *Jacobian* approaches zero.



Figure 4.1: Characterisation of an incompressible, porous material with compaction point (black line), bounded by the limiting deformation  $\tilde{J}_S = 0.5$ , displayed in red, and a non-porous, compressible material (dotted, black line), shown in a qualitative stress-deformation sketch.

As the next step, the introduced volumetric-extension term is investigated by a virtual

tension-compression test leading to an uniaxial state of stress, which is non-zero in  $\mathbf{e}_1$ -direction. Thus, the corresponding deformation gradient is given via

$$\mathbf{F}_{S} = \begin{bmatrix} \lambda & 0 & 0\\ 0 & \lambda_{L} & 0\\ 0 & 0 & \lambda_{L} \end{bmatrix} \mathbf{e}_{i} \otimes \mathbf{e}_{j}, \quad \text{with} \quad J_{S} = \lambda \lambda_{L}^{2}, \tag{4.74}$$

where  $\lambda$  is the prescribed axial stretch and  $\lambda_L$  the unknown lateral stretch. When isothermal conditions are assumed, the axial stress is non-zero, but the normal stress in  $\mathbf{e}_2$ - or  $\mathbf{e}_3$ -direction originating from (4.72) vanishes

$$0 = \frac{\nu^{S}(\tilde{J}_{S}-1)^{2}}{(1-2\nu^{S})(\tilde{J}_{S}^{2}-2\tilde{J}_{S}+2)} \left[ 2\lambda\lambda_{L}^{2} - \frac{2\tilde{J}_{S}}{\tilde{J}_{S}-1} + \frac{2}{\tilde{J}_{S}-(\lambda\lambda_{L}^{2})} \right] + \frac{1}{\lambda} \left( 1 - \frac{1}{\lambda_{L}^{2}} \right), \quad (4.75)$$

resulting in an implicit equation in  $\lambda_L$ . In (4.75), the Lamé constants have been replaced by Young's modulus  $E^S$ , which drops out, and the Poisson ratio  $\nu^S$ , where relations  $\Lambda^S = E^S \nu^S / [(1 + \nu^S)(1 - 2\nu^S)]$  and  $\mu^S = E^S / [2(1 + \nu^S)]$  are utilised for a qualitative comparison. For the numerical case study, a Poisson ratio of  $\nu^S = 0.25$  was chosen, which is within the range that usually applies to plant tissues. For a given prescribed stretch  $\lambda$ , the corresponding lateral stretch  $\lambda_L$  according to (4.75) is displayed in Figure 4.2(a). It shows a rapid increase in lateral stretch  $\lambda_L$  in the compression range ( $\lambda < 1.0$ ).



Figure 4.2: Virtual tension-compression test: (a) Lateral stretch  $\lambda_L$  - axial stretch  $\lambda$  for the introduced test case of uniaxial tension-compression. Note the striking increase in lateral stretch in the compression range ( $\lambda < 1.0$ ). (b) Volumetric deformation  $J_S$  as a function of the applied stretch  $\lambda$ . Note in passing that the axis of abscissa is scaled logarithmically, where the limiting volumetric deformation  $\tilde{J}_S$ , i. e. the compaction point, is indicated in red on the ordinate axis.

Furthermore, the solid Jacobian  $J_S$ , which is given according to  $(4.74)_2$ , is shown in Figure 4.2(b) as a function of the prescribed stretch  $\lambda$ . Note that the volumetric deformation is in the compression range ( $\lambda < 1.0$ ) bounded by the limiting value  $\tilde{J}_S$ , which has been chosen as  $\tilde{J}_S = 0.5$ . Note in passing that stability issues have not been considered for this test case.

Anisotropic contribution: In order to account for the influence of the lignified elements, an anisotropic part  $W^S_{aniso}$  of the solid strain energy has to be introduced, as emphasised in Eurich *et al.* [67]. The approach that is utilised in the current setting has been developed for transversely isotropic materials by Ricken & Bluhm [148], Ricken *et al.* [151], viz.:

$$W_{\text{aniso}}^{S} = \frac{1}{2} \alpha_{S1} \left( J_{S4} - 1 \right)^{\alpha_{S2}}, \qquad (4.76)$$

with the material parameters  $\alpha_{S1}$  accounting for the stiffness in preferred direction and the exponent  $\alpha_{S2}$ . This anisotropic part of the strain-energy function may account for hard tissues, like wood, and soft tissues, like leaves, as well, as it accounts for extension  $(J_{S4} > 1)$  and shrinking  $(J_{S4} < 1)$ . In the present case, the stiffness in the direction of anisotropy is assumed to be deformation-independent, therefore,  $\alpha_{S2} = 2$  needs to be chosen, since the material tangent, which is built by the second derivative with respect to  $J_{S4}$ , is constant in that particular case.

This leads to the anisotropic part of the *Cauchy* stress, which is according to  $(4.63)_2$  given via

$$\mathbf{T}_{\text{aniso}}^{S} = \frac{\rho^{S}}{\rho_{0S}^{S}} \alpha_{S1} \alpha_{S2} \left( J_{S4} - 1 \right)^{\alpha_{S2} - 1} \left( \mathbf{a}^{S} \otimes \mathbf{a}^{S} \right).$$
(4.77)

Thus, it is easily seen that the dehydration of the tissue cells is naturally included in (4.72) and (4.77) by  $\hat{\rho}^{S}$  in (4.14). Note that Ricken *et al.* [150] utilise a similar approach in dealing with porous materials with a growing (or shrinking) solid skeleton.

### 4.4.2 Solid ice

#### **Basic considerations**

There are approaches, particularly in the field of glaciology, where the ice is treated as a non-Newtonian, viscous and incompressible fluid, compare Hutter [98, 99], Morland [130]. For the classification of various types of non-Newtonian fluids, the interested reader is referred to Chhabra [35]. In the work of Hutter [98, 99], distinction is made between cold glaciers with a temperature far below the melting point, where a singlephasic fluid model is assumed, and temperate glaciers with a temperature close to the melting point, where a binary mixture of the ice with percolating or trapped water is considered. These works focus mainly on the gravitation-driven motion or flow of glaciers, which is in the order of magnitude of hundreds of meters per year. This indicates that the relevant time scale is rather in terms of years than in seconds [98]. Consequently, this modelling approach is utilised that is based on the works of Bluhm et al. [16, 18], Liu & Mollo-Christensen [117], Ricken & Bluhm [147], Zheng et al. [195], Zhou & Meschke [196], where the ice is treated as a hyperelastic solid material. In these works, the ice is assumed to be an elastic and isotropic solid.

### Specific properties

In addition to the mentioned property of elasticity, a similar concept as for the solid skeleton in terms of compressibility needs to be developed. Since the volume element is transported by the *Jacobian*  $J_I = \det \mathbf{F}_I = \det (\mathbf{F}_S \mathbf{F}_{S0}^{-1}) = \det \mathbf{F}_S \det \mathbf{F}_{S0}^{-1}$ , which generally differs from 1, a compressible material law has to be considered for the ice as well. However, there is also a limiting volumetric deformation  $\tilde{J}_I$  with regard to the ice, when there is no further shrinking possible, in case the pore space is closed or rather frozen in the given context. In that particular case the behaviour changes from compressible to incompressible. Thus, a very similar volumetric extension to the strain energy  $W^I$  of the ice, compare (4.78), is introduced as done also for the solid skeleton. Finally, the ice strain energy has a part, which is due to the pressure (4.44)<sub>1</sub>, that is in excess to the pore pressure  $p^{FR}$  and formally introduced as the part of the strain energy that is a function of the ice volume fraction, as introduced in the following paragraph.

#### Hyperelastic material law

Additive split: Also for the ice as a solid material, the required properties are considered in terms of the *Helmholtz* free energy  $\psi^I$ , or the strain energy  $W^I$ . These properties are finite deformations, thermoelasticity, the compaction point for the case of a closed pore space, mass interaction describing the formation of ice and the enthalpy of fusion (or similarly the entropy of fusion) that is related to the phase transition. Thus, a customised strain-energy function needs to be proposed to account for all these effects.

Since the ice is also treated as a solid material, the strain-energy function  $W^{I}$  is formally introduced. In contrast to the solid skeleton, it is related via the effective density in the reference configuration of the ice to the *Helmholtz* free energy  $\psi^{I}$ , viz.:

$$W^{I}(\theta, n^{I}, \mathbf{C}_{I}) = \rho_{0I}^{IR} \psi^{I}(\theta, n^{I}, \mathbf{C}_{I}).$$

$$(4.78)$$

The relation of the energies via the effective density  $\rho_{0I}^{IR}$  makes sense insofar, as the material parameters of the ice are usually effective quantities, as the ice is rather tested as a bulk solid material instead of a porous material.

Also for the ice, the strain-energy function does not depend on the right *Cauchy-Green* deformation tensor  $\mathbf{C}_I$ , but rather on its invariants, which suffices and is necessary due to the introduced concepts of objectivity and isotropy. The set of the three principal invariants  $I_{I1}, I_{I2}, I_{I3}$  of  $\mathbf{C}_I$  (or equally for  $\mathbf{B}_I$ ) is given via

$$I_{I1} = \operatorname{tr} \mathbf{C}_{I}, \quad I_{I2} = \operatorname{tr} \left( \operatorname{cof} \mathbf{C}_{I} \right), \quad I_{I3} = \det \mathbf{C}_{I}.$$

$$(4.79)$$

The Jacobian  $J_I$  of the ice is related to the invariant measures via  $J_I = \sqrt{I_{I3}}$ . This leads to the introduction of the strain-energy function in invariant representation via

$$W^{I}(\theta, n^{I}, \mathbf{C}_{I}) \longrightarrow W^{I}(\theta, n^{I}, I_{I1}, I_{I2}, J_{I}).$$
 (4.80)

The respective terms for the formal introduction of the strain energy  $W^{I}$  are based on

the same fundamental works, compare [15, 171], such that

$$W^{I}(\theta, n^{I}, I_{I1}, J_{I}) = U^{I}(J_{I}) - \mu^{IR} \ln J_{I} + \frac{\mu^{IR}}{2} (I_{I1} - 3) - 3 \alpha^{IR} k^{IR} \ln J_{I}(\theta - \theta_{0I}^{I}) - \rho_{0I}^{IR} c_{v}^{IR}(\theta \ln \frac{\theta}{\theta_{0I}^{I}} - \theta + \theta_{0I}^{I}) + W_{n^{I}}^{I}(n^{I}),$$

$$(4.81)$$

where  $\mu^{IR}$  is the effective second *Lamé* constant,  $k^{IR}$  the bulk modulus and  $c_v^{IR}$  the specific heat capacity at constant volume. Similar to the solid skeleton, the compaction point has been included due to the kinematic coupling to the solid skeleton by the volumetric-extension term according to Eurich *et al.* [72], viz.:

$$U^{I}(J_{I}) = \frac{\Lambda^{IR}}{\gamma_{0}^{IR}(\gamma_{0}^{IR} - 1) + \frac{2}{(\tilde{J}_{I} - 1)^{2}}} [J_{I}^{\gamma_{0}^{IR}} - (\gamma_{0}^{IR} + \frac{2}{\tilde{J}_{I} - 1})J_{I} + \gamma_{0}^{IR} + \frac{2}{\tilde{J}_{I} - 1} - 1 + \ln\left(\frac{(\tilde{J}_{I} - 1)^{2}}{(\tilde{J}_{I} - J_{I})^{2}}\right)].$$

$$(4.82)$$

Therein,  $\Lambda^{IR}$  is the effective first Lamé constant and  $\gamma_0^{IR}$  is an additional parameter. However, there is an additional term  $W_{n^I}^I(n^I)$  in (4.81) in comparison to the solid skeleton accounting for the dependency on the volume fraction of the ice, as introduced in (4.78). For the development of the remaining part  $W_{n^I}^I(n^I)$ , condition (4.44)<sub>1</sub> regarding the ice pressure has to be considered. This condition is given via

$$p^{IR} = p^{FR} + \rho^{I} \frac{\partial \psi^{I}}{\partial n^{I}} = p^{FR} + \rho^{I} \frac{\partial W^{I}_{n^{I}}}{\partial n^{I}} =: p^{FR} + p^{IR}_{\theta}, \qquad (4.83)$$

indicating that there is a part  $p_{\theta}^{IR}$  of the pressure  $p^{IR}$  in excess to the pore pressure. As implied in comparable works, for example in Bluhm *et al.* [16], Coussy [39], Koniorczyk *et al.* [106], Zhou & Meschke [196], this additional part  $p_{\theta}^{IR}$  is temperature dependent. Thus, the approach

$$p_{\theta}^{IR} = E_{\text{fus}} \left( \theta_{0I}^{I} - \theta \right) \tag{4.84}$$

is chosen, where  $E_{\text{fus}}$  is the entropy of fusion. The entropy of fusion is the decrease in entropy, when water in a liquid state freezes, compare Atkins & de Paula [6]. Therefore, integration of (4.83) under consideration of (4.84) yields

$$W_{n^{I}}^{I}(n^{I}) = \frac{\rho_{0I}^{IR}}{\rho^{IR}} E_{\text{fus}} \left(\theta_{0I}^{I} - \theta\right) \ln n^{I}.$$
(4.85)

With the in (4.81)-(4.85) introduced strain energy, the *Cauchy* stress is according to  $(4.44)_2$  given as

$$\mathbf{T}_{E\,\mathrm{mech}}^{I} = \frac{\rho^{I}}{\rho_{0I}^{IR}} [2\mu^{IR} \mathbf{K}_{I} - 3\,\alpha^{IR} k^{IR} (\theta - \theta_{0I}^{I}) \mathbf{I} + \frac{\Lambda^{IR}}{\gamma_{0}^{IR} (\gamma_{0}^{IR} - 1) + \frac{2}{(\tilde{J}_{I} - 1)^{2}}} (\gamma_{0}^{IR} J_{I}^{\gamma_{0}^{IR}} - \gamma_{0}^{IR} J_{I} - \frac{2J_{I}}{\tilde{J}_{I} - 1} + \frac{2J_{I}}{\tilde{J}_{I} - J_{I}}) \mathbf{I}],$$

$$(4.86)$$

accounting for the required properties, where the mass production of ice (as phase transformation) is hidden in the density ratio in the beginning, compare also (4.14). **Ice pressure:** As the ice pressure has been constitutively introduced in (4.83) and (4.84) by thermodynamic considerations, its value is consequently given via

$$p^{IR} = p^{FR} + E_{\text{fus}} \left( \theta^{I}_{0I} - \theta \right).$$
(4.87)

This formulation is similar to the one given in Bluhm *et al.* [16], Coussy [39], Koniorczyk *et al.* [106], Zhou & Meschke [196], however, with the difference that these works refer to the liquid pressure and not to the pore pressure, which is due to the partially saturated character of the approach given here.

### 4.4.3 Additional constraints

There is one issue that needs further attention, which is related to the introduction of the compaction point. In particular, the limiting value  $\tilde{J}_{\delta}$  of the volumetric deformation is needed. Yet, due to the utilised formulation of the mass interactions, introduced in **Section 4.7**, there is no analytic expression for the solid volume fractions, which is the reason they have been solved by introducing them as primary fields. Consequently, there is also no analytic expression that uses the condition  $n^S + n^I = 1$  to calculate the limiting value  $\tilde{J}_{\delta}$  of the volumetric deformation that accounts for the actual available pore space. However, when the change in  $J_{\delta}$  that is due to the accumulated volumetric deformation is assumed to be fairly small in comparison to the change that is due to varying volume fractions due to mass interaction, which is the case for the situation at hand, the limiting value of the volumetric deformation can be approximated via

$$\tilde{J}_{\delta} = n^S + n^I, \tag{4.88}$$

as this accounts for the solid and, therefore, the incompressible part of the multiphasic material.

### 4.5 The fluid constituents

In this section, the thermodynamical behaviour of the involved fluids in the macro-pore space is discussed. Since the macro-pore space is filled with two immiscible fluids, a wetting and a non-wetting phase, the concept of capillarity will be concisely addressed. Furthermore, the respective momentum balance of the individual fluid will be utilised to derive the filter velocity, which leads with appropriate assumptions to extended *Darcy* laws. Furthermore, the equations of state of the liquid water and the gaseous air are introduced, along with the *Helmholtz* free energies  $\psi^{\beta}$  based on thermodynamic considerations.

Note that the theory that is utilised within this monograph in relation to the fluids in the macro-pore space of plants has been stated for the ternary model in Eurich *et al.* [67], here, it is applied to the quaternary model.

### 4.5.1 Capillarity

Porous media with a multiphasic pore space have been extensively discussed, inter alia in Bear [10], de Boer & Bluhm [25], Brooks & Corey [33], Ehlers et al. [57], van Genuchten [79], Hassanizadeh & Gray [93], Helmig et al. [94], Joekar-Niasar & Hassanizadeh [101], Niessner *et al.* [135]. Depending on the scope of the investigation, the theory for the inclusion of the action of capillarity varies with regard to the process variables. The capillary pressure, defined as the pressure difference between the non-wetting fluid and the wetting fluid, gas and liquid, is either assumed to be a function of the (liquid) saturation only, or also of internal interfacial areas between the involved fluids. The latter is specifically of interest in case the hysteresis effect needs to be considered. The hysteresis effect with regard to capillarity accounts for the fact that the drainage curve, i. e. describing the displacement of the wetting by the non-wetting fluid, and the imbibition curve, i. e. the opposite displacement scenario, do not coincide in the capillary pressure  $p^{C}$  versus liquid saturation  $s^{L}$  chart. However, since within this monograph there is no interest in alternating liquid or gas fronts moving through the porous medium, this effect can be neglected. A comprehensive discussion concerning these assumptions can be found in Häberle [89], mainly tracing back to Bear [10], Hassanizadeh & Gray [93].

The capillary pressure is defined based on the surface tension in the surface area between the wetting and the non-wetting fluid. This relation is often referred to as *Young-Laplace* equation

$$p^C = \frac{2\,\sigma_s\cos\vartheta}{\tilde{r}}.\tag{4.89}$$

Therein,  $\sigma_s$  is the surface tension,  $\vartheta$  is the contact angle and the representative pore radius is addressed via  $\tilde{r}$ , as shown in Figure 4.3. Therein, the contact angle is defined between the solid skeleton and the fluid interface. A fluid is considered as wetting fluid for contact angles of  $(0^\circ \le \vartheta < 90^\circ)$ , and as non-wetting fluid for contact angles of  $(90^\circ < \vartheta \le 180^\circ)$ , for  $\vartheta = 90^\circ$ , there are no capillary forces, as discussed in Häberle [89].



**Figure 4.3:** Microstructure of the REV with depicted idealised pore indicating the non-wetting fluid (gaseous air) with pressure  $p^{GR}$  and the wetting fluid (liquid water) with pressure  $p^{LR}$ .

There is another possible definition of the capillary pressure that is based on the entropy evaluation. Thus, with the definition of the gas pressure (4.35) and the liquid pressure (4.38), the capillary pressure  $p^{C}$  is obtained as

$$p^{C} = p^{GR} - p^{LR} = -s^{L}\rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}}.$$
(4.90)

Note that this relation will be utilised to derive the energy potential  $\psi^L$  of the liquid water. For this, a constitutive relation of the capillary pressure to the liquid saturation is necessary. In particular, the relation between the (effective) liquid saturation  $s_{\text{eff}}^L$  and the capillary pressure  $p^C$  is chosen according to Brooks & Corey [33] to ensure thermodynamic consistency, as shown in Ehlers & Häberle [58]. Thus, one makes use of

$$s_{\text{eff}}^{L} = \left(\frac{p_d}{p^C}\right)^{\lambda_c} \quad \Longleftrightarrow \quad p^C = p_d \left(s_{\text{eff}}^L\right)^{-\frac{1}{\lambda_c}} \tag{4.91}$$

for  $p^C \ge p_d$ , where  $p_d$  is the entry (or bubbling) pressure and  $\lambda_c$  the pore-size distribution index. As these material parameters are not known for the current investigation, their value has been chosen to account for the initial fluid volume fractions and an assumption regarding  $\lambda_c$ , as discussed in **Chapter 6**. The effective saturation  $s_{\text{eff}}^L$  is according to van Genuchten [79] given via

$$s_{\rm eff}^{L} = \frac{s^{L} - s_{\rm res}^{L}}{1 - s_{\rm res}^{L} - s_{\rm res}^{G}},\tag{4.92}$$

where the residual saturations  $s_{\text{res}}^L$  and  $s_{\text{res}}^G$  have been originally introduced due to physical considerations. It has to be pointed out, that they are also important from a numerical point of view, as a vanishing of one of the fluid saturations may lead to issues in relation to their mass balance, which are utilised in weak form to determine the respective fluid pressures.

Based on the evaluation of the entropy inequality given in  $(4.51)_1$  and  $(4.51)_2$ , the following approaches for the direct momentum productions are admissible

$$\hat{\mathbf{p}}_{E\,\mathrm{dis}}^{L} = -\left(n^{L}\right)^{2} \rho^{LR} g\left(\mathbf{K}_{r}^{L}\right)^{-1} \mathbf{w}_{L}, \quad \hat{\mathbf{p}}_{E}^{G} = -\left(n^{G}\right)^{2} \rho^{GR} g\left(\mathbf{K}_{r}^{G}\right)^{-1} \mathbf{w}_{G}, \tag{4.93}$$

with  $g = |\mathbf{g}|$ . Furthermore, the relative permeabilities  $\mathbf{K}_r^L$  and  $\mathbf{K}_r^G$  are tensors of second order, which generally may consider anisotropies in the permeability. They are defined according to Brooks & Corey [33] as

$$\mathbf{K}_{r}^{L} = \kappa_{r}^{L} \mathbf{K}^{L}, \quad \mathbf{K}_{r}^{G} = \kappa_{r}^{G} \mathbf{K}^{G}, \tag{4.94}$$

where  $\kappa_r^L$  and  $\kappa_r^G$  are relative permeability factors and  $\mathbf{K}^L$  and  $\mathbf{K}^G$  conductivity tensors, that can be related to the intrinsic permeability  $\mathbf{K}^S$  via

$$\mathbf{K}^{L} = \frac{\rho^{LR}g}{\mu^{LR}}\mathbf{K}^{S}, \quad \mathbf{K}^{G} = \frac{\rho^{GR}g}{\mu^{GR}}\mathbf{K}^{S}$$
(4.95)

with  $\mu^{\beta R}$  being the shear viscosity of the respective fluid.

While the relative permeability factors  $\kappa_r^L$  and  $\kappa_r^G$  specifically address the interaction of the involved fluids and are given according to Brooks & Corey [33] via

$$\kappa_r^L = \left(s_{\text{eff}}^L\right)^{\frac{2+3\lambda_c}{\lambda_c}}, \quad \kappa_r^G = \left(1 - s_{\text{eff}}^L\right)^2 \left[1 - \left(s_{\text{eff}}^L\right)^{\frac{2+\lambda_c}{\lambda_c}}\right], \tag{4.96}$$

the intrinsic permeability  $\mathbf{K}^{S}$  in the current configuration is a material property of the solid skeleton and given following Markert [121] via

$$\mathbf{K}^{S} = \left(\frac{n^{F}}{1 - n^{F}} \frac{1 - n^{F}_{0S}}{n^{F}_{0S}}\right)^{\kappa} \mathbf{K}^{S}_{0S},\tag{4.97}$$

where  $\mathbf{K}^{S}$  is related to the intrinsic permeability  $\mathbf{K}_{0S}^{S}$  of the solid reference configuration. Note that  $\kappa$  as a material parameter controling the nonlinearity of the change in available pore space, which is the term in parentheses. With this definition of the intrinsic permeability, anisotropies can be captured, which are caused by inherent material properties and not by deformation.

### 4.5.2 Filter velocities

The velocities of the respective fluid constituents within the macro-pore space are addressed in a modified *Euler*ian setting indicating that the motion of the respective fluid is stated with respect to the solid motion (3.21). The introduced equations are derived based on the evaluation of the constituent-specific momentum balance  $(3.58)_2$ . On the left side of  $(3.58)_2$ , the assumption of creeping-flow conditions has been made, cf. (4.2). On the right side of  $(3.58)_2$ , the stresses are defined via (4.37). Thus, for the liquid water, the momentum balance reads

$$\mathbf{0} = \operatorname{div} \mathbf{T}^{L} + \rho^{L} \mathbf{g} + \hat{\mathbf{p}}^{L} =$$

$$= \operatorname{div} (-n^{L} p^{LR} \mathbf{I}) + \rho^{L} \mathbf{g} + \hat{\mathbf{p}}^{L}_{E \operatorname{dis}} + p^{GR} \operatorname{grad} n^{L} - s^{L} p^{C} \operatorname{grad} n^{F} - \hat{\rho}^{S} \mathbf{x}_{S}^{\prime} - \hat{\rho}^{I} \mathbf{x}_{S}^{\prime} =$$

$$= -(n^{L})^{2} \mu^{LR} (\mathbf{K}^{L})^{-1} \mathbf{w}_{L} - n^{L} \operatorname{grad} p^{LR} + n^{F} p^{C} \operatorname{grad} s^{L} + \rho^{L} \mathbf{g} - \hat{\rho}^{S} \mathbf{x}_{S}^{\prime} - \hat{\rho}^{I} \mathbf{x}_{S},$$

$$(4.98)$$

which yields the filter velocity

$$n^{L}\mathbf{w}_{L} = -\frac{\kappa_{r}^{L}}{\mu^{LR}}\mathbf{K}^{S}\left(\operatorname{grad} p^{LR} - \rho^{LR}\mathbf{g} - \frac{p^{C}}{s^{L}}\operatorname{grad} s^{L} + \frac{\hat{\rho}^{S}}{n^{L}} \mathbf{x}_{S}^{\prime} + \frac{\hat{\rho}^{I}}{n^{L}} \mathbf{x}_{S}^{\prime}\right).$$
(4.99)

This indicates that the filter velocity is determined by several components. In particular, the contribution arising from the water pressure is included by  $\operatorname{grad} p^{LR}$ , the one from gravitational potential via  $\rho^{LR}\mathbf{g}$  and the one from the interaction among the fluids in the macro-pore space via  $(p^C/s^L) \operatorname{grad} s^L$ . Finally,  $(\hat{\rho}^S/n^L) \mathbf{x}_S$  accounts for the momentum production that is caused by cell dehydration and  $(\hat{\rho}^I/n^L) \mathbf{x}_S$  is due to momentum production that originates from the formation of ice, which is orders of magnitudes smaller than the contributions arising from the pressures in the current setting as indicated by

numerical simulations. Concerning the numerical examples presented in this monograph, the dynamics of interest is acting in-plane, such that gravitational forces do not matter, which are acting out-of-plane. Additionally, the contribution originating from momentum interaction that is due to mass production can be neglected.

The question arises, how formulation (4.99) relates to the water-potential concept from biology. Thus, it is sensible to consider the original formulation of *Darcy*'s filter law, cf. e. g. Ehlers [48], viz.:

$$n^F \mathbf{w}_F = -k^F \operatorname{grad} h. \tag{4.100}$$

Therein,  $k^F$  is the hydraulic conductivity for isotropic materials. From (4.100), it can be concluded that the flow of a fluid follows the gradient of the pressure head h, which has to be understood as a flow potential. Following this, one might introduce another potential function  $h_W$  based on (4.99), where its gradient consists of five parts:

$$\operatorname{grad} h_W = \operatorname{grad} p^{LR} - \rho^{LR} \mathbf{g} - \frac{p^C}{s^L} \operatorname{grad} s^L + \frac{\hat{\rho}^S}{n^L} \mathbf{\dot{x}}_S + \frac{\hat{\rho}^I}{n^L} \mathbf{\dot{x}}_S .$$
(4.101)

For the water potential itself, this implies

$$h_W = p^{LR} + U_g + \lambda_c \, p^C + U_{\hat{\rho}^S} + U_{\hat{\rho}^I}, \qquad (4.102)$$

where  $p^{LR}$  is the water pressure potential,  $U_g$  the gravitational potential,  $\lambda_c p^C$  a potential considering the action of capillarity,  $U_{\hat{\rho}^S}$  a potential accounting for the local momentum production that is due to solid mass production and  $U_{\hat{\rho}^I}$  a potential accounting for the local momentum production that is due to the phase transition of water.

For the gaseous constituent, a similar derivation of the filter velocity can be performed. Thus, for the gaseous air, the momentum balance reads with the assumption of creeping flow conditions and equilibrium stresses, viz.:

$$\mathbf{0} = \operatorname{div} \mathbf{T}^{G} + \rho^{G} \mathbf{g} + \hat{\mathbf{p}}^{G} =$$

$$= \operatorname{div} (-n^{G} p^{GR} \mathbf{I}) + \rho^{G} \mathbf{g} + \hat{\mathbf{p}}_{E}^{G} + p^{GR} \operatorname{grad} n^{G} =$$

$$= -(n^{G})^{2} \mu^{GR} (\mathbf{K}^{G})^{-1} \mathbf{w}_{G} - n^{G} \operatorname{grad} p^{GR} + \rho^{G} \mathbf{g},$$
(4.103)

which yields the standard *Darcy* law for the gas

$$n^{G}\mathbf{w}_{G} = -\frac{\kappa_{r}^{G}}{\mu^{GR}}\mathbf{K}^{S}\left(\operatorname{grad} p^{GR} - \rho^{GR}\mathbf{g}\right).$$
(4.104)

#### 4.5.3 Equations of state

An equation of state yields a relation between the state variables density, temperature and pressure. For the (materially incompressible) liquid component, the thermal dependency of the density needs to be accounted for by considering also the density anomaly at 3.98°C. This effect has been described in Bettin & Spieweck [13], Tannaka *et al.* [181], where experimentally based approaches are introduced to address the temperature-dependence

of the liquid density. Due to its simplicity, the approach from Tannaka *et al.* [181] is utilised, where the effective liquid density is given via

$$\rho^{LR}(\tilde{\theta}) = a_5 \left( 1 - \frac{(\tilde{\theta} + a_1)^2 (\tilde{\theta} + a_2)}{a_3 (\tilde{\theta} + a_4)} \right), \tag{4.105}$$

where  $a_1$ - $a_5$  are fitting parameters. Note, that the temperature  $\tilde{\theta}$  is given in °C, such that the conversion  $\tilde{\theta}[^{\circ}C] = \theta[K] - 273.15$  needs to be considered. With this approach, the effective density is in good agreement with the experimental data, obtained from <u>a technical</u> report of the Physikalisch-Technische Bundesanstalt [144], shown in Figure 4.4. Furthermore, this figure displays also the density of water below the freezing point including the chosen analytical ansatz and experimental data for comparison. The jump in density accross the singular surface  $\Gamma$  is shown by the black vertical line at 0 °C.



Figure 4.4: The density of water. For temperatures  $\tilde{\theta} > 0$  °C as liquid constituent with a comparison of the approach by Tannaka *et al.* [181] and experimental data from [144]. For temperatures  $\tilde{\theta} < 0$  °C as ice with a comparison of the approach introduced in (4.19)<sub>2</sub> with experimental data from [66]. The vertical black line represents the jump in density accross the singular surface  $\Gamma$ . Note that the material parameters of the ice are given in Table 6.2.

For the gaseous component, the ideal gas law in the form of *Boyle-Mariotte* is applied as equation of state, which is according to Ehlers [49] given in the current setting via

$$\rho^{GR} = \frac{p^{GR} + p_0}{\bar{R}^G \theta} \longrightarrow p^{GR} = (\rho^{GR} - \rho^{GR}_{0G})\bar{R}^G \theta, \qquad (4.106)$$

where  $p_0$  the ambient pressure. Therefore,  $p^{GR}$  is the excess gas pressure compared to the ambient pressure,  $\bar{R}^G$  is the gas constant of air.

### 4.5.4 *Helmholtz* free energies

The procedure for the derivation of the *Helmholtz* free energies  $\psi^{\beta}$  is inspired by the works of Ehlers [49], Ghadiani [81] or Häberle [89]. Based on the restrictions from the entropy inequality, compare  $(4.32)_3$  and  $(4.32)_4$ , together with the definition of the gaseous pressure in (4.35) as well as the capillary pressure in (4.90), the *Helmholtz* free energies will be derived.

Therefore, there are two constraints for the liquid water that have to be fulfilled, one originating from the entropy inequality, which results in

$$\frac{\partial \psi^L}{\partial s^L} = -\frac{p^C}{s^L \rho^{LR}}.$$
(4.107)

Furthermore, the definition of the specific heat capacity  $c_v^{LR}$  at contant volume is utilised, viz.:

$$c_v^{LR} = -\theta \,\frac{\partial^2 \psi^L}{\partial \theta^2}.\tag{4.108}$$

Here, the assumption is made that  $c_v^{LR}$  is contant within the temperature range of interest. In that particular case, (4.108) will be formally integrated. This yields the thermal part of the *Helmholtz* free energy of the liquid via

$$\frac{\partial \psi_{\theta}^{L}}{\partial \theta} = -c_{v}^{LR} \ln\left(\frac{\theta}{\theta_{0S}^{S}}\right) \longrightarrow \psi_{\theta}^{L} = -c_{v}^{LR} \left[\theta \ln\left(\frac{\theta}{\theta_{0S}^{S}}\right) - \theta + \theta_{0S}^{S}\right] + \psi_{\theta 0}^{L}.$$
(4.109)

Therein, the additional constant energy term  $\psi_{\theta 0}^L$  is considered. When the effective saturation is assumed to be approximately equal to the saturation, i. e.  $s_{\text{eff}}^L \approx s^L$ , the saturation-part of the *Helmholtz* free energy is, under consideration of (4.91), given via

$$\frac{\partial \psi_{s^L}^L}{\partial s^L} = -\frac{p_d}{\rho^{LR}} (s^L)^{-\frac{1}{\lambda_c} - 1} \longrightarrow \psi_{s^L}^L = \frac{p_d}{\rho^{LR}} \lambda_c (s^L)^{-\frac{1}{\lambda_c}} + \psi_{s^L 0}^L = \frac{\lambda_c p^C}{\rho^{LR}} + \psi_{s^L 0}^L, \quad (4.110)$$

where  $\psi^L_{s^L0}$  is a constant reference energy. Therefore, the total energy is given via

$$\psi^{L} = \frac{\lambda_{c} p^{C}}{\rho^{LR}} - c_{v}^{LR} \left[ \theta \ln \left( \frac{\theta}{\theta_{0S}^{S}} \right) - \theta + \theta_{0S}^{S} \right] + \psi_{0}^{L}, \qquad (4.111)$$

where the reference energy potential is the sum of the introduced potentials and chosen as  $\psi_0^L = p_0^{FR}/\rho_0^{SR} - \lambda_c p_0^C/\rho_0^{LR} - p_0^{LR}/\rho_0^{LR}$ , such that there is initially no solid mass production, indicating that the initial difference in chemical potential in (4.150) vanishes.

A very similar procedure as for the liquid water is carried out also for the gaseous constituent. Also the definition of the specific heat capacity  $c_v^{GR}$  at constant volume is utilised, whereby it is assumed to be constant within the given temperature range as well, viz.:

$$c_v^{GR} = -\theta \,\frac{\partial^2 \psi^G}{\partial \theta^2}.\tag{4.112}$$

When (4.112) is integrated twice with respect to the temperature, the thermal part of  $\psi^{G}$  can be derived via

$$\frac{\partial \psi_{\theta}^{G}}{\partial \theta} = -c_{v}^{GR} \ln\left(\frac{\theta}{\theta_{0S}^{S}}\right) \longrightarrow \psi_{\theta}^{G} = -c_{v}^{GR} \left[\theta \ln\left(\frac{\theta}{\theta_{0S}^{S}}\right) - \theta + \theta_{0S}^{S}\right].$$
(4.113)

The density-part of  $\psi^G$  is also formally integrated, when (4.35) and (4.106) are combined, viz.:

$$\frac{\partial \psi_{\rho^{GR}}^G}{\partial \rho^{GR}} = \bar{R}^G \theta \left( \frac{1}{\rho^{GR}} - \frac{\rho_{0G}^{GR}}{(\rho^{GR})^2} \right) \longrightarrow \psi_{\rho^{GR}}^G = \bar{R}^G \theta \left[ \ln \left( \frac{\rho^{GR}}{\rho_{0G}^{GR}} \right) + \frac{\rho_{0G}^{GR}}{\rho^{GR}} - 1 \right].$$
(4.114)

This leads to the total *Helmholtz* free energy of the gaseous constituent

$$\psi^{G} = \bar{R}^{G} \theta \left[ \ln \left( \frac{\rho^{GR}}{\rho_{0G}^{GR}} \right) + \frac{\rho_{0G}^{GR}}{\rho^{GR}} - 1 \right] - c_{v}^{GR} \left[ \theta \ln \left( \frac{\theta}{\theta_{0S}^{S}} \right) - \theta + \theta_{0S}^{S} \right], \quad (4.115)$$

which vanishes in the reference state. Further additional constant energy terms are not needed for the gaseous constituent.

### 4.6 Heat flux

The assumption of slow processes enables the simplification of a common temperature of all the constituents at a certain location. This implies that only the energy balance of the overall aggregate has to be evaluated, which will be discussed in detail in **Section 4.8**. Moreover, it implies that the partial heat fluxes  $\mathbf{q}^{\alpha}$  differ only in a factor, which can be concluded from the evaluation of the entropy inequality (4.51)<sub>3</sub>. This leads to *Fourier* laws for the heat flux of each constituent, viz.:

$$\mathbf{q}^{\alpha} = -\mathbf{H}^{\alpha} \operatorname{grad} \theta, \quad \text{where} \quad \mathbf{H}^{\alpha} = n^{\alpha} \mathbf{H}^{\alpha R}.$$
 (4.116)

Therein,  $\mathbf{H}^{\alpha}$  is the partial thermal conductivity and  $\mathbf{H}^{\alpha R}$  the effective constituent-specific thermal conductivity, in which anisotropies that are caused by the microstructure of the material can be taken into account. In order to ensure thermodynamic consistency,  $\mathbf{H}^{\alpha R}$ has to be positive definite. Note that for the case of isotropy, the thermal conductivity is given by a single value via

$$\mathbf{H}^{\alpha R} = H^{\alpha R} \mathbf{I}. \tag{4.117}$$

### 4.7 Mass interactions

The final and somehow most crucial part of the constitutive setting is concerned with a proper decription of the mass-interaction terms to address the phase transition of water in the intercellular space via  $\hat{\rho}^{I}$  and the consequent dehydration of the cells via  $\hat{\rho}^{S}$ .

### 4.7.1 Solid-liquid phase transition of water

From the evaluation of the entropy inequality with regard to the phase transition of water (4.50), two options are possible, viz.:

(a): 
$$\mathcal{D}_{\hat{\rho}^{I}} = -\hat{\rho}^{I}(\psi^{I} + \frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{p^{IR}}{\rho^{IR}} - \frac{p^{LR}}{\rho^{LR}}) > 0$$
  
(b):  $\mathcal{D}_{\hat{\rho}^{I}} = -\hat{\rho}^{I}(\psi^{I} + \frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{p^{IR}}{\rho^{IR}} - \frac{p^{LR}}{\rho^{LR}}) = 0.$ 
(4.118)

When option (a) is considered, the phase transition of water is regarded as non-equilibrium process. Thus, there is an increase in entropy. In that case, the process is often described as a spontaneous process, where the direction of phase transition is automatically determined, such that below the freezing point of  $\theta = 273.15$  K under atmospheric pressure, liquid water transforms to solid ice and above the freezing point vice versa.

However, when option (b) is considered, the phase transition of water is regarded as an equilibrium process meaning that there is no entropy production. Thus, when there is no mass production, i. e.  $\hat{\rho}^I = 0$ ,  $(4.118)_2$  is obviously fulfilled. In case there is mass production, i. e.  $\hat{\rho}^I \neq 0$ , the term in parenthesis has to vanish indicating that the chemical potentials of the ice and the liquid are identical. It also indicates that the direction of the process is not a priori clear, in fact, liquid and solid are in equilibrium. So the direction of the process depends on the fact whether energy or heat is leaving or entering the system. Utilising the derivation of the mass-production term according to Häberle [89] allows to consider the phase-transition process as an equilibrium process. In fact, option (b) is the process that is considered within this monograph, compare also Graf [83], Komarova [105]. Note that equilibrium freezing has also been reported for plant tissues, compare Beck et al. [11]. As already mentioned, prerequisite for this non-spontaneous process is that ice forms under the assumption of atmospheric pressure at a temperature of  $\theta = 273.15$  K. Note in passing that the freezing point generally may depend on the proteins or solutes dissolved in water [166], or also on pressure [149]. However, these dependences are not considered in this context, which is also supported by Beck *et al.* [11]. Moreover, also the enthalpy and entropy of fusion are considered as constant [149]. For further explanations regarding the thermodynamics of phase transitions of a pure substance, the interested reader is referred to Atkins & de Paula [6], Moran & Shapiro [129] regarding a general thermodynamic framework, or with regard to porous media, such as Bluhm et al. [18], de Boer [21], Coussy [39], Ehlers & Häberle [58], Koniorczyk et al. [106], Talamucci [180].

Having this in mind, further considerations are necessary to describe the ice formation in the porous plant tissue.

#### Derivation of the surface-specific term

As already introduced, the derivation of the mass-interaction term is based on the work of Ehlers & Häberle [58], Häberle [89]. Therein, the assumption is made that only the in the phase transition involved constituents are affected by the phase transition at the singular surface. Hence, in this context, the jump relations  $(3.83)_2 - (3.85)_2$  apply to the water component  $\varphi^W = \varphi^I \cup \varphi^L$  only. Thus, the balance relation of mass  $(3.83)_2$  yields for water

$$\left[\!\left[\rho^{W}\mathbf{w}_{W\Gamma}\right]\!\right]\cdot\mathbf{n}_{\Gamma} = 0 \quad \longrightarrow \quad \left(\rho^{W+}\mathbf{w}_{W\Gamma}^{+} - \rho^{W-}\mathbf{w}_{W\Gamma}^{-}\right)\cdot\mathbf{n}_{\Gamma} = 0, \quad (4.119)$$

where  $\varphi^{W+} = \varphi^L$  and  $\varphi^{W-} = \varphi^I$ . Having this categorisation in mind, relation (4.119)<sub>2</sub> can be rewritten as

$$(\rho^L \mathbf{w}_{L\Gamma} - \rho^I \mathbf{w}_{I\Gamma}) \cdot \mathbf{n}_{\Gamma} = 0.$$
(4.120)

This mass flux over the internal interface  $\Gamma$  can be interpreted as the interfacial term of phase transition, compare Ehlers & Häberle [58], Häberle [89]. This idea traces mainly

back to the work of Whitaker [191], where

$$\hat{\varrho}_{\Gamma}^{L} = \rho^{L} \mathbf{w}_{L\Gamma} \cdot \mathbf{n}_{\Gamma}^{L} = \rho^{L} \mathbf{w}_{L\Gamma} \cdot \mathbf{n}_{\Gamma}, 
\hat{\varrho}_{\Gamma}^{I} = \rho^{I} \mathbf{w}_{I\Gamma} \cdot \mathbf{n}_{\Gamma}^{I} = -\rho^{I} \mathbf{w}_{I\Gamma} \cdot \mathbf{n}_{\Gamma}.$$
(4.121)

This yields inserted into (4.120)

$$\hat{\varrho}_{\Gamma}^{L} + \hat{\varrho}_{\Gamma}^{I} = 0. \tag{4.122}$$

Note that the volume-specific mass production  $\hat{\rho}^I$  of the ice is solely given by the surfacespecific mass production  $\hat{\varrho}_{\Gamma}^L$  of the liquid, which needs to be homogenised, viz.:

$$\hat{\rho}^{I} dv = \hat{\varrho}_{\Gamma}^{L} da_{\Gamma} \longrightarrow \hat{\rho}^{I} = \hat{\varrho}_{\Gamma}^{L} \frac{da_{\Gamma}}{dv} = \hat{\varrho}_{\Gamma}^{L} a_{\Gamma}, \qquad (4.123)$$

where the phase-change surfaces with respect to the volume is given by

$$a_{\Gamma} = \frac{\mathrm{d}a_{\Gamma}}{\mathrm{d}v}.\tag{4.124}$$

However, for the volume-specific mass production of liquid water, the constraint  $(3.57)_1$  needs to be considered, which indicates

$$\hat{\rho}^L + \hat{\rho}^S = -\hat{\rho}^I = -a_{\Gamma} \,\hat{\varrho}^L_{\Gamma} = a_{\Gamma} \,\hat{\varrho}^I_{\Gamma}. \tag{4.125}$$

Thus, the volume-specific mass production of liquid water is given via

$$\hat{\rho}^L = a_\Gamma \,\hat{\varrho}^I_\Gamma - \hat{\rho}^S. \tag{4.126}$$

This indicates that the mass production of the liquid has a part  $a_{\Gamma} \hat{\varrho}_{\Gamma}^{I}$  originating from the phase transition at the interface  $\Gamma$  and a part  $\hat{\rho}^{S}$  that is due to cell dehydration.

The interfacial mass production  $\hat{\varrho}_{\Gamma}^{L}$  (or  $\hat{\varrho}_{\Gamma}^{I}$ ) can be derived by considering the jump relations once again. In particular, the energy jump of the water component  $\varphi^{W}$  yields

$$\left[ \rho^{W}(\varepsilon^{W} + \frac{1}{2} \mathbf{\dot{x}}_{W} \cdot \mathbf{\dot{x}}_{W}) \mathbf{w}_{W\Gamma} - \mathbf{T}^{W} \mathbf{\dot{x}}_{W} + \mathbf{q}^{W} \right] \cdot \mathbf{n}_{\Gamma} = 0.$$
(4.127)

Note the symmetry of the stress tensors  $\mathbf{T}^W = (\mathbf{T}^W)^T$ . The evaluation of the jump condition yields

$$\left[\rho^{L}\left(\varepsilon^{L}+\frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L}\right) \mathbf{w}_{L\Gamma}-\mathbf{T}^{L} \mathbf{x}_{L}+\mathbf{q}^{L}\right] \cdot \mathbf{n}_{\Gamma}-\left[\rho^{I}\left(\varepsilon^{I}+\frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S}\right) \mathbf{w}_{S\Gamma}-\mathbf{T}^{I} \mathbf{x}_{S}+\mathbf{q}^{I}\right] \cdot \mathbf{n}_{\Gamma}=0.$$

$$(4.128)$$

Recalling the definitions of the interfacial mass productions via  $\hat{\varrho}_{\Gamma}^{L} = \rho^{L} \mathbf{w}_{L\Gamma} \cdot \mathbf{n}_{\Gamma}$  and  $\hat{\varrho}_{\Gamma}^{I} = -\rho^{I} \mathbf{w}_{I\Gamma} \cdot \mathbf{n}_{\Gamma}$  leads, together with (4.122), to the form

$$\hat{\varrho}_{\Gamma}^{L}(\varepsilon^{L} + \frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L} - \varepsilon^{I} - \frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S}) = (\mathbf{T}^{L} \mathbf{x}_{L} - \mathbf{q}^{L}) \cdot \mathbf{n}_{\Gamma} - (\mathbf{T}^{I} \mathbf{x}_{S} - \mathbf{q}^{I}) \cdot \mathbf{n}_{\Gamma} \quad (4.129)$$

and finally to

$$\hat{\varrho}_{\Gamma}^{L} = \frac{-(\mathbf{q}^{L} - \mathbf{q}^{I}) \cdot \mathbf{n}_{\Gamma} + (\mathbf{T}^{L} \mathbf{\dot{x}}_{L} - \mathbf{T}^{I} \mathbf{\dot{x}}_{S}) \cdot \mathbf{n}_{\Gamma}}{(\varepsilon^{L} + \frac{1}{2} \mathbf{\dot{x}}_{L} \cdot \mathbf{\dot{x}}_{L} - \varepsilon^{I} - \frac{1}{2} \mathbf{\dot{x}}_{S} \cdot \mathbf{\dot{x}}_{S})}.$$
(4.130)

The enthalpies of water  $\zeta^w = \varepsilon^w + \frac{p^{wR}}{\rho^{wR}}$  are introduced based on a *Legendre* transformation, yielding

$$\hat{\varrho}_{\Gamma}^{L} = \frac{-(\mathbf{q}^{L} - \mathbf{q}^{I}) \cdot \mathbf{n}_{\Gamma} + (\mathbf{T}^{L} \mathbf{\dot{x}}_{L} - \mathbf{T}^{I} \mathbf{\dot{x}}_{S}) \cdot \mathbf{n}_{\Gamma}}{(\zeta^{L} - \frac{p^{LR}}{\rho^{LR}} + \frac{1}{2} \mathbf{\dot{x}}_{L} \cdot \mathbf{\dot{x}}_{L} - \zeta^{I} + \frac{p^{IR}}{\rho^{IR}} - \frac{1}{2} \mathbf{\dot{x}}_{S} \cdot \mathbf{\dot{x}}_{S})}.$$
(4.131)

As the thermal quantities determine mainly the phase transition process, several components in (4.131) can be neglected, therefore, the interfacial mass transfer is stated, according to [58, 89], in its final form via

$$\hat{\varrho}_{\Gamma}^{L} \approx \frac{-(\mathbf{q}^{L} - \mathbf{q}^{I}) \cdot \mathbf{n}_{\Gamma}}{\zeta^{L} - \zeta^{I}} = \frac{-(\mathbf{q}^{L} - \mathbf{q}^{I}) \cdot \mathbf{n}_{\Gamma}}{\Delta \zeta_{\text{fus}}}.$$
(4.132)

Therein, the enthalpy of fusion  $\Delta \zeta_{\text{fus}}$  has been introduced. The direction  $\mathbf{n}_{\Gamma}$  of the interfacial area is oriented along the density gradient, which is for incompressible constituents given by the temperature gradient and, therefore, for the case of ice formation given via

$$\mathbf{n}_{\Gamma} = -\frac{1}{|\operatorname{grad}\theta|}\operatorname{grad}\theta.$$
(4.133)

#### Specific surface $a_{\Gamma}$ of phase transition

The derived mass-interaction term (4.132) is a surface-specific quantity accounting for the physics of that process. However, the coupling of the set of balance equations (3.58) is facilitated with volume-specific quantities, in particular with  $\hat{\rho}^{\alpha}$ . Thus, volume-specific averaging processes are needed in order to get an idea, which quantities actually effect the internal interface  $a_{\Gamma}$  of phase transition.

For the derivation of the specific surface  $a_{\Gamma}$  of phase transition from liquid water to solid ice, and vice versa, further assumptions regarding the microstructure are necessary. As introduced in **Section 4.5**, cylindrically shaped capillary tubes are considered as idealised (macro-)pore space. The basic assumption is that the main direction of anisotropy of the whole biological structure (twig or branch) is the longitudinal direction of the in Figure 4.5 depicted idealised pores. Consequently, the applied ambient temperature is acting predominantly perpendicular to the longitudinal direction. Thus, the ice front moves transversally through the pore, indicating an increasing  $\tilde{h}$  within  $0 \leq \tilde{h} \leq 2\tilde{r}$  in Figure 4.6, until the water is frozen. The specific surface  $a_{\Gamma}$  of phase transition is the ratio of the interfacial area  $A_{\rm IL}$  with respect to the overall volume V, given via

$$a_{\Gamma} = \frac{A_{\rm IL}}{V}.\tag{4.134}$$

Therein, the interfacial area  $A_{\rm IL}$  is given via

$$A_{\rm IL} = \tilde{s} \, l_1, \tag{4.135}$$

where  $\tilde{s}$  is the chord length of the projected cylinder, cf. Figure 4.6, and  $l_1$  the length of the water-filled part of the pore, liquid or solid, cf. Figure 4.5. The overall volume V can be derived considering the definition of the pore volume  $V^P$ 

$$V^{P} = \pi \,\tilde{r}^{2} \,l_{2} = (1 - n^{S}) \,V \implies V = \frac{\pi \,\tilde{r}^{2} \,l_{2}}{1 - n^{S}}.$$
(4.136)



**Figure 4.5:** Idealised longitudinal section of the in Figure 4.3 depicted idealised cylindrical pore with representative radius  $\tilde{r}$ , where its total length is given via  $l_2$ , the length of the water-filled part with  $l_1$  and x as coordinate in vertical direction. Furthermore, the direction at which the temperature gradient applies is indicated.



**Figure 4.6:** Cross section within  $0 \le x \le l_1$  of the idealised pore with radius  $\tilde{r}$ , cf. Figure 4.5. The ice-filled part of the cross section with height  $\tilde{h}$  and chord length  $\tilde{s}$  is depicted by  $A_{\text{ice}}$ , the liquid-ice interface via  $A_{\text{IL}}$  (out-of-plane).

Therein,  $\tilde{r}$  is the representative radius of the pore and  $l_2$  its total length. With (4.135) and (4.136), the specific surface is given via

$$a_{\Gamma} = \frac{\tilde{s} \left(1 - n^{S}\right)}{\pi \,\tilde{r}^{2}} \frac{l_{1}}{l_{2}}.\tag{4.137}$$

In (4.137), the chord length  $\tilde{s}$  as well as the ratio  $l_1/l_2$  needs to be specified. In this regard, the gaseous volume fraction  $n^G$  is defined via

$$n^{G} = \frac{V^{G}}{V} = \frac{\pi \,\tilde{r}^{2}(l_{2} - l_{1})(1 - n^{S})}{\pi \,\tilde{r}^{2} \,l_{2}} = (1 - \frac{l_{1}}{l_{2}})(1 - n^{S}). \tag{4.138}$$

Consequently, the length ratio  $l_1/l_2$  is given via

$$\frac{l_1}{l_2} = 1 - \frac{n^G}{1 - n^S}.$$
(4.139)

The length ratio (4.139) yields with (4.137) an important interim result, viz.:

$$a_{\Gamma} = \frac{\tilde{s}\left(1 - n^{S}\right)}{\pi \,\tilde{r}^{2}} \left(1 - \frac{n^{G}}{1 - n^{S}}\right) = \frac{\tilde{s}}{\pi \,\tilde{r}^{2}} \left(1 - n^{S} - n^{G}\right) = \frac{\tilde{s}}{\pi \,\tilde{r}^{2}} \,n^{W},\tag{4.140}$$

where  $a_{\Gamma}$  compares the chord length  $\tilde{s}$  to the overall cross sectional area of the pore with respect to the water component  $n^W$ . The ice volume fraction  $n^I$  is defined via

$$n^{I} = \frac{V^{I}}{V} = \frac{A_{\text{ice}} \left(1 - n^{S}\right)}{\pi \,\tilde{r}^{2}} \frac{l_{1}}{l_{2}} = \frac{A_{\text{ice}}}{\pi \,\tilde{r}^{2}} \, n^{W}, \tag{4.141}$$

where the area of the ice-filled part  $A_{\rm ice}$  of the cross section with area  $\pi \tilde{r}^2$  is with trigonometric considerations given via

$$A_{\rm ice} = \arccos\left(1 - \frac{\tilde{h}}{\tilde{r}}\right)\tilde{r}^2 - \sqrt{2\,\tilde{r}\,\tilde{h} - \tilde{h}^2}\,(\tilde{r} - \tilde{h}),\tag{4.142}$$

such that the relative amount of water  $n_W^I$ , i. e. the frozen part of the water, is with (4.141) and (4.142) given as a function of  $\tilde{h}$ , viz.:

$$n_W^I = \frac{n^I}{n^W} = \frac{A_{\rm ice}}{\pi \,\tilde{r}^2} = \frac{\arccos\left(1 - \frac{\tilde{h}}{\tilde{r}}\right)\tilde{r}^2 - \sqrt{2\,\tilde{r}\,\tilde{h} - \tilde{h}^2}\,(\tilde{r} - \tilde{h})}{\pi\,\tilde{r}^2}.\tag{4.143}$$

Figure 4.7 shows that relation (4.143) is fairly linear with respect to  $\tilde{h}$ , such that it can be approximated by a linear function, which is given via

$$n_W^I \approx \frac{1}{2\,\tilde{r}}\,\tilde{h},\tag{4.144}$$

which is also shown in Figure 4.7. When (4.144) is inverted,  $\hat{h}$  is given via



**Figure 4.7:** Comparison of the exact geometrical solution, depicted by the dotted black line, of the  $n_W^I - \tilde{h}$  – relation and the linearised geometrical solution, depicted as black line. It is shown for a representative pore radius of  $\tilde{r} = 0.02 \text{ mm}$ , however, the qualitative behaviour is independent of this chosen value.

$$\tilde{h} \approx 2\,\tilde{r}\,n_W^I.\tag{4.145}$$

Following this, trigonometric considerations reveal a relation of the chord length  $\tilde{s}$  to the height  $\tilde{h}$ , cf. Figure 4.6, via

$$\tilde{s} = 2\sqrt{2\,\tilde{r}\,\tilde{h} - \tilde{h}^2},$$
(4.146)

where (4.145) can be inserted into (4.146), and this, finally into (4.140) yielding

$$a_{\Gamma} = \frac{2\sqrt{2\,\tilde{r}\,\tilde{h} - \tilde{h}^2}}{\pi\,\tilde{r}^2}\,n^W = \frac{2\sqrt{2\,\tilde{r}\,(2\,\tilde{r}\,n_W^I) - (2\,\tilde{r}\,n_W^I)^2}}{\pi\,\tilde{r}^2}\,n^W.$$
(4.147)

Finally, the relation of the specific surface  $a_{\Gamma}$  is a function of the relative amount of ice  $n_W^I$ , the effective pore radius  $\tilde{r}$  and the amount of the water component  $n^W$ , viz.:

$$a_{\Gamma} = \frac{4}{\pi \,\tilde{r}} \,\sqrt{n_W^I - (n_W^I)^2} \, n^W. \tag{4.148}$$

In Figure 4.8, the approach (4.148) for the specific surface  $a_{\Gamma}$  is shown as a function of the relative amount of ice  $n_W^I$ . However, this geometric solution is not feasible for numerical implementation, as the slope of the function is very high in the vicinity of the starting and end point for values close to zero and unity in terms of  $n_W^I$ . Therefore, a customised approach is utilised for implementation with the same maximum value that accounts also for the constraint close to zero or unity in terms of  $n_W^I$ . The approximation, also shown in Figure 4.8, is given via

$$a_{\Gamma} = \begin{cases} 12.19326 \, (n_W^I - 0.05)^2 \, (0.95 - n_W^I)^2 & \text{for : } 0.05 \le n_W^I \le 0.95, \\ 0 & \text{else.} \end{cases}$$
(4.149)



**Figure 4.8:** Specific surface  $a_{\Gamma}$ . The geometric solution with a representative pore radius of  $\tilde{r} = 0.02 \text{ mm}$  and a constant water content of  $n^W = 0.1$  is depicted in dotted black. The black line is utilised for computations, as this approach accounts also for the physical boundaries and residual volume fractions of the involved constituents.

### 4.7.2 Double-porosity induced cell dehydration

From a biological point of view, water may move through the cell wall by diffusion of individual water molecules or by a bulk water flow through water-permeable pores. It has been shown that water moves much faster due to the latter mentioned mechanism, cf. Kramer & Boyer [111], Schäffner [159], Taiz & Zeiger [179], Tyerman *et al.* [185], Weig *et al.* [189]. Therefore, the dehydration of the tissue cells occurs predominantly through the micro pores in the cell wall, which may lead to a shrinkage of the cells. Note that the number of cells obviously remains constant during this process, thus, there is no real growth of solid material but rather mass exchange in terms of water. For further reading regarding the impact of structural properties in relation to the water status of tissue cells, the interested reader is also referred to Cosgrove [38], Nonami & Boyer [139] and Steudle [177].

In contrast to the double-porosity models of Gerke & van Genuchten [80], Dykhuizen [42], Borja & Choo [26], Borja & Koliji [27], Choo & Borja [36], Choo *et al.* [37], Zhang *et al.* [194], or in a thermo-hydro-mechanical framework by Khalili & Selvadurai [103], who consider individual fluid constituents at two porosity scales with individual states of motion and mass exchange of a respective fluid across the scales, a customised quasi double-porosity model is introduced in Eurich *et al.* [67] and adjusted in this context to account for Model I and Model II, where the flow of water within the micro pores of the cell wall is in both cases solely homogenised towards the mass-interaction term of the solid skeleton. A model with independent states of motion at two porosity scales is not necessary in the current setting, since the water is either confined to the solid skeleton as cell water or it is mobile within the macro-pore space.

Having these considerations in mind, similar to the notions regarding the phase transition in terms of the mass-production term  $\hat{\rho}^I$ , i. e. (4.118), it is also generally possible to consider the cell dehydration, which is represented by the mass-production term  $\hat{\rho}^S$ , as a process in equilibrium or not. However, in the current setting, the flow in the micro-pores is considered as non-equilibrium process, as is also the flow in the macro-pores, which is bio-physically the same process. Therefore, based on the entropy inequality (4.52)<sub>1</sub>, the flow at the microscale, i. e.  $\hat{\rho}^S$ , follows the difference in chemical potential between the intracellular space and the extracellular space. Hence, the mass production is given via

$$\hat{\rho}^{S} = -\kappa^{SL}\omega L_{p} \left(\rho^{SR}\right)^{2} \left(\psi^{S} + \frac{p^{FR}}{\rho^{SR}} + \frac{1}{2} \mathbf{\dot{x}}_{S} \cdot \mathbf{\dot{x}}_{S} - \psi^{L} - \frac{p^{LR}}{\rho^{LR}} - \frac{1}{2} \mathbf{\dot{x}}_{L} \cdot \mathbf{\dot{x}}_{L}\right), \quad (4.150)$$

where  $\kappa^{SL} \ge 0$  is a parameter accounting for the effective permeability of the cell wall, inter alia by accounting for the change in effective surface area. This function is highly plant-specific and is introduced as

$$\kappa^{SL} = \begin{cases} \kappa_0^{SL} \left( n^S - n_{\rm res}^S \right)^2 \left( 1 - n_{\rm res}^F - n^S \right)^2 & \text{for : } n_{\rm res}^S \le n^S \le 1 - n_{\rm res}^F, \\ 0 & \text{else.} \end{cases}$$
(4.151)

This ansatz is admissible and accounts for the physical constraints of dehydration and rehydration, compare Figure 4.9 for the cases that are considered for numerical investigation. These constraints are particularly a residual solid tissue material  $n_{\rm res}^S$  and a residual

pore space  $n_{\text{res}}^F$ . In particular, the parameters for the ansatz given in (4.151) are as noted in Table 4.1.

Case (a) applied to Section 6.1	Case (b) applied to Section 6.2
$\kappa_0^{SL} = 256$	$\kappa_0^{SL} = 39.0625$
$n_{\rm res}^S = 0.4$	$n_{ m res}^S=0.1$
$n_{ m res}^F=0.1$	$n_{ m res}^F=0.1$

 Table 4.1: Parameters for the ansatz given in (4.151)
 (4.151)

The parameters for case (a), cf. Figure 4.9, are utilised for the simulation shown in **Section 6.1**, whereas the parameters for case (b), cf. Figure 4.9, are utilised for the simulation shown in **Section 6.2**.



**Figure 4.9:** Effective permeability coefficient  $\kappa^{SL}$  as a function of the solid volume fraction representing the degree of hydration of the tissue cells. Note that in (a), the water content of the solid skeleton is rather moderate, whereas in (b), the water content of the solid skeleton is high.

Furthermore, in (4.150)  $\omega$  is the volume-specific surface area of the cells in natural conditions through which the cell dehydrates. Note that the kinetic energy terms in (4.150) will be ignored for the numerical examples presented in this monograph as their impact is negligible.

Note in passing that the formulation of the cell dehydration (4.150) is very similar to the standard formulation for cell dehydration and rehydration (2.2) in most biology-based articles, compare, for example [111, 177], which has been also discussed in **Chapter 2**.

### 4.8 Adapted balance relations

In general, for a quaternary model with a common temperature for all constituents, four mass balances can be set up, four balance relations for linear momentum, four balance relations for angular momentum and one energy balance for the overall aggregate. However, when *Cauchy* continua are considered, the balance relations for angular momentum are

automatically fulfilled due to the underlying symmetry of the *Cauchy* stress tensors  $\mathbf{T}^{\alpha}$ . Furthermore, since the ice is assumed to be kinematically coupled to the solid skeleton, the balance relation of linear momentum for the ice does not need to be evaluated seperately, since the motion of the ice is already defined by the actual motion of the solid skeleton, when its initial solid motion until phase transition starts is considered, as introduced in **Subsection 3.3.4**. Therefore, the governing balance relations with the corresponding primary variables, which are solved with the indicated equation, are given as follows.

- 1. Momentum balance of the overall aggregare, cf. (4.154)  $\longrightarrow$   $\mathbf{u}_S$
- 2. Mass balance of the liquid in the macro-pore space, cf. (4.156)  $\longrightarrow p^{LR}$
- 3. Mass balance of the gas in the macro-pore space, cf. (4.157)  $\longrightarrow p^{GR}$
- 4. Mass balance of the solid skeleton, cf. (4.158)  $\longrightarrow n^S$
- 5. Mass balance of the solid ice, cf. (4.159)  $\longrightarrow n^{I}$
- 6. Energy balance of the overall aggregate, cf. (4.161)  $\longrightarrow \theta$

Additionally, with appropriate assumptions regarding the fluid flow within the macro-pore space, the filter velocities  $n^{\beta} \mathbf{w}_{\beta}$  are determined directly (and not with weak forms) via the respective momentum balance.

- 1. Momentum balance of the liquid in the macro-pore space, cf. (4.99)  $\longrightarrow n^L \mathbf{w}_L$
- 2. Momentum balance of the gas in the macro-pore space, cf. (4.104)  $\longrightarrow n^G \mathbf{w}_G$

With the introduced assumptions and considerations thus far, the adapted strong forms of the governing equations of the quaternary model are specified below.

The balance of linear momentum of the overall aggregate  $\varphi$  is derived by summing up the individual momentum balances  $(3.58)_2$  of the respective constituents  $\varphi^{\alpha}$ . In the case of quasi-static conditions, this results in

$$\mathbf{0} = \sum_{\alpha} [\operatorname{div} \mathbf{T}^{\alpha} + \rho^{\alpha} \, \mathbf{g} + \hat{\mathbf{p}}^{\alpha}].$$
(4.152)

Therein, the summation yields with  $(3.9)_3$ , (3.10),  $(3.57)_1$ ,  $(3.57)_2$  and  $(3.59)_1$ 

$$\sum_{\alpha} \mathbf{T}^{\alpha} = \mathbf{T}^{S} + \mathbf{T}^{I} + \mathbf{T}^{L} + \mathbf{T}^{G},$$

$$\sum_{\alpha} \rho^{\alpha} = n^{S} \rho^{SR} + n^{I} \rho^{IR} + n^{L} \rho^{LR} + n^{G} \rho^{GR} =: \rho,$$

$$\sum_{\alpha} \hat{\mathbf{p}}^{\alpha} = \sum_{\alpha} (\mathbf{s}^{\alpha} - \hat{\rho}^{\alpha} \mathbf{x}_{\alpha}') = \hat{\rho}^{S} \mathbf{w}_{L} + \hat{\rho}^{I} \mathbf{w}_{L}.$$
(4.153)

Finally, this results in the momentum balance of the overall aggregate  $\varphi$ 

$$\mathbf{0} = \operatorname{div} \left( \mathbf{T}^{S} + \mathbf{T}^{I} + \mathbf{T}^{L} + \mathbf{T}^{G} \right) + \rho \,\mathbf{g} + \hat{\rho}^{S} \,\mathbf{w}_{L} + \hat{\rho}^{I} \,\mathbf{w}_{L}.$$
(4.154)

Note in passing that the overall *Cauchy* stress **T** is defined in  $(3.60)_5$ . The sum of the partial stresses is given via

$$\sum_{\alpha} \mathbf{T}^{\alpha} = \mathbf{T}^{S} + \mathbf{T}^{I} + \mathbf{T}^{L} + \mathbf{T}^{G} = \mathbf{T}^{S}_{E \operatorname{mech}} + \mathbf{T}^{I}_{E \operatorname{mech}} - n^{I} E_{\operatorname{fus}} \left(\theta^{I}_{0I} - \theta\right) \mathbf{I} - p^{FR} \mathbf{I}.$$
(4.155)

The mass balances are stated for each constituent according to  $(3.58)_1$ . The mass balance of the liquid water in the macro-pore space is given via

$$(n^{L})'_{S} \rho^{LR} + n^{L} (\rho^{LR})'_{S} + \operatorname{div} (n^{L} \rho^{LR} \mathbf{w}_{L}) + n^{L} \rho^{LR} \operatorname{div} (\mathbf{u}_{S})'_{S} = \hat{\rho}^{L}, \qquad (4.156)$$

when the transformation rule for material derivatives (3.22) is applied. Since  $(3.57)_1$  requires the sum of the mass production terms to vanish,  $\hat{\rho}^L = -\hat{\rho}^S - \hat{\rho}^I$  holds. Since the gaseous constituent is not interacting with the other constituents in terms of mass, i. e.  $\hat{\rho}^G = 0, (3.58)_1$  simplifies to

$$(n^{G})'_{S}\rho^{GR} + n^{G}(\rho^{GR})'_{S} + \operatorname{div}(n^{G}\rho^{GR}\mathbf{w}_{G}) + n^{G}\rho^{GR}\operatorname{div}(\mathbf{u}_{S})'_{S} = 0.$$
(4.157)

For the solid skeleton, the mass balance reads due to the mass interaction and the temperature dependency of the density  $\rho^{SR}$ , viz.:

$$(n^{S})'_{S} \rho^{SR} + n^{S} (\rho^{SR})'_{S} + n^{S} \rho^{SR} \operatorname{div} (\mathbf{u}_{S})'_{S} = \hat{\rho}^{S}.$$
(4.158)

The mass balance of the ice is given, when additionally the kinematic coupling (3.37) is taken into consideration, via

$$(n^{I})'_{S} \rho^{IR} + n^{I} (\rho^{IR})'_{S} + n^{I} \rho^{IR} \operatorname{div} (\mathbf{u}_{S})'_{S} = \hat{\rho}^{I}.$$
(4.159)

Furthermore, the energy balance of the overall aggregate  $\varphi$  will be utilised, since there is a common temperature  $\theta$ . It is obtained by summing up the respective energy balances (3.58)<sub>4</sub> of the constituents  $\varphi^{\alpha}$ , viz.:

$$\sum_{\alpha} \rho^{\alpha} (\varepsilon^{\alpha})'_{\alpha} = \sum_{\alpha} [\mathbf{T}^{\alpha} \cdot \mathbf{L}_{\alpha} - \operatorname{div} \mathbf{q}^{\alpha} + \rho^{\alpha} r^{\alpha} - \hat{\mathbf{p}}^{\alpha} \cdot \mathbf{x}'_{\alpha} - \hat{\rho}^{\alpha} (\varepsilon^{\alpha} + \frac{1}{2} \mathbf{x}'_{\alpha} \cdot \mathbf{x}'_{\alpha})]. \quad (4.160)$$

Therein, the direct energy production  $\hat{\varepsilon}^{\alpha}$  has been replaced by  $(3.59)_3$ , when condition  $(3.57)_4$  for the overall energy production is used. There is still energy exchange due to frictional interactions of the constituents in  $\hat{\mathbf{p}}^{\alpha} \cdot \mathbf{\dot{x}}_{\alpha}$  and energy exchange that goes along with mass interactions in the term  $\hat{\rho}^{\alpha}(\varepsilon^{\alpha} + \frac{1}{2} \mathbf{\dot{x}}_{\alpha} \cdot \mathbf{\dot{x}}_{\alpha})$ . According to the introduced preliminary assumptions, effects due to radiation are neglected, i. e. (4.7), such that the strong formulation of the energy balance is given via

$$\rho^{S}(\varepsilon^{S})'_{S} + \rho^{I}(\varepsilon^{I})'_{S} + \rho^{L}(\varepsilon^{L})'_{L} + \rho^{G}(\varepsilon^{G})'_{G} = \mathbf{T}^{S}_{E \operatorname{mech}} \cdot \mathbf{L}_{S} + \mathbf{T}^{I}_{E \operatorname{mech}} \cdot \mathbf{L}_{S} - p^{FR} \operatorname{div}(\mathbf{u}_{S})'_{S} - n^{I}E_{\operatorname{fus}}(\theta^{I}_{0I} - \theta) \operatorname{div}(\mathbf{u}_{S})'_{S} + n^{L}\operatorname{grad} p^{LR} \cdot \mathbf{w}_{L} + n^{G}\operatorname{grad} p^{GR} \cdot \mathbf{w}_{G} - \operatorname{div}(\mathbf{q}^{S} + \mathbf{q}^{I} + \mathbf{q}^{L} + \mathbf{q}^{G} + n^{L}p^{LR}\mathbf{w}_{L} + n^{G}p^{GR}\mathbf{w}_{G}) - n^{F}p^{C}\operatorname{grad} s^{L} \cdot \mathbf{w}_{L} - \hat{\mathbf{p}}^{L}_{E\operatorname{dis}} \cdot \mathbf{w}_{L} - \hat{\mathbf{p}}^{G}_{E} \cdot \mathbf{w}_{G} - \rho^{S}(\varepsilon^{S} + \frac{1}{2}\mathbf{x}'_{S} \cdot \mathbf{x}'_{S} - \varepsilon^{L} - \frac{1}{2}\mathbf{x}'_{L} \cdot \mathbf{x}'_{L}) - \hat{\rho}^{I}(\varepsilon^{I} + \frac{1}{2}\mathbf{x}'_{S} \cdot \mathbf{x}'_{S} - \varepsilon^{L} - \frac{1}{2}\mathbf{x}'_{L} \cdot \mathbf{x}'_{L}).$$

$$(4.161)$$

## 4.9 Reduced model

### 4.9.1 Motivation

As outlined in **Subsection 3.2.1**, two TPM models are introduced to assess the impact of ice formation on plant tissues. This allows to make a distinction between localised and rather dispersed ice. In this section, the impact of localised ice formation is treated. For the case of local ice accumulation within more extensive intercellular spaces, as for example in *Equisetum hyemale* [167], the impact of ice formation onto the porous tissue aggregate can be modelled by imposing appropriate boundary conditions at the locations of ice formation. These are specifically *Dirichlet* water pressure boundary conditions that are based on experimental investigations. Thus, this section aims at assessing the water management of plant tissues in a freezing environment with a focus on the water status with respect to both porosity scales.

Note that the reduced model, which is shortly addressed within this section, is accompanied by the proof of thermodynamic consistency in **Appendix A**. The corresponding results are presented in **Section 6.2**.

### 4.9.2 Discussion of the reduced quasi-double-porosity model

The (reduced) ternary modelling approach applied to the thermo-hydro-mechanical processes in plant tissues allows for the simulation of the water management and especially of the cell dehydration, which is regarded as the crucial mechanism of frost resistance. In particular, the model proceeds from a solid skeleton  $\varphi^S$  and two fluids in the macro-pore space, which are liquid water  $\varphi^L$  and gaseous air  $\varphi^G$ , with the properties discussed in previous sections of this chapter, see Figure 4.10.

Note that the considerations regarding the homogenisation of Model I apply also to Model II, however, for the reduced number of constituents. Thus,

$$\varphi = \bigcup_{\alpha} \varphi^{\alpha} = \varphi^{S} \cup \varphi^{L} \cup \varphi^{G}, \qquad (4.162)$$

where the saturation condition holds:

$$\sum_{\alpha} n^{\alpha} = n^{S} + n^{L} + n^{G} = 1.$$
(4.163)

Note, furthermore, that the considerations and assumptions in **Chapter 3** and **Chapter 4** thus far are valid, however, for the reduced set of constituents, cf. (4.162). The interested reader will notice in the remainder of this monograph that Model I is downward compatible, meaning that neglecting the quantities related to the ice will lead to Model II. This indicates particularly, that in the set of the governing equations (4.152)-(4.161) of the quaternary model, the quantities related to the ice vanish to obtain the governing equations (4.165)-(4.169) of the ternary model, such that

$$n^{I} = 0, \qquad (n^{I})'_{S} = 0, \qquad \rho^{IR} = 0, \qquad (\rho^{IR})'_{S} = 0, \qquad \hat{\rho}^{I} = 0,$$
  
$$\mathbf{T}^{I} = \mathbf{0}, \qquad \mathbf{T}^{I}_{E \,\mathrm{mech}} = \mathbf{0}, \qquad \varepsilon^{I} = 0, \qquad (\varepsilon^{I})'_{S} = 0, \qquad \mathbf{q}^{I} = \mathbf{0}.$$
  
(4.164)



**Figure 4.10:** *REV* with schematically shown microstructure and resulting macroscopic ternary TPM model specifying the volume fractions.

Consequently, the mass balance of the ice (4.159) as part of the quaternary model is omitted for the ternary model.

### 4.9.3 Set of governing equations

For the ternary model with a common temperature for all constituents, there are three mass balances, one for each constituent, three balance relations of linear momentum, from which the one of the overall aggregate will be utilised as well as the two fluid momentum balances to determine the state of motion of the respective constituent and, finally, the energy balance of the overall aggregate is necessary. In detail, the following set of governing balance equations will be utilised to solve the indicated primary variables.

- 1. Momentum balance of the overall aggregate, cf. (4.165)  $\longrightarrow$   $\mathbf{u}_S$
- 2. Mass balance of the liquid in the macro-pore space, cf. (4.166)  $\longrightarrow p^{LR}$
- 3. Mass balance of the gas in the macro-pore space, cf. (4.167)  $\longrightarrow p^{GR}$
- 4. Mass balance of the solid skeleton, cf. (4.168)  $\longrightarrow n^S$
- 5. Energy balance of the overall aggregate, cf. (4.169)  $\longrightarrow \theta$

For the sake of completeness, the relevant balance equations are stated also for the ternary model, however, without derivations in order to omit too much repetition. Therefore, the momentum balance of the overall aggregate  $\varphi$  is given by the sum of the constituent-specific equations via

$$\mathbf{0} = \operatorname{div}\left(\mathbf{T}_{E \operatorname{mech}}^{S} - p^{FR}\mathbf{I}\right) + \rho \,\mathbf{g} + \hat{\rho}^{S} \,\mathbf{w}_{L}.$$
(4.165)

The strong formulations of the constituent-specific balance relations of mass are given via

$$(n^{L})'_{S} \rho^{LR} + n^{L} (\rho^{LR})'_{S} + \operatorname{div} (n^{L} \rho^{LR} \mathbf{w}_{L}) + n^{L} \rho^{LR} \operatorname{div} (\mathbf{u}_{S})'_{S} = \hat{\rho}^{L}, \qquad (4.166)$$

for the liquid in the macro-pore space, yielding the same equation as for the quaternary model, which is also valid for the gas phase, viz.:

$$(n^{G})'_{S}\rho^{GR} + n^{G}(\rho^{GR})'_{S} + \operatorname{div}(n^{G}\rho^{GR}\mathbf{w}_{G}) + n^{G}\rho^{GR}\operatorname{div}(\mathbf{u}_{S})'_{S} = 0.$$
(4.167)

Finally, the mass balance of the solid skeleton reads

$$(n^{S})'_{S} \rho^{SR} + n^{S} (\rho^{SR})'_{S} + n^{S} \rho^{SR} \operatorname{div} (\mathbf{u}_{S})'_{S} = \hat{\rho}^{S}, \qquad (4.168)$$

which is also identical to the one for the quaternary model. The strong formulation of the energy balance of the overall aggregate  $\varphi$  is given via

$$\rho^{S}(\varepsilon^{S})'_{S} + \rho^{L}(\varepsilon^{L})'_{L} + \rho^{G}(\varepsilon^{G})'_{G} - \mathbf{T}^{S}_{E \operatorname{mech}} \cdot \mathbf{L}_{S} + p^{FR} \operatorname{div}(\mathbf{u}_{S})'_{S} - - n^{L} \operatorname{grad} p^{LR} \cdot \mathbf{w}_{L} - n^{G} \operatorname{grad} p^{GR} \cdot \mathbf{w}_{G} + + \operatorname{div}(\mathbf{q}^{S} + \mathbf{q}^{L} + \mathbf{q}^{G} + n^{L} p^{LR} \mathbf{w}_{L} + n^{G} p^{GR} \mathbf{w}_{G}) + + \hat{\mathbf{p}}^{L}_{E \operatorname{dis}} \cdot \mathbf{w}_{L} + n^{F} p^{C} \operatorname{grad} s^{L} \cdot \mathbf{w}_{L} + \hat{\mathbf{p}}^{G}_{E} \cdot \mathbf{w}_{G} + + \hat{\rho}^{S}(\varepsilon^{S} + \frac{1}{2} \mathbf{x}'_{S} \cdot \mathbf{x}'_{S} - \varepsilon^{L} - \frac{1}{2} \mathbf{x}'_{L} \cdot \mathbf{x}'_{L}) = 0.$$

$$(4.169)$$

Additionally, with appropriate assumptions regarding the fluid flow within the macropore space, the filter velocities  $n^{\beta} \mathbf{w}_{\beta}$  are determined directly (and not with their weak formulations) via the respective fluid momentum balance.

- 1. Momentum balance of the liquid in the macro-pore space, cf. (4.170)  $\longrightarrow n^L \mathbf{w}_L$
- 2. Momentum balance of the gas in the macro-pore space, cf. (4.171)  $\longrightarrow n^G \mathbf{w}_G$

These customised balance relations yield for the liquid

$$n^{L}\mathbf{w}_{L} = -\frac{\kappa_{r}^{L}}{\mu^{LR}}\mathbf{K}^{S}\left(\operatorname{grad} p^{LR} - \rho^{LR}\mathbf{g} - \frac{p^{C}}{s^{L}}\operatorname{grad} s^{L} + \frac{\hat{\rho}^{S}}{n^{L}} \mathbf{x}_{S}'\right)$$
(4.170)

and for the gas

$$n^{G}\mathbf{w}_{G} = -\frac{\kappa_{r}^{G}}{\mu^{GR}}\mathbf{K}^{S}\left(\operatorname{grad} p^{GR} - \rho^{GR}\mathbf{g}\right).$$
(4.171)

# Chapter 5: Numerical treatment

As the next step, the derived set of coupled partial differential equations (PDEs) has to be solved, in the case at hand monolithically in order to account for the coupled character of the governing equations. This is done by utilising the Finite-Element Method (FEM), which is the standard tool within solid mechanics. For a comprehensive and mathematically somehow rigorous introduction of the foundations of the FEM, the interested reader is referred to the standard works of Bathe [9], Braess [32], Schwarz [169], Zienkiewicz *et al.* [197]. Nevertheless, in this chapter, the primary variables of initial-boundaryvalue-problems for Model I as well as for Model II are specified and basic considerations regarding the type of boundary conditions are introduced. Furthermore, the weak formulations of the governing equations are introduced for Model I and Model II. Finally, the discretisation in space and time is given for the sake of completeness.

For numerical simulations, the in-house FE tool PANDAS is utilised. The tool has been implemented and set up by Ammann [3], Eipper [63], Ellsiepen [65] and extended since then in application to a variety of topics.

Note that this chapter provides a summary of the necessary steps and considerations in terms of the numerical procedure, as described in Häberle [89], Koch [104], Wagner [187], however, here in application to the solution of initial-boundary-value problems within plant biomechanics.

### 5.1 Application of the Finite-Element Method

In order to formulate meaningful initial-boundary-value problems, two sets of primary variables are defined corresponding to Model I and Model II. Therefore, the two sets of primary variables,  $\mathbf{u}_1$  and  $\mathbf{u}_2$ , are given via

$$\boldsymbol{u}_{1} = [\boldsymbol{u}_{S}, p^{LR}, p^{GR}, n^{S}, n^{I}, \theta]^{T}, \quad \boldsymbol{u}_{2} = [\boldsymbol{u}_{S}, p^{LR}, p^{GR}, n^{S}, \theta]^{T},$$
(5.1)

where  $u_1$  corresponds to Model I and  $u_2$  to Model II. Generally, regarding the use of the constituent-specific mass balances, one might also consider to state the turgor pressure  $p^{FR}$  as one of the primary variables in combination with one of the fluid pressures  $p^{\beta R}$  or a saturation  $s^{\beta}$ . However, in the context of an investigation of plants at subzero temperatures, the water pressure  $p^{LR}$  as one of the unknown fields (to address the no-flux condition of Model I or the drop in water pressure in application to Model II, compare **Chapter 6**) and the gas pressure  $p^{GR}$  as another primary variable (to prescribe the gas pressure as the ambient pressure, compare **Chapter 6**) is much more sensible. Furthermore, the solid volume fractions  $n^{\delta}$  have to introduced as unknown fields due to the non-vanishing mass-interaction term in (4.18).

Then, boundary conditions have to be defined corresponding to the primary variables,

this is done solely for the more general Model I in order to avoid too much repetition. For each of the primary variables, the boundary  $\partial\Omega$  of the spatial domain  $\Omega$  is partitioned into an (essential) *Dirichlet* boundary  $\partial\Omega_D$  to address the primary variable itself and a (natural) *Neumann* boundary  $\partial\Omega_N$  to address the corresponding flux, where the following applies, viz.:

$$\partial \Omega_{\mathbf{u}_{S}} = \partial \Omega_{D}^{\mathbf{u}_{S}} \cup \partial \Omega_{N}^{\tilde{\mathbf{t}}}, \qquad \emptyset = \partial \Omega_{D}^{\mathbf{u}_{S}} \cap \partial \Omega_{N}^{\tilde{\mathbf{t}}}, 
\partial \Omega_{p^{LR}} = \partial \Omega_{D}^{p^{LR}} \cup \partial \Omega_{N}^{\tilde{m}^{L}}, \qquad \emptyset = \partial \Omega_{D}^{p^{LR}} \cap \partial \Omega_{N}^{\tilde{m}^{L}}, 
\partial \Omega_{p^{GR}} = \partial \Omega_{D}^{p^{GR}} \cup \partial \Omega_{N}^{\tilde{m}^{G}}, \qquad \emptyset = \partial \Omega_{D}^{p^{GR}} \cap \partial \Omega_{N}^{\tilde{m}^{G}}, 
\partial \Omega_{n^{S}} = \partial \Omega_{D}^{n^{S}} \cup \partial \Omega_{N}^{\tilde{v}^{S}}, \qquad \emptyset = \partial \Omega_{D}^{n^{S}} \cap \partial \Omega_{N}^{\tilde{v}^{S}}, 
\partial \Omega_{n^{I}} = \partial \Omega_{D}^{n^{I}} \cup \partial \Omega_{N}^{\tilde{v}^{I}}, \qquad \emptyset = \partial \Omega_{D}^{n^{I}} \cap \partial \Omega_{N}^{\tilde{v}^{I}}, 
\partial \Omega_{\theta} = \partial \Omega_{D}^{\theta} \cup \partial \Omega_{N}^{\tilde{q}}, \qquad \emptyset = \partial \Omega_{D}^{\theta} \cap \partial \Omega_{N}^{\tilde{q}}.$$
(5.2)

From the right column of (5.2) it is seen, that the respective boundaries, denoted by the placeholder  $\partial \Omega_D$  and  $\partial \Omega_N$ , of the corresponding primary variables are mutually exclusive meaning that you have to define one of them, but cannot define both of them. The respective flux at the *Neumann* boundary is further discussed in **Section 5.2**.

### 5.2 Weak formulations of the governing equations

As the FEM is utilised, the ansatz (or trial) spaces  $\mathcal{A}$  as well as the test spaces  $\mathcal{T}$  have to be defined for the corresponding primary variables. Therefore, the respective ansatz spaces are given via

$$\begin{aligned}
\mathcal{A}^{\mathbf{u}_{S}}(t) &:= \{ \mathbf{u}_{S} \in \mathcal{H}^{1}(\Omega)^{d} : \mathbf{u}_{S}(\mathbf{x},t) = \bar{\mathbf{u}}_{S}(\mathbf{x},t) \text{ on } \partial\Omega_{D}^{\mathbf{u}_{S}} \}, \\
\mathcal{A}^{p^{LR}}(t) &:= \{ p^{LR} \in \mathcal{H}^{1}(\Omega) : p^{LR}(\mathbf{x},t) = \bar{p}^{LR}(\mathbf{x},t) \text{ on } \partial\Omega_{D}^{p^{LR}} \}, \\
\mathcal{A}^{p^{GR}}(t) &:= \{ p^{GR} \in \mathcal{H}^{1}(\Omega) : p^{GR}(\mathbf{x},t) = \bar{p}^{GR}(\mathbf{x},t) \text{ on } \partial\Omega_{D}^{p^{GR}} \}, \\
\mathcal{A}^{n^{S}}(t) &:= \{ n^{S} \in \mathcal{H}^{1}(\Omega) : n^{S}(\mathbf{x},t) = \bar{n}^{S}(\mathbf{x},t) \text{ on } \partial\Omega_{D}^{n^{S}} \}, \\
\mathcal{A}^{n^{I}}(t) &:= \{ n^{I} \in \mathcal{H}^{1}(\Omega) : n^{I}(\mathbf{x},t) = \bar{n}^{I}(\mathbf{x},t) \text{ on } \partial\Omega_{D}^{n^{I}} \}, \\
\mathcal{A}^{\theta}(t) &:= \{ \theta \in \mathcal{H}^{1}(\Omega) : \theta(\mathbf{x},t) = \bar{\theta}(\mathbf{x},t) \text{ on } \partial\Omega_{D}^{\theta} \}
\end{aligned}$$
(5.3)

and the respective test spaces are given via

$$\mathcal{T}^{\mathbf{u}_{S}} := \{ \delta \mathbf{u}_{S} \in \mathcal{H}^{1}(\Omega)^{d} : \delta \mathbf{u}_{S}(\mathbf{x}) = \mathbf{0} \text{ on } \partial \Omega_{D}^{\mathbf{u}_{S}} \},$$

$$\mathcal{T}^{p^{LR}} := \{ \delta p^{LR} \in \mathcal{H}^{1}(\Omega) : \delta p^{LR}(\mathbf{x}) = 0 \text{ on } \partial \Omega_{D}^{p^{LR}} \},$$

$$\mathcal{T}^{p^{GR}} := \{ \delta p^{GR} \in \mathcal{H}^{1}(\Omega) : \delta p^{GR}(\mathbf{x}) = 0 \text{ on } \partial \Omega_{D}^{p^{GR}} \},$$

$$\mathcal{T}^{n^{S}} := \{ \delta n^{S} \in \mathcal{H}^{1}(\Omega) : \delta n^{S}(\mathbf{x}) = 0 \text{ on } \partial \Omega_{D}^{n^{S}} \},$$

$$\mathcal{T}^{n^{I}} := \{ \delta n^{I} \in \mathcal{H}^{1}(\Omega) : \delta n^{I}(\mathbf{x}) = 0 \text{ on } \partial \Omega_{D}^{n^{I}} \},$$

$$\mathcal{T}^{\theta} := \{ \delta \theta \in \mathcal{H}^{1}(\Omega) : \delta \theta(\mathbf{x}) = 0 \text{ on } \partial \Omega_{D}^{\theta} \}.$$

$$(5.4)$$

Therein,  $\mathcal{H}^1$  represents the *Sobolev* space in order to ensure square-integrability for the involved ansatz and test functions as well as for their gradients. Furthermore,  $d \in \{1, 2, 3\}$  represents the dimension of the physical problem, for the numerical examples presented in **Chapter 6**, there are generally three dimensions considered, i. e. d = 3. Note that the respective primary variable equals the corresponding ansatz function at the *Dirichlet* boundary, the test function, however, vanishes at the corresponding *Dirichlet* boundary.

### 5.2.1 Quaternary model with ice formation

The strong formulations of the governing equations of the quaternary model are given in (4.154), (4.156), (4.157), (4.158), (4.159) and (4.161). For the solution of the set of primary variables  $\mathbf{u}_1$ , these strong formulations need to be transferred into their respective weak formulation. These are obtained by multiplying the strong formulation with the respective test function  $\delta \mathbf{u}_S$ ,  $\delta p^{LR}$ ,  $\delta p^{GR}$ ,  $\delta n^S$ ,  $\delta n^I$  and  $\delta \theta$ , and a subsequent integration over the domain  $\Omega$ . In particular, the weak formulation of the momentum balance of the overall aggregate  $\varphi$  is obtained by multiplying (4.154) with  $\delta \mathbf{u}_S$ , which results after some manipulations in

$$\mathcal{G}_{\mathbf{u}_{S}}(\boldsymbol{u}_{1},\delta\mathbf{u}_{S}) \equiv \int_{\Omega} (\mathbf{T}_{E\,\mathrm{mech}}^{S} + \mathbf{T}_{E\,\mathrm{mech}}^{I} - n^{I}E_{\mathrm{fus}}\left(\theta_{0I}^{I} - \theta\right)\mathbf{I} - p^{FR}\mathbf{I}) \cdot \mathrm{grad}\,\delta\mathbf{u}_{S}\,\mathrm{d}v - \int_{\Omega} (\rho\,\mathbf{g} + \hat{\rho}^{S}\mathbf{w}_{L} + \hat{\rho}^{I}\mathbf{w}_{L}) \cdot \delta\mathbf{u}_{S}\,\mathrm{d}v - \int_{\partial\Omega_{N}^{\tilde{\mathbf{t}}}} \tilde{\mathbf{t}} \cdot \delta\mathbf{u}_{S}\,\mathrm{d}a = 0,$$

$$(5.5)$$

where  $\tilde{\mathbf{t}} = (\mathbf{T}^S + \mathbf{T}^I + \mathbf{T}^L + \mathbf{T}^G) \mathbf{n}$  is the stress vector acting at the *Neumann* boundary  $\partial \Omega_N^{\tilde{\mathbf{t}}}$  of the porous aggregate  $\Omega$ . With regard to the primary variables  $p^{LR}$ ,  $p^{GR}$ ,  $n^S$  and  $n^I$ , the corresponding weak formulation of the mass balances are obtained in a similar
way and are given via

$$\begin{aligned} \mathcal{G}_{p^{LR}}(\boldsymbol{u}_{1},\delta p^{LR}) &\equiv \int_{\Omega} \left[ (n^{L})'_{S} \,\rho^{LR} + n^{L} (\rho^{LR})'_{S} + \rho^{L} \operatorname{div} (\mathbf{u}_{S})'_{S} - \hat{\rho}^{L} \right] \delta p^{LR} \,\mathrm{d}v - \\ &- \int_{\Omega} \rho^{L} \mathbf{w}_{L} \cdot \operatorname{grad} \delta p^{LR} \,\mathrm{d}v + \int_{\partial \Omega_{N}^{\tilde{m}^{L}}} \tilde{m}^{L} \delta p^{LR} \,\mathrm{d}a = 0, \\ \mathcal{G}_{p^{GR}}(\boldsymbol{u}_{1},\delta p^{GR}) &\equiv \int_{\Omega} \left[ (n^{G})'_{S} \,\rho^{GR} + n^{G} (\rho^{GR})'_{S} + \rho^{G} \operatorname{div} (\mathbf{u}_{S})'_{S} \right] \delta p^{GR} \,\mathrm{d}v - \\ &- \int_{\Omega} \rho^{G} \mathbf{w}_{G} \cdot \operatorname{grad} \delta p^{GR} \,\mathrm{d}v + \int_{\partial \Omega_{N}^{\tilde{m}^{G}}} \tilde{m}^{G} \delta p^{GR} \,\mathrm{d}a = 0, \end{aligned}$$

$$\mathcal{G}_{n^{S}}(\boldsymbol{u}_{1},\delta n^{S}) \equiv \int_{\Omega} [(n^{S})'_{S} + \frac{n^{S}}{\rho^{SR}}(\rho^{SR})'_{S} - \frac{\hat{\rho}^{S}}{\rho^{SR}} - (\mathbf{u}_{S})'_{S} \cdot \operatorname{grad} n^{S}] \,\delta n^{S} \,\mathrm{d}v - - \int_{\Omega} n^{S}(\mathbf{u}_{S})'_{S} \cdot \operatorname{grad} \delta n^{S} \,\mathrm{d}v + \int_{\partial \Omega_{N}^{\tilde{\nu}^{S}}} \tilde{\nu}^{S} \delta n^{S} \,\mathrm{d}a = 0,$$
(5.6)

$$\mathcal{G}_{n^{I}}(\boldsymbol{u}_{1},\delta n^{I}) \equiv \int_{\Omega} [(n^{I})'_{S} + \frac{n^{I}}{\rho^{IR}}(\rho^{IR})'_{S} - \frac{\hat{\rho}^{I}}{\rho^{IR}} - (\mathbf{u}_{S})'_{S} \cdot \operatorname{grad} n^{I}] \,\delta n^{I} \,\mathrm{d}v - \int_{\Omega} n^{I}(\mathbf{u}_{S})'_{S} \cdot \operatorname{grad} \delta n^{I} \,\mathrm{d}v + \int_{\partial \Omega_{N}^{\tilde{\nu}^{I}}} \tilde{\nu}^{I} \delta n^{I} \,\mathrm{d}a = 0.$$

Therein,  $\tilde{m}^{\beta} = \rho^{\beta} \mathbf{w}_{\beta} \cdot \mathbf{n}$  is the fluid mass efflux through the Neumann boundary  $\partial \Omega_N^{\tilde{m}^{\beta}}$ . Regarding the solid skeleton and the ice, there is no volume flux through the Neumann boundary  $\partial \Omega_N^{\tilde{v}^{\delta}}$  that has to be considered, therefore,  $\tilde{v}^S = n^S(\mathbf{u}_S)'_S \cdot \mathbf{n} = 0$  as well as  $\tilde{v}^I = n^I(\mathbf{u}_S)'_S \cdot \mathbf{n} = 0$ , which is due to the Lagrangean formulation of the solid skeleton and the ice (via its kinematic coupling to the solid skeleton). In contrast, the introduced mass efflux of the fluids  $\tilde{m}^{\beta}$  is generally non-vanishing due to the modified Eulerian description with an Eulerian domain that deforms with the solid skeleton, cf. [67]. Finally, the temperature  $\theta$  is determined using the weak formulation of the energy balance of the overall aggregate  $\varphi$ . Thus,

$$\begin{aligned} \mathcal{G}_{\theta}(\boldsymbol{u}_{1},\delta\theta) &\equiv \int_{\Omega} \left[ \rho^{S}(\varepsilon^{S})_{S}' + \rho^{I}(\varepsilon^{I})_{S}' + \rho^{L}(\varepsilon^{L})_{L}' + \rho^{G}(\varepsilon^{G})_{G}' - \right. \\ &\left. - \mathbf{T}_{E\,\mathrm{mech}}^{S} \cdot \mathbf{L}_{S} - \mathbf{T}_{E\,\mathrm{mech}}^{I} \cdot \mathbf{L}_{S} + p^{FR} \operatorname{div}(\mathbf{u}_{S})_{S}' + \right. \\ &\left. + n^{I}E_{\mathrm{fus}}\left(\theta_{0I}^{I} - \theta\right) \operatorname{div}(\mathbf{u}_{S})_{S}' - n^{L} \mathrm{grad} p^{LR} \cdot \mathbf{w}_{L} - n^{G} \mathrm{grad} p^{GR} \cdot \mathbf{w}_{G} + \right. \\ &\left. + n^{F}p^{C} \mathrm{grad} s^{L} \cdot \mathbf{w}_{L} + \hat{\mathbf{p}}_{E\,\mathrm{dis}}^{L} \cdot \mathbf{w}_{L} + \hat{\mathbf{p}}_{E}^{G} \cdot \mathbf{w}_{G} + \right. \\ &\left. + \hat{\rho}^{S}(\varepsilon^{S} + \frac{1}{2} \, \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \varepsilon^{L} - \frac{1}{2} \, \mathbf{x}_{L} \cdot \mathbf{x}_{L}) + \right. \\ &\left. + \hat{\rho}^{I}(\varepsilon^{I} + \frac{1}{2} \, \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \varepsilon^{L} - \frac{1}{2} \, \mathbf{x}_{L} \cdot \mathbf{x}_{L}) \right] \delta\theta \, \mathrm{d}v - \right. \\ &\left. - \int_{\Omega} \left( \mathbf{q}^{S} + \mathbf{q}^{I} + \mathbf{q}^{L} + \mathbf{q}^{G} + n^{L} p^{LR} \, \mathbf{w}_{L} + n^{G} p^{GR} \, \mathbf{w}_{G} \right) \cdot \mathrm{grad} \, \delta\theta \, \mathrm{d}v + \right. \\ &\left. + \int_{\partial\Omega_{N}^{\tilde{q}}} \tilde{q} \, \delta\theta \, \mathrm{d}a = 0. \end{aligned}$$

$$\tag{5.7}$$

Therein, the heat flux  $\tilde{q} = (\mathbf{q}^S + \mathbf{q}^I + \mathbf{q}^L + \mathbf{q}^G + n^L p^{LR} \mathbf{w}_L + n^G p^{GR} \mathbf{w}_G) \cdot \mathbf{n}$  is defined at the *Neumann* boundary  $\partial \Omega_N^{\tilde{q}}$ .

### 5.2.2 Ternary (reduced) model

The procedure to obtain the weak formulations of the governing equations of the reduced model is generally the same, however, the notions in **Section 4.9** need to be considered. Therefore, the strong formulations (4.165)-(4.169) are transformed into their weak counterparts by multiplying them with the corresponding test functions and a subsequent integration over the domain  $\Omega$ . For the case of the momentum balance of the overall aggregate  $\varphi$ , the weak formulation is given via

$$\mathcal{G}_{\mathbf{u}_{S}}(\boldsymbol{u}_{2},\delta\mathbf{u}_{S}) \equiv \int_{\Omega} (\mathbf{T}_{E\,\mathrm{mech}}^{S} - p^{FR}\mathbf{I}) \cdot \operatorname{grad} \delta\mathbf{u}_{S} \,\mathrm{d}v - \int_{\Omega} (\rho\,\mathbf{g} + \hat{\rho}^{S}\mathbf{w}_{L}) \cdot \delta\mathbf{u}_{S} \,\mathrm{d}v - \int_{\Omega} \mathbf{\tilde{t}} \cdot \delta\mathbf{u}_{S} \,\mathrm{d}a = 0,$$

$$(5.8)$$

where  $\tilde{\mathbf{t}} = (\mathbf{T}^S + \mathbf{T}^L + \mathbf{T}^G) \cdot \mathbf{n}$  is the stress vector acting at the Neumann boundary  $\partial \Omega_N^{\tilde{\mathbf{t}}}$  of the domain  $\Omega$ . Furthermore, the respective mass balances in their weak formulation

are given via

$$\mathcal{G}_{p^{LR}}(\boldsymbol{u}_2, \delta p^{LR}) \equiv \int_{\Omega} \left[ (n^L)'_S \, \rho^{LR} + n^L (\rho^{LR})'_S + \rho^L \operatorname{div} (\mathbf{u}_S)'_S + \hat{\rho}^S \right] \delta p^{LR} \, \mathrm{d}v - \\ - \int_{\Omega} \rho^L \mathbf{w}_L \cdot \operatorname{grad} \delta p^{LR} \, \mathrm{d}v + \int_{\partial \Omega_N^{\tilde{m}L}} \tilde{m}^L \delta p^{LR} \, \mathrm{d}a = 0,$$

$$\mathcal{G}_{p^{GR}}(\boldsymbol{u}_{2},\delta p^{GR}) \equiv \int_{\Omega} \left[ (n^{G})_{S}^{\prime} \rho^{GR} + n^{G} (\rho^{GR})_{S}^{\prime} + \rho^{G} \operatorname{div}(\mathbf{u}_{S})_{S}^{\prime} \right] \delta p^{GR} \, \mathrm{d}v - \int_{\Omega} \rho^{G} \mathbf{w}_{G} \cdot \operatorname{grad} \delta p^{GR} \, \mathrm{d}v + \int_{\partial \Omega_{N}^{\tilde{m}^{G}}} \tilde{m}^{G} \delta p^{GR} \, \mathrm{d}a = 0,$$

$$(5.9)$$

$$\mathcal{G}_{n^{S}}(\boldsymbol{u}_{2},\delta n^{S}) \equiv \int_{\Omega} \left[ (n^{S})_{S}' + \frac{n^{S}}{\rho^{SR}} (\rho^{SR})_{S}' - \frac{\hat{\rho}^{S}}{\rho^{SR}} - (\mathbf{u}_{S})_{S}' \cdot \operatorname{grad} n^{S} \right] \delta n^{S} \, \mathrm{d}v - \int_{\Omega} n^{S} (\mathbf{u}_{S})_{S}' \cdot \operatorname{grad} \delta n^{S} \, \mathrm{d}v + \int_{\partial \Omega_{N}^{\tilde{v}^{S}}} \tilde{v}^{S} \delta n^{S} \, \mathrm{d}a = 0.$$

Therein, the fluid mass flux is accordingly defined via  $\tilde{m}^{\beta} = \rho^{\beta} \mathbf{w}_{\beta} \cdot \mathbf{n}$ , the solid volume flux is zero,  $\tilde{v}^{S} = n^{S}(\mathbf{u}_{S})'_{S} \cdot \mathbf{n} = 0$ , as there is no transport of solid matter through the surface  $\partial \Omega_{N}^{\tilde{v}^{S}}$ . Finally, the energy balance of the overall aggregate  $\varphi$  needs to be posed in its weak formulation, viz.:

$$\begin{aligned} \mathcal{G}_{\theta}(\boldsymbol{u}_{2},\delta\theta) &\equiv \int_{\Omega} \left[ \rho^{S}(\varepsilon^{S})_{S}' + \rho^{L}(\varepsilon^{L})_{L}' + \rho^{G}(\varepsilon^{G})_{G}' - \mathbf{T}_{E\,\mathrm{mech}}^{S} \cdot \mathbf{L}_{S} + \\ &+ p^{FR} \operatorname{div}(\mathbf{u}_{S})_{S}' - n^{L} \operatorname{grad} p^{LR} \cdot \mathbf{w}_{L} - n^{G} \operatorname{grad} p^{GR} \cdot \mathbf{w}_{G} + \\ &+ \hat{\mathbf{p}}_{E\,\mathrm{dis}}^{L} \cdot \mathbf{w}_{L} + n^{F} p^{C} \operatorname{grad} s^{L} \cdot \mathbf{w}_{L} + \hat{\mathbf{p}}_{E}^{G} \cdot \mathbf{w}_{G} + \\ &+ \hat{\rho}^{S}(\varepsilon^{S} + \frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \varepsilon^{L} - \frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L}) \right] \delta\theta \, \mathrm{d}v - \\ &- \int_{\Omega} (\mathbf{q}^{S} + \mathbf{q}^{L} + \mathbf{q}^{G} + n^{L} p^{LR} \mathbf{w}_{L} + n^{G} p^{GR} \mathbf{w}_{G}) \cdot \operatorname{grad} \delta\theta \, \mathrm{d}v + \\ &+ \int_{\partial\Omega_{N}^{\tilde{q}}} \tilde{q} \, \delta\theta \, \mathrm{d}a = 0. \end{aligned}$$

$$(5.10)$$

Therein, the heat efflux  $\tilde{q} = (\mathbf{q}^S + \mathbf{q}^L + \mathbf{q}^G + n^L p^{LR} \mathbf{w}_L + n^G p^{GR} \mathbf{w}_G) \cdot \mathbf{n}$  is defined at the *Neumann* boundary  $\partial \Omega_N^{\tilde{q}}$ .

## 5.3 Discretisation

### 5.3.1 Spatial descretisation

The main idea of the FEM is to approximate the continuous domain  $\Omega$  by  $\Omega^h$ , which is composed of non-overlapping subdomains, the so-called finite elements  $\Omega^e$ , such that

$$\Omega \approx \Omega^h = \bigcup_e \Omega^e, \tag{5.11}$$

where each element  $\Omega^e$  is composed of connected nodal points  $P^j$ . Note the smaller the element  $\Omega^e$ , the smaller the introduced error. The introduction of a discretised domain  $\Omega^h$  requires the introduction of discretised ansatz and test spaces for each primary variable, denoted by  $\mathcal{A}^h$  and  $\mathcal{T}^h$ , respectively. Thus, the discretised ansatz functions are given via

$$\mathbf{u}_{S}(\mathbf{x},t) \approx \mathbf{u}_{S}^{h}(\mathbf{x},t) = \bar{\mathbf{u}}_{S}^{h}(\mathbf{x},t) + \sum_{j=1}^{N} \phi_{\mathbf{u}_{S}}^{j}(\mathbf{x}) \mathbf{u}_{S}^{j}(t) \in \mathcal{A}^{\mathbf{u}_{S}h}(t),$$

$$p^{LR}(\mathbf{x},t) \approx p^{LRh}(\mathbf{x},t) = \bar{p}^{LRh}(\mathbf{x},t) + \sum_{j=1}^{N} \phi_{p^{LR}}^{j}(\mathbf{x}) p^{LRj}(t) \in \mathcal{A}^{p^{LR}h}(t),$$

$$p^{GR}(\mathbf{x},t) \approx p^{GRh}(\mathbf{x},t) = \bar{p}^{GRh}(\mathbf{x},t) + \sum_{j=1}^{N} \phi_{p^{GR}}^{j}(\mathbf{x}) p^{GRj}(t) \in \mathcal{A}^{p^{GR}h}(t),$$

$$n^{S}(\mathbf{x},t) \approx n^{Sh}(\mathbf{x},t) = \bar{n}^{Sh}(\mathbf{x},t) + \sum_{j=1}^{N} \phi_{n^{S}}^{j}(\mathbf{x}) n^{Sj}(t) \in \mathcal{A}^{n^{S}h}(t),$$

$$n^{I}(\mathbf{x},t) \approx n^{Ih}(\mathbf{x},t) = \bar{n}^{Ih}(\mathbf{x},t) + \sum_{j=1}^{N} \phi_{n^{I}}^{j}(\mathbf{x}) n^{Ij}(t) \in \mathcal{A}^{n^{I}h}(t),$$

$$\theta(\mathbf{x},t) \approx \theta^{h}(\mathbf{x},t) = \bar{\theta}^{h}(\mathbf{x},t) + \sum_{j=1}^{N} \phi_{\theta}^{j}(\mathbf{x}) \theta^{j}(t) \in \mathcal{A}^{\theta h}(t).$$
(5.12)

Furthermore, the corresponding discretised test functions are given via

$$\begin{split} \delta \mathbf{u}_{S}(\mathbf{x}) &\approx \delta \mathbf{u}_{S}^{h}(\mathbf{x}) &= \sum_{j=1}^{N} \phi_{\mathbf{u}_{S}}^{j}(\mathbf{x}) \delta \mathbf{u}_{S}^{j} \in \mathcal{T}^{\mathbf{u}_{S}h}, \\ \delta p^{LR}(\mathbf{x}) &\approx \delta p^{LRh}(\mathbf{x}) &= \sum_{j=1}^{N} \phi_{p^{LR}}^{j}(\mathbf{x}) \delta p^{LRj} \in \mathcal{T}^{p^{LR}h}, \\ \delta p^{GR}(\mathbf{x}) &\approx \delta p^{GRh}(\mathbf{x}) &= \sum_{j=1}^{N} \phi_{p^{GR}}^{j}(\mathbf{x}) \delta p^{GRj} \in \mathcal{T}^{p^{GR}h}, \\ \delta n^{S}(\mathbf{x}) &\approx \delta n^{Sh}(\mathbf{x}) &= \sum_{j=1}^{N} \phi_{n^{S}}^{j}(\mathbf{x}) \delta n^{Sj} \in \mathcal{T}^{n^{S}h}, \\ \delta n^{I}(\mathbf{x}) &\approx \delta n^{Ih}(\mathbf{x}) &= \sum_{j=1}^{N} \phi_{n^{I}}^{j}(\mathbf{x}) \delta n^{Ij} \in \mathcal{T}^{n^{I}h}, \\ \delta \theta(\mathbf{x}) &\approx \delta \theta^{h}(\mathbf{x}) &= \sum_{j=1}^{N} \phi_{\theta}^{j}(\mathbf{x}) \delta \theta^{j} \in \mathcal{T}^{\theta h}. \end{split}$$
(5.13)

In (5.12) and (5.13), the set  $\{\bar{\mathbf{u}}_{S}^{h}, \bar{p}^{LRh}, \bar{p}^{GRh}, \bar{n}^{Sh}, \bar{n}^{Ih}, \bar{\theta}^{h}\}$  is defined by the value of the corresponding *Dirichlet* boundary condition. As the *Bubnov-Galerkin* method is utilised, the global basis functions  $\{\phi_{\mathbf{u}_{S}}^{j}, \phi_{p^{LR}}^{j}, \phi_{p^{GR}}^{j}, \phi_{n^{S}}^{j}, \phi_{n^{I}}^{j}, \phi_{\theta}^{j}\}$  apply to the ansatz functions as well as to the test functions, where j = 1, ..., N with in total N number of nodes. Note that the basis functions are equal to one at a certain node and vanish at all other nodes. The application of the so-called partition-of-unity principle requires the sum of all basis functions to be equal to one at each point. Finally, the set of variables  $\{\mathbf{u}_{S}^{j}, p^{LRj}, p^{GRj}, n^{Sj}, n^{Ij}, \theta^{j}\}$  defines the nodal degrees of freedom (DOF). Note that the applied procedure yields a system of  $N \times \text{DOF}$  linearly independent equations.

In order to avoid stability issues that are related to the Ladyzhenskaya-Babuška-Brezzi (LBB) condition, quadratic basis functions are utilised for the solid displacement  $\mathbf{u}_{S}^{h}$ , and linear basis functions for the other unknown fields, specifically for the fluid pressures  $p^{LRh}$  and  $p^{GRh}$ , for the solid volume fractions  $n^{Sh}$  and  $n^{Ih}$  as well as for the temperature  $\theta^{h}$ . This sort of mixed finite element is usually referred to as extended *Taylor-Hood* element, as depicted in Figure 5.1.



Figure 5.1: Extended hexahedral Taylor-Hood element.

Note that an isoparametric concept is applied, meaning that the same ansatz functions are utilised for the displacement as well as for the geometry transformation. A geometry transformation is necessary, as the computations are conducted at the element level. Details regarding the spatial discretisation in the context of the FE tool PANDAS can be found, for example, in Häberle [89], Koch [104], Wagner [187].

### 5.3.2 Temporal discretisation

At this stage of the numerical procedure, the initial-boundary-value problem is spatially discretised, but not yet regarding time. Thus, this semi-discrete numerical problem has the form

$$\mathcal{F}(t, \boldsymbol{y}, \boldsymbol{y}') = [\boldsymbol{D}\boldsymbol{y}' + \boldsymbol{k}(\boldsymbol{y}) - \boldsymbol{f}] \stackrel{!}{=} \boldsymbol{0}.$$
(5.14)

Therein, D is the generalised damping matrix, k(y) is the generalised stiffness vector, and f is the vector of external forces containing the values of the *Neumann* boundary

conditions. Note that  $\boldsymbol{y}$  contains the nodal degrees of freedom and  $\boldsymbol{y}'$  their derivatives. As in the corresponding weak formulations of the governing equations the only derivative is always the one regarding the motion of the solid,  $(\cdot)'_{S}$  is replaced by  $(\cdot)'$ .

As outlined, the time discretisation utilised within the FE tool PANDAS has been implemented by Ammann [3], Eipper [63], Ellsiepen [65], it is described in detail in Häberle [89], Koch [104], Wagner [187] as well as Acartürk [1], therefore, in this context a brief summary of the notions regarding temporal discretisation is given for the sake of completeness.

For the time discretisation of the system of differential-algebraic equations (DAEs), the implicit *Euler* (or backward *Euler*) time integration scheme is applied. This yields with the application of a backward *Taylor* series, when terms of higher order are neglected, viz.:

$$\boldsymbol{y}_n = \boldsymbol{y}_{n+1} - h_n \, \boldsymbol{y}'_{n+1} \longrightarrow \boldsymbol{y}'_{n+1} = \frac{1}{h_n} (\boldsymbol{y}_{n+1} - \boldsymbol{y}_n).$$
 (5.15)

Therein,  $y_{n+1}$  is the solution vector corresponding to the current time  $t_{n+1}$ ,  $y'_{n+1}$  is the derivative of the solution vector at the current time,  $y_n$  is the solution vector from the previous time  $t_n$  and  $h_n$  the actual time step defined via  $h_n = t_{n+1} - t_n$ . Applying this implicit *Euler* strategy to (5.14) yields

$$\boldsymbol{\mathcal{F}}_{n+1}(t_{n+1}, \boldsymbol{y}_{n+1}, \boldsymbol{y}'_{n+1}(\boldsymbol{y}_{n+1})) = [\boldsymbol{D}(\boldsymbol{y}_{n+1}) \, \boldsymbol{y}'_{n+1} + \boldsymbol{k}(\boldsymbol{y}_{n+1}) - \boldsymbol{f}_{n+1}] \stackrel{!}{=} \boldsymbol{0}.$$
(5.16)

This is, in turn, solved with the *Newton-Raphson* method, where the computation of the residual tangent  $D\mathcal{F}_{n+1}^k$  is required. It is defined via

$$D\boldsymbol{\mathcal{F}}_{n+1}^{k} := \frac{\mathrm{d}\boldsymbol{\mathcal{F}}_{n+1}^{k}}{\mathrm{d}\boldsymbol{y}_{n+1}^{k}} = \frac{\partial\boldsymbol{\mathcal{F}}_{n+1}^{k}}{\partial\boldsymbol{y}_{n+1}^{k}} + \frac{1}{h_{n}} \frac{\partial\boldsymbol{\mathcal{F}}_{n+1}^{k}}{\partial(\boldsymbol{y}')_{n+1}^{k}}$$
(5.17)

and is computed numerically at the current Newton step k within the scope of this monograph. Furthermore, the so-called stage increment  $\Delta y_{n+1}^k$  is calculated by solving

$$D\boldsymbol{\mathcal{F}}_{n+1}^{k} \Delta \boldsymbol{y}_{n+1}^{k} = -\boldsymbol{\mathcal{F}}_{n+1}^{k}.$$
(5.18)

With this increment, the solution vector can be updated

$$\boldsymbol{y}_{n+1}^{k+1} = \boldsymbol{y}_{n+1}^{k} + \Delta \boldsymbol{y}_{n+1}^{k}, \qquad (5.19)$$

whereby the iteration continues, until the norm  $\| \mathcal{F}_{n+1}^{k+1} \|$  of the residuum is smaller than a certain pre-defined tolerance  $\epsilon_{tol}$ , viz.:

$$\| \boldsymbol{\mathcal{F}}_{n+1}^{k+1} \| < \epsilon_{\text{tol}}.$$

$$(5.20)$$

When condition (5.20) is fulfilled, the computation at the next time step starts.

**Concluding remark:** Before discussing the numerical examples in the following chapter, one final remark regarding the numerical procedure is necessary, as the application of the reduced Model II requires in (6.6) the *Dirichlet* boundary of the liquid pressure to be a linear function of the temperature, another primary variable. As discussed in detail later in this monograph, this enables to model the impact of the ice pressure on the porous tissue. Both, liquid pressure and temperature, constitute essential boundary conditions at the surface of interest. However, as there have not been any oscillations, a weak implementation of the *Dirichlet* boundary condition of the pressure (or potentially also of the temperature) is not necessary. This has been introduced by Acartürk [1], where the *Dirichlet* boundary conditions depend also on the current state of the material. Hence, in this context, it may be concluded, that this applies just for the case where the *Dirichlet* boundary condition of another primary field.

# Chapter 6: Numerical examples

This chapter includes two numerical examples that show the feasibility of the introduced theoretical TPM models to address the behaviour of plant tissues in a subzero environment. Thus, as described in detail in this monograph so far, two examples are shown, one regarding the quaternary Model I to address dispersed ice, and one regarding the reduced ternary Model II to address the impact of localised ice. Although the models are somehow fundamentally different, the idea for both models and numerical examples is the same: Understanding the coupled thermo-hydro-mechanical behaviour of plant tissues in a subzero environment with a focus on the water management at two porosity scales.

Note that for each model one representative plant has been chosen that exhibits one of the two mentioned ice-formation patterns. The plants have been selected after consultations with scientists from the State Museum of Natural History in Stuttgart<sup>1</sup> as part of the cooperation within CRC  $141^2$ .

Note furthermore that the numerical results in this chapter have been computed with the Finite-Element code PANDAS.

### 6.1 The formation of dispersed ice in *Betula nana*

The numerical example that is shown in this section is based on the quaternary TPM model (Model I) to address the formation of dispersed intercellular ice and the consequences of the phase transition on the availability of water in the micro-pore space and the macro-pore space with application to *Betula nana*. *Betula nana* belongs to the class of woody species with trivial name dwarf birch, as discussed in Schott & Roth-Nebelsick [166]. Therein, it is described as a small shrub, which is up to 1 m high and has its natural habitat in the cold tundra.

The focus of this numerical example is in the ice formation in the intercellular space. The ice formation, in turn, has consequences on the water pressure, which controls the water management at the microscale and at the macroscale as well. It has also consequences on the deformation and stress of the specimen, which will be also discussed, with appropriate figures concerning the behaviour in the whole cross section, as depicted in Figure 6.1.

<sup>&</sup>lt;sup>1</sup>Schott [165], Schott & Roth-Nebelsick [166], Schott et al. [167]

<sup>&</sup>lt;sup>2</sup>Collaborative Research Center CRC 141: Biological Design and Integrative Structures - Analysis, Simulation and Implementation in Architecture funded by the German Research Foundation (DFG). More information is available on www.trr141.de (retrieved 10 September 2020).

### 6.1.1 Problem description

In this numerical example, the ice formation in the stem cross section is examined. The geometry of an idealised cross section of *Betula nana* is given in Figure 6.1. Therein, a quarter of the cross section is shown with dimensions within the range as reported by Schott & Roth-Nebelsick [166], Weijers *et al.* [190]. The boundaries are labelled with Roman numerals, where the respective boundary conditions are given in Table 6.1.



Figure 6.1: Quarter of the idealised cross section of *Betula nana*, with radius of 2.0 mm. The boundaries are denoted by the Roman numerals (I-V), cf. Table 6.1.

Due to symmetry, only a quarter of the stem cross section needs to be considered. The symmetry conditions in terms of no-flux conditions and no circumferential displacements are listed along with all other boundary conditions in Table 6.1 corresponding to the boundaries defined in Figure 6.1.

The initial conditions for the primary variables  $\mathbf{u}_S$ ,  $n^S$ ,  $n^I$ ,  $p^{LR}$ ,  $p^{GR}$  and  $\theta$  for initialboundary-value problems are given via

$$\mathbf{u}_{S0} = \mathbf{0} \, [\text{mm}], 
 n_{0S}^{S} = 0.75, 
 n_{0I}^{I} = 0.01, 
 p_{0}^{LR} = -0.8 \, [\text{MPa}], 
 p_{0}^{GR} = 0 \, [\text{MPa}], 
 \theta_{0S}^{S} = 278.15 \, [\text{K}],$$
 (6.1)

where  $(6.1)_2$  is after [126, 186],  $(6.1)_3$  is an arbitrary small value (zero is not possible, since a vanishing mass balance of the ice is not feasible within the numerical campaign),

**Table 6.1:** Boundary conditions for the boundaries I-V of Figure 6.1 applied to the initialboundary-value problems of Betula nana. Note that  $t_1$ ,  $t_2$  and  $t_3$  represent the components of the surface traction  $\tilde{\mathbf{t}}$  in the directions  $\mathbf{e}_1$ ,  $\mathbf{e}_2$  and  $\mathbf{e}_3$ , respectively.

Ι	II	III	IV	V
$t_1 = 0$	$u_1 = 0$	$t_1 = 0$	$t_1 = 0$	$t_1 = 0$
$t_2 = 0$	$t_2 = 0$	$u_2 = 0$	$t_2 = 0$	$t_2 = 0$
$t_3 = 0$	$u_3 = 0$	$u_3 = 0$	$u_3 = 0$	$u_3 = 0$
$\tilde{m}^L = 0$	$\tilde{m}^L = 0$	$\tilde{m}^L = 0$	$\tilde{m}^L = 0$	$\tilde{m}^L=0$
$p^{GR} = p_0^{GR}$	$\tilde{m}^G=0$	$\tilde{m}^G=0$	$\tilde{m}^G=0$	$\tilde{m}^G=0$
$\tilde{v}^S = 0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$
$\tilde{v}^I = 0$	$\tilde{v}^{I} = 0$	$\tilde{v}^I = 0$	$\tilde{v}^I = 0$	$\tilde{v}^I=0$
$\theta = \theta_D$	$\tilde{q} = 0$	$\tilde{q} = 0$	$\tilde{q} = 0$	$\tilde{q} = 0$

 $(6.1)_4$  is in accordance to [140], the gaseous initial pressure is the ambient pressure, and  $(6.1)_6$  is suggested by [166]. Furthermore, the *Dirichlet* boundary condition in terms of temperature  $(\theta_D)$  at boundary I, cf. in Table 6.1, is prescribed by

$$\theta_D = \begin{cases} \theta_{0S}^S - \frac{\theta_{\text{diff}}}{t_{\text{diff}}} t & \text{for : } t \le t_{\text{diff}}, \\ \theta_{0S}^S - \theta_{\text{diff}} & \text{else,} \end{cases}$$
(6.2)

with  $\theta_{\text{diff}} = 15 \text{ K}$  and  $t_{\text{diff}} = 27,000 \text{ s}$ , as suggested by Schott & Roth-Nebelsick [166], Schott *et al.* [167] to account for the necessary acclimatisation of the specimen, see also [67]. Note that in the set of initial conditions (6.1) as well as in the set of material parameters in Table 6.2, the given values refer to the genus *Betula* (birch), as the values are not fully given to the best of the author's knowledge for the more specific *Betula nana*. Thus, the set of material parameters is given in Table 6.2. Therein, the approximated initial effective liquid saturation of  $s_{\text{eff},0}^L = 0.1$  is implemented by considering a pore size distribution index of  $\lambda_c = 0.6$  and an emerging bubbling pressure of  $p_d = 0.0172355 \text{ MPa}$ . The value for the pore size distribution index chosen here stands for rather poorly sorted porous materials, compare also [89]. The emerging bubbling pressure is due to the initial liquid pressure, given in [140]. The hydraulic anisotropy is accounted for by introducing the intrinsic permeability tensor  $\mathbf{K}_{0S}^{S}$ :

$$\mathbf{K}_{0S}^{S} = \begin{pmatrix} 10^{-8} & 0 & 0\\ 0 & 10^{-8} & 0\\ 0 & 0 & 10^{-6} \end{pmatrix} \mathbf{e}_{i} \otimes \mathbf{e}_{j} \,[\mathrm{mm}^{2}].$$
(6.3)

With this permeability tensor, according to the mechanical transverse isotropy, one preferred flow direction is defined, which is the out-of-plane direction of the numerical example discussed in this section.

Parameter	Value	Unit	Remark/Reference
$p_0$	0.101	MPa	Atmospheric pressure in (4.106)
$\theta_{0S}^S$	278.15	Κ	Initial temperature of experiment [166]
$\theta^{I}_{0I}$	273.15	Κ	Freezing point [66]
$n_{0S}^S$	0.75	_	Initial solid volume fraction after [126, 186]
$n_{0I}^I$	0.01	_	Initial ice volume fraction
$s_{ m res}^L$	0.05	_	Residual saturation of $\varphi^L$ in (4.92)
$s^G_{ m res}$	0.05	_	Residual saturation of $\varphi^G$ in (4.92)
$s^L_{\mathrm{eff},0}$	0.1	—	Accounting for $(6.1)$ after [140]
$\lambda_c$	0.6	—	Accounting for $(6.1)$ after [140]
$\rho_{0S}^{SR}$	$1.15\times10^{-6}$	$\rm kg/mm^3$	Density of fresh plant after [126, 186]
$\rho_{0I}^{IR}$	$9.16\times 10^{-7}$	$\rm kg/mm^3$	Density of ice at $0.0^{\circ}$ C [66]
$a_1$	-3.983035	$^{\circ}\mathrm{C}$	Parameter in $(4.105)$ [181]
$a_2$	301.797	$^{\circ}\mathrm{C}$	Parameter in $(4.105)$ [181]
$a_3$	$5.225289\times 10^5$	$^{\circ}\mathrm{C}^{2}$	Parameter in $(4.105)$ [181]
$a_4$	69.34881	$^{\circ}\mathrm{C}$	Parameter in $(4.105)$ [181]
$a_5$	$9.9997495 \times 10^{-7}$	$\rm kg/mm^3$	Parameter in $(4.105)$ [181]
$L_p$	$1.0 \times 10^{-4}$	$\mathrm{mm}/(\mathrm{sMPa})$	Hydraulic micro-conductivity [111]
ω	100.0	$1/\mathrm{mm}$	Specific surface of cells [111]
$\tilde{r}$	0.02	mm	Pore radius after [69]
$\Delta \zeta_{\rm fus}$	$3.33  imes 10^8$	m Nmm/kg	Enthalpy of fusion of water [66]
$E_{\rm fus}$	1.12	MPa/K	Entropy of fusion of water [64]
$\bar{R^G}$	$2.87 \times 10^5$	$N \mathrm{mm}/(\mathrm{kg}\mathrm{K})$	Specific gas constant of air [66]
$\mu^{LR}$	$1.7 \times 10^{-9}$	$N  s/mm^2$	Viscosity of water at $0.01^{\circ}C$ [66]
$\mu^{GR}$	$1.7 \times 10^{-11}$	$N  s/mm^2$	Viscosity of air at $0.0^{\circ}$ C [66]
$\Lambda^S$	1485.15	MPa	In-plane stiffness after [156]
$\mu^S$	282.88	MPa	In-plane stiffness after [156]
$k^S$	1673.75	MPa	In-plane stiffness after [156]
$\gamma_0^S$	2.0	_	Exponent in $(4.71)$ after $[172]$
$\alpha_{S1}$	5150.0	MPa	Out-of-plane stiffness after [156]
$\alpha_{S2}$	2.0	_	Out-of-plane stiffness after [156]
$\Lambda^{IR}$	3460.0	MPa	Stiffness of ice after [117]
$\mu^{IR}$	2310.0	MPa	Stiffness of ice after [117]
$k^{IR}$	5000.0	MPa	Stiffness of ice after [117]
$\gamma_0^{IR}$	2.0	_	Exponent in $(4.82)$ after $[172]$
$\kappa$	1.0	_	Exponent compaction point in $(4.97)$
$\alpha^S$	$1.75 \times 10^{-5}$	1/K	Thermal expansion of plant after [188]
$\alpha^{IR}$	$5.0 \times 10^{-5}$	1/K	Thermal expansion of ice [120]
$c_v^S$	$1.9 \times 10^6$	$N \mathrm{mm}/(\mathrm{kg}\mathrm{K})$	Specific heat after [66]
$c_v^{IR}$	$2.05 \times 10^6$	$N \mathrm{mm}/(\mathrm{kg}\mathrm{K})$	Specific heat after [66]
$c_v^{LR}$	$4.2 \times 10^6$	$N \mathrm{mm}/(\mathrm{kg}\mathrm{K})$	Specific heat at $0.01^{\circ}C$ [66]
$c_v^{GR}$	$7.2 \times 10^5$	$N \mathrm{mm}/(\mathrm{kg}\mathrm{K})$	Specific heat at 0.0°C [66]
$H^{SR}$	0.18	N/(sK)	At a $M_C$ of 18% after [156]
$H^{IR}$	2.22	N/(sK)	For ice at $0.0^{\circ}$ C [66]
$H^{LR}$	0.556	N/(sK)	For water at $0.01^{\circ}$ C [66]
$H^{GR}$	0.024	N/(sK)	For air at $0.0^{\circ}$ C [66]

 Table 6.2: Material parameters of the quaternary TPM model

### 6.1.2 Results & Discussion

#### Ice formation in the intercellular space

First of all, the formation of ice in the intercellular space is addressed, as this is somehow influencing all other effects in *Betula nana* as well. Thus, for the case discussed here, meaningful time steps have been selected, which are given in the caption of the respective figure.



**Figure 6.2:** Ice formation for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time. The maximum value of the ice production is decreasing from boundary I to the centre of the cross section, so is also the velocity of the ice formation front.

From Figure 6.2, it is seen that the ice formation front in terms of  $\hat{\rho}^{I}$  propagates from boundary I through the porous plant tissue following the temperature gradient, where the drop in temperature is prescribed at boundary I. From the outside (boundary I) to the centre of the cross section, the maximum value of the ice production is decreasing, so is also the velocity of the ice formation front. The ice mass production leads to an increase in ice volume fraction  $n^{I}$ , as it is seen in Figure 6.3. Note that the ice volume fraction is not starting to increase in the most outer layer of elements, as seen on the second frame from the left in the upper row, which is assumed to be a numerical artefact that is related to the *Neumann* boundary condition. In this context, it should be also mentioned that the cells need to dehydrate before the macro-pore water can further freeze, however, as it is seen later, the dehydration occurs rather fast, which leads to a rapid ice formation and not to a process over many hours.



**Figure 6.3:** Ice volume fraction  $n^{I}$  for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time.

### Double-porosity induced water management

The formation of ice effects also via the mass-production terms the evolution of the water pressure  $p^{LR}$ . This is the most important quantity that determines the water management at the microscopic scale as well as at the macroscopic scale. At the microscopic scale, the water management is represented through the solid mass production  $\hat{\rho}^S$ , that describes biologically the dehydration of the tissue cells, and is given in Figure 6.5.

The water management at the microscopic scale leads to a decrease in solid volume fraction  $n^S$ , where it is worth mentioning that the numerical example in this section considers a plant that has a rather high amount of lignified elements, such that the stiffness is rather high. However, this also indicates that the water content of the solid skeleton is rather low, which is shown by the high minimum value of  $n^S$  in Figure 6.6, this remaining solid volume fraction does not consist of water, that may be subjected to dehydration. The fact that the decrease does not start at the most outer layer of elements, as seen in the second left time frame in the upper row, is also assumed to be related to the Neumann boundary condition.

The water management at the macroscopic scale is described by an extended *Darcy* law, that has been derived in (4.99) describing the filter velocity  $n^L \mathbf{w}_L$  of the water in the macro-pore space. Figure 6.7 shows that the filter velocity is always oriented towards the ice front, an effect that has been frequently described as frost suction, compare Coussy [39], Coussy & Monteiro [40], Ricken & Bluhm [147], the ice attracts more and more water to the freezing site.



 $p^{LR}$ 

**Figure 6.4:** Water pressure for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time.



**Figure 6.5:** Cell dehydration  $\hat{\rho}^S$  for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time. It is determined by the hydraulic conductivity  $L_p$  of the cell wall as well as the water pressure.



**Figure 6.6:** Solid volume fraction  $n^S$  for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time. The lower boundary in solid volume fraction represents the biological tissue material.



Figure 6.7: Ice volume fraction distribution (colour-coded) and resulting filter velocity  $n^L \mathbf{w}_L$  (blue arrows) in an enlarged view for time steps 268 min and 328 min. Smaller arrows indicate a lower filter velocity, longer arrows indicate a higher velocity. Note that the same magnification for the arrows is utilised for both time frames. The filter velocity represents the frost suction, as the flow of liquid water in the macro-pore space is always oriented towards the ice front.

#### Deformation and corresponding stresses

In order to assess the deformation of the underlying cross section, several processes have to be considered. First of all, there is the decrease in temperature that lead to a shrinkage of the cross section of the plant due to the thermal dependencies of the respective effective density of the constituents. Additionally, there is a net mass efflux out of the domain, as it will be shown later by the filter velocity of the gas phase in Figure 6.10, which also generally contributes to a shrinkage. However, the phase transition of the water from liquid to solid leads to an expansion due to the associated decrease in density of the ice, as shown in Figure 4.4. The result of these processes is shown in Figure 6.8, where the in-plane deformation pattern is given along with the ice volume fraction to acknowledge specifically this effect of volume expansion during ice formation. The expansion due to ice formation starts with the most outer layer of elements, as shown in the third time frame from left in the upper row, and then propagates through the plant cross section to its centre. At some time, the expansion due to ice formation is larger than the mentioned thermal and hydraulic effects that generally cause shrinkage.



**Figure 6.8:** In-plane deformation pattern of a cross section for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time. The initial configuration of the cross section is shown in light grey, the cross section in the actual configuration is shown in the colour-coded deformed shape, scaled by a factor of 1500 per vector component. The colour, which is somehow represented in a dull way, represents the evolution of the volume fraction of the ice. Note the striking deformation of the most outer row of elements of the third frame from left in the upper row, as there is already ice formation in this outer region, however, not yet in the whole cross section. From there on, the ice front propagates through the cross section, so is the expansion of the elements.

Having this deformation pattern in mind, one might wonder why the shrinkage is initially rather high in comparison to the expansion that is caused by ice formation. This is mainly for two reasons. The first reason is related to the choice of the material parameters that have been utilised for simulation, specifically with regard to the high thermal expansion coefficient of the solid skeleton. But emphasis is on the other reason that is based on the partial saturation of the macro-pore space of liquid and gas. In fact, as shown in Figure 6.9, the gas volume fraction is decreasing in regions where ice formation is observed.



**Figure 6.9:** Gas volume fraction  $n^G$  for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time. Note the boundary effect in the second and third time frame from left in the upper row. When ice formation starts, the decrease in gas volume fraction can be observed, compare Figure 6.8.

Note that the gas is also slightly compressed and as a reaction forced out of the cross section, which is shown in Figure 6.10. Thereon, the evolution of the ice volume fraction is related to the filter velocity  $n^G \mathbf{w}_G$  of the gas.

Finally, the stresses in the solid skeleton are shown in Figure 6.11, specifically, the normal stress in  $\mathbf{e}_1$ -direction in terms of the mechanical extra stress  $\mathbf{T}_{E\,\mathrm{mech}}^S$  of the solid skeleton, as defined in (4.62). Due to symmetry, the normal stress in  $\mathbf{e}_2$ -direction is behaving in the same way. Initially, when there is no ice, the stress is approximately zero, as the solid skeleton can deform freely due to the applied temperature drop. However, when the ice volume fraction is increasing, the tensile stresses of the solid skeleton are increasing as well, which is due to the expansion that is associated to the ice formation. Yet, it should be noted that the stresses are far below the strength of the material, compare Ross [156]. High tensile stresses in the solid skeleton are frequently responsible for frost damage in construction materials, as discussed in Azmatch *et al.* [7], Ming *et al.* [127].



Figure 6.10: Ice volume fraction distribution (colour-coded) and resulting filter velocity  $n^G \mathbf{w}_G$  (blue arrows) in an enlarged view for time steps 268 min and 328 min. Smaller arrows indicate a lower filter velocity, longer arrows indicate a higher velocity. Note that the same magnification for the arrows is utilised for both time frames.



Figure 6.11: Normal stress in  $\mathbf{e}_1$ -direction for time steps 120 min, 228 min, 232 min, 244 min, 268 min, 288 min, 328 min and 440 min increasing from top left to bottom right regarding time. In detail, it is the mentioned component of  $\mathbf{T}_{E \,\mathrm{mech}}^S$  of the solid skeleton, as defined in (4.62).

## 6.2 The impact of localised ice in *Equisetum hyemale*

Note that the numerical example presented in this section is based on the TPM model, which has been introduced as reduced model (or Model II) in **Section 4.9**. Furthermore, note that parts of the numerical example shown in this section are part of Eurich *et al.* [67]. Therein, the introduced test protocol in terms of the prescribed temperature, the geometrical dimensions as well as the estimation of the initial volume fractions via image analysis has been contributed by scientists from the State Museum of Natural History<sup>3</sup>.

### 6.2.1 Problem description

The plant that is being investigated is *Equisetum hyemale*, common name winter scouring rush, which has shoots of up to 1 m height. It mostly grows in moist habitats, such as wetlands or swamps, as discussed in Schott *et al.* [167]. Its geometry is depicted in Figure 6.12. Therein, a quarter of the idealised cross section is shown, where the boundaries are labelled with Roman numerals, for which the *Dirichlet* or *Neumann* boundary condition is defined according to Table 6.3. Boundary I is at the pith cavity, while boundary V is at the vallecular canals.



Figure 6.12: Quarter of the idealised cross section of Equisetum hyemale including dimensions of the hollow cylinder and vallecular canals with 0.22 mm diameter. For the discussion of results, points A, B and C are indicated, the boundaries are denoted by the Roman numerals (I-VII), cf. Table 6.3.

<sup>&</sup>lt;sup>3</sup>The analysis of the respective plant tissues has been carried out at the State Museum of Natural History in Stuttgart, Germany under the supervision of Anita Roth-Nebelsick and got published, inter alia, in Schott [165], Schott & Roth-Nebelsick [166], Schott *et al.* [167].

It has been reported by Schott *et al.* [167], that the main locations of ice formation in *Equisetum hyemale* are at the surface to the pith cavity and the vallecular canals. According to Figure 6.12, the diameter of the pith cavity is 3.8 mm and of the vallecular canals 0.22 mm, which are distributed within the cross section of width 0.5 mm. Furthermore, three more or less arbitrary, but from the locations somehow representative points within the cross section are indicated with coordinates, namely A (1.3435, 1.3435, 0.025), B (1.452, 1.447, 0.025) and C (1.583, 1.586, 0.025), given in [mm]. Due to symmetry, only a quarter of the cross section has to be considered. The symmetry conditions, which are no-flux conditions and no circumferential displacements, are listed with the other boundary conditions in Table 6.3 for an idealised cross section.

**Table 6.3:** Boundary conditions for the boundaries I-VII indicated in Figure 6.12. Note that  $t_1, t_2$  and  $t_3$  represent the components of the surface traction  $\tilde{\mathbf{t}}$  in  $\mathbf{e}_1$ ,  $\mathbf{e}_2$  and  $\mathbf{e}_3$ , respectively.

I	II	III	IV	V	VI	VII
	4 0		4 0	,	4 0	+
$u_1 = 0$	$t_1 = 0$	$u_1 = 0$	$t_1 = 0$	$t_1 = 0$	$t_1 \equiv 0$	$t_1 = 0$
$u_2 = 0$	$t_2 = 0$	$t_2 = 0$	$u_2 = 0$	$t_2 = 0$	$t_2 = 0$	$t_2 = 0$
$t_3 = 0$	$t_3 = 0$	$u_3 = 0$	$u_3 = 0$	$t_3 = 0$	$u_3 = 0$	$u_3 = 0$
$p^{LR} = p_D^{LR}$	$\tilde{m}^L = 0$	$\tilde{m}^L=0$	$\tilde{m}^L=0$	$p^{LR} = p_D^{LR}$	$\tilde{m}^L=0$	$\tilde{m}^L=0$
$\tilde{m}^G=0$	$p^{GR} = p_0^{GR}$	$\tilde{m}^G=0$	$\tilde{m}^G=0$	$\tilde{m}^G=0$	$\tilde{m}^G=0$	$\tilde{m}^G=0$
$\tilde{v}^S=0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$	$\tilde{v}^S=0$
$\tilde{q} = 0$	$\theta = \theta_D$	$\tilde{q} = 0$	$\tilde{q} = 0$	$\tilde{q} = 0$	$\tilde{q} = 0$	$\tilde{q} = 0$

Furthermore, the initial conditions for the primary variables  $\mathbf{u}_S$ ,  $n^S$ ,  $p^{LR}$ ,  $p^{GR}$  and  $\theta$  are given via

$$\mathbf{u}_{S0} = \mathbf{0} \, [\text{mm}], 
 n_{0S}^{S} = 0.6, 
 p_{0}^{LR} = -0.11 \, [\text{MPa}], 
 p_{0}^{GR} = 0 \, [\text{MPa}], 
 \theta_{0S}^{S} = 278.15 \, [\text{K}].$$
(6.4)

Finally, the *Dirichlet* boundary condition in terms of temperature  $(\theta_D)$  at boundary II, cf. in Table 6.3, is prescribed by

$$\theta_D = \begin{cases} \theta_{0S}^S - \frac{\theta_{\text{diff}}}{t_{\text{diff}}} t & \text{for : } t \le t_{\text{diff}}, \\ \theta_{0S}^S - \theta_{\text{diff}} & \text{else,} \end{cases}$$
(6.5)

with  $\theta_{\text{diff}} = 15 \text{ K}$  and  $t_{\text{diff}} = 27,000 \text{ s}$ , as suggested by Schott & Roth-Nebelsick [166], Schott *et al.* [167] to account for the necessary acclimatisation of the specimen. Note that the onset of ice formation introduces a drop in water potential, cf. Niklas [136]. Hence, according to the considerations thus far, a drop in water pressure is applied at the boundaries to larger ice bodies at the pith cavity as well as the vallecular canals. Here, the interpolated values from the experimental investigation of Niklas [136] have been utilised for the *Dirichlet* pressure boundary condition  $\partial \Omega_D^{p^{LR}}$  at the mentioned pith cavity (boundary I) as well as the vallecular canals (boundary V), viz.:

$$p_D^{LR} = \begin{cases} p_0^{LR} + p_{\text{diff}} \left( \theta - \theta_{0I}^I \right) & \text{for} : \theta < \theta_{0I}^I, \\ p_0^{LR} & \text{else,} \end{cases}$$
(6.6)

with  $p_{\text{diff}} = 0.007 \text{ MPa}$ . This shows exemplarily the strong coupling of the underlying thermo-hydro-mechanical model, as the pressure drop is a function of the local temperature at the given boundaries of ice formation.

Finally, the model requires the knowledge of all material parameters, that have been introduced. The approximated initial effective liquid saturation of  $s_{\text{eff},0}^L = 0.1$  is implemented by considering a pore size distribution index of  $\lambda_c = 0.6$  and an emerging bubbling pressure of  $p_d = 0.00237$  MPa. Note that the influence of the compaction point can be neglected for this example, as the porosity will be increasing during the simulation as a consequence of cell dehydration. Note that the material parameters of the solid skeleton and the pore water are mostly similar due to the high water content of the solid skeleton. In some cases, when there is no data available for the solid skeleton, the values of the water have been utilised instead. In addition to the mechanical anisotropy, also the hydraulic anisotropy at the macroscale with one preferred direction is taken into account by the intrinsic permeability tensor  $\mathbf{K}_{0S}^S$ :

$$\mathbf{K}_{0S}^{S} = \begin{pmatrix} 10^{-8} & 0 & 0\\ 0 & 10^{-8} & 0\\ 0 & 0 & 10^{-6} \end{pmatrix} \mathbf{e}_{i} \otimes \mathbf{e}_{j} \,[\mathrm{mm}^{2}].$$
(6.7)

### 6.2.2 Results & Discussion

Of special interest for initial-boundary-value problems applied to *Equisetum hyemale* are the temperature-induced effects on the hydraulics in the micro- and macro-pore space, where the mentioned double-porosity feature leads to water management at two porosity scales. The resulting deformation pattern is also discussed, as is the location of the maximum ice accumulation.

#### Thermally induced hydraulics in the micro- and macro-pore space

Based on the temperature evolution, the pressure is the most important quantity controlling the hydraulics in the micro-pore space and the macro-pore space as well. Thus, with the initial condition of the effective water pressure  $p^{LR}$ , cf. (6.4)<sub>3</sub>, Figure 6.13 shows the water pressure  $p^{LR}$  distribution in the displayed cross section for meaningful time steps. These are 1.5 h, 4.5 h, 7.5 h, 10 h, 15.5 h, 20 h, 32 h and 50 h increasing from top left to bottom right. In particular, when the temperature  $\theta$  within the vallecular canals and the pith cavity reaches a value below the assumed freezing point of 273.15 K, the prescribed change in water pressure according to (6.6) is due to the onset of ice formation describing the frost suction. From there on, the pressure drop propagates from boundaries I and

Parameter	Value	Unit	Remark/Reference
$p_0$	0.101	MPa	Atmospheric pressure in (4.106)
$\theta_{0S}^S$	278.15	Κ	Initial temperature of experiment [165, 167]
$n_{0S}^S$	0.6	_	Initial solid volume fraction [165, 167]
$s_{ m res}^L$	0.05	_	Residual saturation of $\varphi^L$ in (4.92)
$s^G_{ m res}$	0.05	_	Residual saturation of $\varphi^G$ in (4.92)
$s^L_{\mathrm{eff},0}$	0.1	_	Accounting for $(6.4)$ , after $[136]$
$\lambda_c$	0.6	_	Accounting for $(6.4)$ , after $[136]$
$\rho_{0S}^{SR}$	$1.0 \times 10^{-6}$	$\rm kg/mm^3$	Density of watery plant [4]
$a_1$	-3.983035	$^{\circ}\mathrm{C}$	Parameter in $(4.105)$ [181]
$a_2$	301.797	$^{\circ}\mathrm{C}$	Parameter in $(4.105)$ [181]
$a_3$	$5.225289\times10^5$	$^{\circ}\mathrm{C}^{2}$	Parameter in $(4.105)$ [181]
$a_4$	69.34881	$^{\circ}\mathrm{C}$	Parameter in $(4.105)$ [181]
$a_5$	$9.9997495 \times 10^{-7}$	$\rm kg/mm^3$	Parameter in $(4.105)$ [181]
$L_p$	$1.0 \times 10^{-5}$	$\rm mm/(sMPa)$	Hydraulic micro-conductivity [111]
ω	100.0	$1/\mathrm{mm}$	Specific surface of cells [111]
$\bar{R^G}$	$2.87\times 10^5$	$\rm Nmm/(kgK)$	Specific gas constant of air [66]
$\mu^{LR}$	$1.7  imes 10^{-9}$	${ m Ns/mm^2}$	Viscosity of water at $0.01^{\circ}C$ [66]
$\mu^{GR}$	$1.7\times 10^{-11}$	${ m Ns/mm^2}$	Viscosity of air at $0.0^{\circ}$ C [66]
$\Lambda^S$	12.0	MPa	In-plane stiffness after $[137, 138, 174]$
$\mu^S$	12.0	MPa	In-plane stiffness after $[137, 138, 174]$
$k^S$	20.0	MPa	In-plane stiffness after $[137, 138, 174]$
$\gamma_0^S$	2.0	_	Exponent in $(4.71)$ after $[172]$
$\tilde{J}_S$	0.0	_	Neglect compaction point in $(4.71)$
$\alpha_{S1}$	300.0	MPa	Out-of-plane stiffness after [137, 138, 174]
$\alpha_{S2}$	2.0	_	Out-of-plane stiffness after [137, 138, 174]
$\kappa$	1.0	_	Exponent compaction point in $(4.97)$
$\alpha^S$	$1.0  imes 10^{-5}$	1/K	Thermal expansion of watery plant [170]
$c_v^S$	$4.2\times 10^6$	$\rm Nmm/(kgK)$	Suggested value of water at $0.01^{\circ}C$ [66]
$c_v^{LR}$	$4.2  imes 10^6$	$\rm Nmm/(kgK)$	For water at $0.01^{\circ}$ C [66]
$c_v^{GR}$	$7.2\times 10^5$	$\rm Nmm/(kgK)$	For air at $0.0^{\circ}$ C [66]
$H^{SR}$	0.556	$\rm N/(sK)$	Suggested value of water at $0.01^{\circ}C$ [66]
$H^{LR}$	0.556	$\rm N/(sK)$	For water at $0.01^{\circ}C$ [66]
$H^{GR}$	0.024	$\rm N/(sK)$	For air at $0.0^{\circ}$ C [66]

 Table 6.4:
 Material parameters of the ternary TPM model

V through the whole cross section, where the intrinsic permeability  $\mathbf{K}^{S}$  determines how fast. The minimum value of  $p^{LR}$  is -0.18 MPa according to the experimental results of Niklas [136].

The emerging change in water pressure has an immediate effect on the flow macro-pore space, which is shown by the resulting filter velocity  $n^L \mathbf{w}_L$  represented by blue arrows in Figure 6.14.



**Figure 6.13:** Water pressure  $p^{LR}$  distribution within the cross section of Equisetum hyemale for time steps 1.5 h, 4.5 h, 7.5 h, 10 h, 15.5 h, 20 h, 32 h and 50 h increasing from top left to bottom right regarding time.



**Figure 6.14:** Characteristic water pressure  $p^{LR}$  distribution and resulting filter velocity  $n^L \mathbf{w}_L$  (blue arrows) in an enlarged view. Smaller arrows indicate a lower filter velocity, longer arrows indicate a higher velocity.

According to (4.170), the pressure distribution in Figure 6.13 causes a *Darcy* flow of water through the macro-pore space into the vallecular canals and the pith cavity, which is depicted in Figure 6.14 in a detailed view. Note that this is a qualitative, but representative pressure and flow pattern and is, therefore, displayed without units. It shows the distribution of the filter velocity  $n^L \mathbf{w}_L$  in the region of interest close to the pith cavity and the vallecular canals. Note in passing that the gas exchange at the pith cavity and the vallecular canals is neglected, as stated in Table 6.3, at the other boundaries it is generally possible and occurs in order to mantain equilibrium.

Clearly, a change in water pressure  $p^{LR}$  effects also the flow in the micro-pore space. The flow in the micro-pore space is biologically given as cell dehydration and included into the modelling approach via the mass production term  $\hat{\rho}^S$  according to (4.150), which is displayed in Figure 6.15. Therein, the onset of the micro-pore flow follows the change in water pressure at the surface to the pith cavity and the vallecular canals. As the pressure gradient in these regions is higher, also indicated by the higher filter velocity in Figure 6.14, the cell dehydration is more pronounced, but also decreasing faster, cf. Figure 6.15. In this figure, it is also seen, that the change or degree of dehydration follows the pressure gradient.



**Figure 6.15:** Cell dehydration for time steps 1.5 h, 4.5 h, 7.5 h, 10 h, 15.5 h, 20 h, 32 h and 50 h increasing from top left to bottom right regarding time. It is governed by the pressure gradient and the micro porosity, in particular, by the effective hydraulic conductivity of the cell wall.

As discussed so far, the solid volume fraction is always a degree for the hydration of the tissue cells. Thus, the initial solid volume fraction, here  $n_{0S}^S = 0.6$ , accounts for a high degree of hydration in the natural state of a specific plant, *Equisetum hyemale* in that particular case. The solid volume fraction reduces due to cell dehydration to a minimal value of 0.1, which corresponds to the (physically solid) biological tissue material. In that

final state, there is no water in the cells anymore that might be subjected to dehydration. This shows the dehydration of the solid skeleton as the consequence of the involved thermohydro-mechanical processes. On the one hand, this has been recognised as one of the key features of frost hardiness, on the other hand, excess dehydration might be an issue, when this state continues for too long.



**Figure 6.16:** Solid volume fraction  $n^S$  for time steps 1.5 h, 4.5 h, 7.5 h, 10 h, 15.5 h, 20 h, 32 h and 50 h increasing from top left to bottom right regarding time. The solid volume fraction approaches a minimum value of 0.1, which corresponds to the amount of biological tissue material in the solid skeleton.

The evolution of the liquid volume fraction  $n^L$  is a bit more involved, as it arises as a consequence of the involved micro-pore flow and macro-pore flow. It is depicted in Figure 6.17 for meaningful time steps. Note that there is initially a slight drop in liquid volume fraction at 4.5 h close to the pith cavity as well as the vallecular canals, compare also the nodal values in Figure 6.22, which is due to the instantaneous onset of the macro-pore flow. The cell dehydration cannot compensate for this initial effect. However, this depends on the relation between the involved hydraulic conductivities at the microscale and at the macroscale. The increase in available pore water in the macro-pore space in terms of  $n^L$  for later time steps is due to the increasing cell dehydration.

The presented results so far are further supported by the evaluation of the nodal values at three points A, B and C within the cross section, as introduced in Figure 6.12. In particular, the nodal values of the temperature  $\theta$ , the water pressure  $p^{LR}$ , the solid mass production  $\hat{\rho}^S$ , the solid volume fraction  $n^S$  and the liquid volume fraction  $n^L$  will be discussed at these representatively distributed points in the cross section. For the discussion concerning the liquid volume fraction, these results have already been considered.



**Figure 6.17:** Evolution of the liquid volume fraction  $n^L$  for time steps 1.5 h, 4.5 h, 7.5 h, 10 h, 15.5 h, 20 h, 32 h and 50 h increasing from top left to bottom right regarding time.

The temperature evolution is very similar for all points, indicating that there is just a small temperature gradient over the cross section at a certain instant of time, compare Figure 6.18.



**Figure 6.18:** Temperature  $\theta$  close to the pith cavity (Point A), in the middle of the cross section (Point B) and close to the outer surface (Point C), cf. Figure 6.12. Note that the curves overlap indicating that the temperature evolution over time is very similar for the chosen locations within the cross section.

As Point A is at the boundary to the pith cavity, where the water pressure drop is prescribed, the pressure decreases linearly for temperatures below the freezing point  $\theta_{0I}^{I}$  according to (6.6). For points B and C, which are a bit further away from that boundary, the pressure arises with time shift as a consequence of the involved thermo-hydro-mechanical processes, but mainly due to the permeability at the macroscale, compare Figure 6.19. The water pressure and the permeability at the microscale determine the cell dehydration, as depicted in Figure 6.20.



**Figure 6.19:** Water pressure  $p^{LR}$  for the selected points A, B and C. The pressure at Point A is defined by the prescribed pressure  $p_D^{LR}$ . The pressure at Point B and Point C result from the <u>coupled processes</u>, but, in particular, by the chosen permeability at the macroscale.



**Figure 6.20:** The solid mass production  $\hat{\rho}^S$  at points A, B and C as a consequence of the pressure difference between the intracellular space and the extracellular space and the effective hydraulic conductivity at the microscale.

At Point A, although the pressure drop leads initially to the dehydration of the tissue cells, displayed in Figure 6.20 and 6.21, there is still a drop in liquid volume fraction within the <u>macro-pore space</u>, cf. Figure 6.22, due to the macro-pore flow. For later time steps, there is an increase in liquid volume fraction, as the dehydration is getting more pronounced. As already discussed, this illustrates the double-porosity feature of the material. Note that the time shift of the pressure at locations B and even more at C is also reflected in the mass production and the corresponding volume fractions.



**Figure 6.21:** Solid volume fraction  $n^S$  at points A, B and C. Due to the time shift of the solid mass production  $\hat{\rho}^S$ , cf. Figure 6.20, the cells close to the pith cavity dehydrate faster in relation to locations B and C.



**Figure 6.22:** Liquid volume fraction  $n^L$  at points A, B and C. The double-porosity effect is evident for the time evolution of  $n^L$  at Point A, however, this effect is hardly visible at Point B, and not at all at Point C.

### Location of maximum ice accumulation

With the knowledge of the involved flow of water at both scales, the location of maximum ice accumulation can be determined by comparing the water efflux into the vallecular canals and the pith cavity. It turns out that the fraction of the total amount of water leaving the tissue material into the vallecular canals is 0.73, the efflux into the pith cavity is, consequently, 0.27. These numbers are qualitatively supported by the experimental findings of Schott *et al.* [167] showing that there is more ice in the vallecular canals, as it attracts more water in freezing conditions. The corresponding volumetric efflux into the vallecular canals is always higher compared to the volumetric efflux into the pith cavity.



Figure 6.23: Comparison of the volumetric flow rate  $[mm^3/s]$  into the vallecular canals, marked in blue, and the pith cavity, marked in red.

One reason for the higher amount of water leaving the tissue into the vallecular canals is the higher surface area. In order to find out, whether this is the only reason, the volumetric efflux of water in relation to its surface in terms of  $[mm^3/mm^2 s]$  is compared, cf. Figure 6.24. This reveals, that the higher total amount of water in the vallecular canals is not just an effect that can be traced back to its larger surface area. In fact, the pressure gradient and the amount of available water in the macro-pore space has to be higher in the vicinity of the vallecular canals.

#### Deformation

Finally, as a consequence of the involved thermo-hydro-mechanical processes, the deformation of the cross section of *Equisetum hyemale* is depicted in Figure 6.25 exhibiting a representative in-plane deformation pattern after 8 h, 20 h, 32 h and 50 h, where initially the deformation is mostly due to the temperature drop and for later time steps rather due to the dehydration of the tissue cells into the pith cavity and the vallecular canals. This type of behaviour has also been observed by Schott *et al.* [167] as a result of their



Figure 6.24: Comparison of the volumetric flow rate per surface area  $[mm^3/mm^2 s]$  into the vallecular canals, marked in blue, and the pith cavity, marked in red.

experiments indicating an oval shape of the vallecular canals in the deformed configuration, compare also Figure 3 in [167]. It is the result of the coupled thermo-mechanical deformation and the outflow of water into the vallecular canals and the pith cavity, which leads to shrinkage of the plant.



Figure 6.25: The undeformed cross section of Equisetum hyemale is depicted in light grey, the qualitative in-plane deformation pattern, taken at time steps t = 8 h, t = 20 h, t = 32 h and t = 50 h from left to right, is shown with the adapted mesh in blue, scaled by a factor of 150 per vector component.

# Chapter 7: Summary and outlook

## 7.1 Summary

plants.

In this thesis, a modelling approach for frost-resistant plants has been introduced that is based on the macroscopic Theory of Porous Media. It allows to distinguish between rather dispersed ice formation in the whole domain of interest and localised ice formation at internal cavities of the plant by introducing a reduced model without the ice as individual constituent, that addresses the impact of ice formation on the porous plant. However, it has been shown that the quaternary model for dispersed ice is downward compatible obtaining the reduced ternary model for localised ice.

Thus, the more general quaternary model proceeds from a multiphase solid skeleton that is comprised of lignified elements as well as tissue cells, which contain generally water. The physical behaviour of such a solid material is rather complex, as it involves a number of effects: anisotropy due to the lignified elements, thermoelasticity, the compaction point and mass interaction describing the double porosity, all of this in the framework of finite deformations. The inclusion of the compaction point might be of importance insofar, as it allows for a comparison of the stresses that are related to a shrinking pore space at the macroscopic scale, specifically due to ice formation, for porous materials with and without a smart water management. However, such a comparison is not sensible at the current stage of the investigation, as the damage (avoidance) mechanisms and related material properties are not yet established. The ice is also treated as a solid material in the framework of finite deformations. Further important effects are thermoelasticity, the compaction point and the phase transition of water, which is included by the massinteraction term as well as by an ansatz that accounts for the enthalpy of fusion. In the macro-pore space, there is liquid water and gaseous air indicating the action of capillarity. In general, the interaction of all the constituents is included in terms of mass by considering the phase transition of water and the dehydration of the cells as the consequence. The inclusion of the momentum interaction leads to extended *Darcy* laws for the perfusion of the porous material. In these interactions terms so far, the biology-inspired concept of water potential is recovered for the water status at the microscale as well as at the macroscale. Furthermore, as there is just one energy balance utilised, the one for the overall aggregate due to the common temperature of the constituents, there is no direct energy interaction. However, there are energy-interaction terms that are due to mass interaction and momentum interaction. This modelling approach may also apply

The derived set of thermodynamically consistent equations is solved monolithically using the Finite-Element Method. In detail, the quaternary model addresses the ice formation explicitly in the whole cross section. The corresponding numerical example reveals the

to a variety of other porous materials, which exhibit similar properties as the introduced

strong dependency on the internal surfaces of ice formation. It also reveals the influence of the ice formation on the water pressure, which is the most important quantity that drives the water management at the microscopic scale and at the macroscopic scale as well. Therefore, the cells dehydrate as a consequence of the ice formation. The water at the macroscopic scale is drawn towards the ice-formation front. This effect has been frequently reported. This numerical example is also capable of addressing the deformation pattern. After initial shrinkage, the formation of ice leads to an expansion. However, the expansion has been found to be rather low, since the gas volume fraction reduces at the same time dramatically due to the ice formation. It is assumed, that this effect is mainly responsible for the moderate tensile stresses in the solid skeleton in the zone of ice formation. In fact, the tensile stress is far below the strength of the material. Generally, it is well known that excess tensile stresses are responsible for damage in freezing porous construction materials.

The other numerical example aims at assessing the impact of localised ice formation on the porous plant tissue with a reduced ternary model without the ice as an individual modelling constituent. Therefore, the focus is on the water management at two porosity scales. Furthermore, the location of the maximum ice accumulation can be determined, which is an interesting result. Note that the accumulation of water in regions, where ice formation is not a threat for the structural integrity of the plant is a crucial factor with regard to their frost hardiness.

# 7.2 Outlook

With these results, the macroscopic theory for ice formation in plant tissues is set up, which includes crucial properties of frost resistance. This model can be easily transferred to other porous materials in subzero environments, such as porous construction materials. However, it is not yet clear, how the new frost resistant construction material would be like that is based on the mechanisms of plant tissues that goes beyond the well-known strategy of air spaces in the material.

In general, the mechanisms of frost resistance of plants, especially those that are based on the formation of extracellular ice, which dehydrates the tissue cells based on the micro porosity of the cell wall, are quite well established. However, the relation of the (changes in) microstructure and/or material parameters to the involved bio-physical processes is not yet fully understood to the best of the author's knowledge. Especially the time sequence of the involved bio-physical processes, the change in the microstructure, and how it relates to the frost resistance of the plants is not yet established.

Furthermore, the homogenisation of the mass-interaction terms from surface-specific quantities towards volume-specific quantities is crucial. As of now, unit-cell models are applied, however, their accuracy is not clear. Thus, homogenisation methods that are much closer to the plant tissue, potentially based on image analysis and non-invasive experimental procedures, would be desirable. Also, a loop back to the plant analysis is needed in terms of model calibration and model validation.

With this knowledge, more meaningful simulations beyond the revelation of the basic

processes may be conducted. This, however, might also lead to the necessity to further develop the numerical procedure. In detail, more complex geometries might be necessary with a higher number of degrees of freedom. Thus, a parallelisation of the computations in PANDAS would be essential, the results within this monograph were obtained with computations on one CPU. However, a coupling of PANDAS to commercial software packages has already been conducted for other material elements.

Finally, an investigation is required what kind of engineering material is necessary, that fulfils the set of properties that is known from plants.

# Appendix A: Proof of thermodynamic consistency of the reduced model

For the sake of completeness, the evaluation of the entropy inequality of the reduced ternary model is stated in this appendix. Note that an excerpt of this evaluation is part of Eurich *et al.* [67]. In this context, the procedure includes specifically the necessary restrictions for the response functions in context of the ternary Model II. Note that for Model II, the number of governing equations is reduced compared to Model I, corresponding to the number of constituents, compare **Section 4.8** with **Subsection 4.9.3**.

The saturation constraint and effective stress principle: The establishment of the necessary restrictions to develop the material-specific equations for the ternary model are based on the very same considerations as for the quaternary model. Therefore, starting point is the entropy inequality in *Clausius-Duhem* form (A.1) for the overall, here ternary, aggregate, viz.:

$$\sum_{\alpha} \{-\rho^{\alpha}[(\psi^{\alpha})'_{\alpha} + \theta'_{\alpha}\eta^{\alpha}] - \hat{\mathbf{p}}^{\alpha} \cdot \mathbf{\dot{x}}_{\alpha} - \hat{\rho}^{\alpha}(\psi^{\alpha} + \frac{1}{2} \mathbf{\dot{x}}_{\alpha} \cdot \mathbf{\dot{x}}_{\alpha}) + \mathbf{T}^{\alpha} \cdot \mathbf{L}_{\alpha} - \frac{1}{\theta} \mathbf{q}^{\alpha} \cdot \operatorname{grad} \theta - \mathcal{P}(n^{\alpha})'_{S}\} \ge 0.$$
(A.1)

Therein, the saturation condition has already been included as a side condition by means of the time derivative  $(\cdot)'_S$  of (4.163) multiplied with the *Lagrange*an multiplier  $\mathcal{P}$ . The saturation condition yields the following expression

$$\sum_{\alpha} (n^{\alpha})'_{S} = (n^{S})'_{S} + (n^{L})'_{L} + (n^{G})'_{G} - \operatorname{grad} n^{L} \cdot \mathbf{w}_{L} - \operatorname{grad} n^{G} \cdot \mathbf{w}_{G} =$$

$$= \frac{\hat{\rho}^{S}}{\rho^{SR}} - n^{S} \mathbf{I} \cdot \mathbf{D}_{S} - \frac{n^{S}}{\rho^{SR}} \frac{\partial \rho^{SR}}{\partial \theta} \theta'_{S} -$$

$$- \frac{\hat{\rho}^{S}}{\rho^{LR}} - n^{L} \mathbf{I} \cdot \mathbf{D}_{L} - \frac{n^{L}}{\rho^{LR}} \frac{\partial \rho^{LR}}{\partial \theta} \theta'_{L} - \operatorname{grad} n^{L} \cdot \mathbf{w}_{L} -$$

$$- n^{G} \mathbf{I} \cdot \mathbf{D}_{G} - \frac{n^{G}}{\rho^{GR}} (\rho^{GR})'_{G} - \operatorname{grad} n^{G} \cdot \mathbf{w}_{G} = 0.$$
(A.2)
The saturation condition (A.2) will be inserted into (A.1), which yields

$$\begin{split} &(\underbrace{\mathbf{T}^{S} + n^{S}\mathcal{P}\mathbf{I}}_{\mathbf{T}_{E}^{S}}) \cdot \mathbf{D}_{S} - \rho^{S}(\psi^{S})_{S}^{\prime} - \rho^{S}[\underbrace{\eta^{S} - \mathcal{P}\frac{1}{(\rho^{SR})^{2}}\frac{\partial\rho^{SR}}{\partial\theta}}]\theta_{S}^{\prime} + \\ &+ \underbrace{(\underbrace{\mathbf{T}^{L} + n^{L}\mathcal{P}\mathbf{I}}_{\mathbf{T}_{E}^{L}}) \cdot \mathbf{D}_{L} - \rho^{L}(\psi^{L})_{L}^{\prime} - \rho^{L}[\underbrace{\eta^{L} - \mathcal{P}\frac{1}{(\rho^{LR})^{2}}\frac{\partial\rho^{LR}}{\partial\theta}}]\theta_{L}^{\prime} + \\ &+ \underbrace{(\underbrace{\mathbf{T}^{G} + n^{G}\mathcal{P}\mathbf{I}}_{\mathbf{T}_{E}^{G}}) \cdot \mathbf{D}_{G} - \rho^{G}(\psi^{G})_{G}^{\prime} - \rho^{G}\eta^{G}\theta_{G}^{\prime} + \mathcal{P}\frac{n^{G}}{\rho^{GR}}(\rho^{GR})_{G}^{\prime} - \\ &- \underbrace{(\underbrace{\hat{\mathbf{p}}^{L} - \mathcal{P}\operatorname{grad}n^{L}}_{\mathbf{p}_{E}^{L}}) \cdot \mathbf{w}_{L} - \widehat{\rho^{S}}\overset{\prime}{\mathbf{x}}_{S} \cdot \mathbf{w}_{L} - \\ &- \underbrace{(\underbrace{\hat{\mathbf{p}}^{G} - \mathcal{P}\operatorname{grad}n^{G}}_{\mathbf{p}_{E}^{G}}) \cdot \mathbf{w}_{G} - \frac{1}{\theta}(\mathbf{q}^{S} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \operatorname{grad}\theta - \\ &- \widehat{\rho^{S}}(\psi^{S} + \frac{1}{2}\overset{\prime}{\mathbf{x}}_{S} \cdot \overset{\prime}{\mathbf{x}}_{S} - \psi^{L} - \frac{1}{2}\overset{\prime}{\mathbf{x}}_{L} \cdot \overset{\prime}{\mathbf{x}}_{L} + \frac{\mathcal{P}}{\rho^{SR}} - \frac{\mathcal{P}}{\rho^{LR}}) \ge 0. \end{split}$$

Therein, the extra quantities, as defined in (4.23), are defined for the ternary model accordingly via

$$\mathbf{T}_{E}^{S} = \mathbf{T}^{S} + n^{S} \mathcal{P} \mathbf{I}, \qquad \mathbf{T}_{E}^{L} = \mathbf{T}^{L} + n^{L} \mathcal{P} \mathbf{I}, \qquad \mathbf{T}_{E}^{G} = \mathbf{T}^{G} + n^{G} \mathcal{P} \mathbf{I},$$
$$\hat{\mathbf{p}}_{E}^{L} = \hat{\mathbf{p}}^{L} - \mathcal{P} \operatorname{grad} n^{L}, \qquad \hat{\mathbf{p}}_{E}^{G} = \hat{\mathbf{p}}^{G} - \mathcal{P} \operatorname{grad} n^{G}, \qquad \eta_{E}^{S} = \eta^{S} - \mathcal{P} \frac{1}{(\rho^{SR})^{2}} \frac{\partial \rho^{SR}}{\partial \theta},$$
$$\eta_{E}^{L} = \eta^{L} - \mathcal{P} \frac{1}{(\rho^{LR})^{2}} \frac{\partial \rho^{LR}}{\partial \theta}. \qquad (A.4)$$

These extra quantities, in turn, are inserted into the entropy inequality (A.3), what leads to the form of the entropy inequality as follows

$$\mathbf{T}_{E}^{S} \cdot \mathbf{D}_{S} - \rho^{S}(\psi^{S})_{S}^{\prime} - \rho^{S}\eta_{E}^{S}\theta_{S}^{\prime} + \mathbf{T}_{E}^{L} \cdot \mathbf{D}_{L} - \rho^{L}(\psi^{L})_{L}^{\prime} - \rho^{L}\eta_{E}^{L}\theta_{L}^{\prime} + + \mathbf{T}_{E}^{G} \cdot \mathbf{D}_{G} - \rho^{G}(\psi^{G})_{G}^{\prime} - \rho^{G}\eta^{G}\theta_{G}^{\prime} + \mathcal{P}\frac{n^{G}}{\rho^{GR}}(\rho^{GR})_{G}^{\prime} - - \hat{\mathbf{p}}_{E}^{L} \cdot \mathbf{w}_{L} - \hat{\rho}^{S} \stackrel{\prime}{\mathbf{x}}_{S} \cdot \mathbf{w}_{L} - \hat{\mathbf{p}}_{E}^{G} \cdot \mathbf{w}_{G} - \frac{1}{\theta}(\mathbf{q}^{S} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \operatorname{grad} \theta - - \hat{\rho}^{S}(\psi^{S} + \frac{1}{2}\stackrel{\prime}{\mathbf{x}}_{S} \cdot \stackrel{\prime}{\mathbf{x}}_{S} - \psi^{L} - \frac{1}{2}\stackrel{\prime}{\mathbf{x}}_{L} \cdot \stackrel{\prime}{\mathbf{x}}_{L} + \frac{\mathcal{P}}{\rho^{SR}} - \frac{\mathcal{P}}{\rho^{LR}}) \geq 0.$$
(A.5)

**Thermodynamical principles and process variables:** Those quantities, that cannot directly be determined from the initial state, the primary variables or their derivatives, need to be introduced as response functions for which constitutive equations need to be found. In particular, these are given via

$$\mathcal{R} = \{\psi^{\alpha}, \mathbf{T}_{E}^{\alpha}, \eta_{E}^{S}, \eta_{E}^{L}, \eta^{G}, \hat{\mathbf{p}}_{E}^{\beta}, \hat{\rho}^{S}, \mathbf{q}^{\alpha}\}.$$
(A.6)

The set of process variables that need to be considered are given in (4.26). For the given problem at hand, a reduced set is sufficient, where the respective process variables for a specific constituent are given via

$$\psi^{S} = \psi^{S}(\theta, \operatorname{grad} \theta, \mathbf{C}_{S}, \operatorname{Grad}_{S} \mathbf{C}_{S}, \mathcal{M}^{S}),$$
  

$$\psi^{L} = \psi^{L}(\theta, \operatorname{grad} \theta, s^{L}, \operatorname{grad} s^{L}, \mathbf{w}_{L}, \mathbf{D}_{L}),$$
  

$$\psi^{G} = \psi^{G}(\theta, \operatorname{grad} \theta, \rho^{GR}, \operatorname{grad} \rho^{GR}, \mathbf{w}_{G}, \mathbf{D}_{G}),$$
  
(A.7)

when phase separation is assumed. The material time derivatives of the *Helmholtz* free energies  $\psi^{\alpha}$  are determined by making use of the chain rule, viz.:

$$\begin{aligned} (\psi^{S})'_{S} &= \frac{\partial \psi^{S}}{\partial \theta} \,\theta'_{S} + \frac{\partial \psi^{S}}{\partial \text{grad} \theta} \cdot (\text{grad} \,\theta)'_{S} + \frac{\partial \psi^{S}}{\partial \mathbf{C}_{S}} \cdot (\mathbf{C}_{S})'_{S} + \frac{\partial \psi^{S}}{\partial \text{Grad}_{S} \,\mathbf{C}_{S}} \cdot (\text{Grad}_{S} \,\mathbf{C}_{S})'_{S}, \\ (\psi^{L})'_{L} &= \frac{\partial \psi^{L}}{\partial \theta} \,\theta'_{L} + \frac{\partial \psi^{L}}{\partial \text{grad} \,\theta} \cdot (\text{grad} \,\theta)'_{L} + \frac{\partial \psi^{L}}{\partial s^{L}} (s^{L})'_{L} + \frac{\partial \psi^{L}}{\partial \text{grad} \,s^{L}} \cdot (\text{grad} \,s^{L})'_{L} + \\ &+ \frac{\partial \psi^{L}}{\partial \mathbf{w}_{L}} \cdot (\mathbf{w}_{L})'_{L} + \frac{\partial \psi^{L}}{\partial \mathbf{D}_{L}} \cdot (\mathbf{D}_{L})'_{L}, \\ (\psi^{G})'_{G} &= \frac{\partial \psi^{G}}{\partial \theta} \,\theta'_{G} + \frac{\partial \psi^{G}}{\partial \text{grad} \,\theta} \cdot (\text{grad} \,\theta)'_{G} + \frac{\partial \psi^{G}}{\partial \rho^{GR}} (\rho^{GR})'_{G} + \frac{\partial \psi^{G}}{\partial \text{grad} \,\rho^{GR}} \cdot (\text{grad} \,\rho^{GR})'_{G} + \\ &+ \frac{\partial \psi^{G}}{\partial \mathbf{w}_{G}} \cdot (\mathbf{w}_{G})'_{G} + \frac{\partial \psi^{G}}{\partial \mathbf{D}_{G}} \cdot (\mathbf{D}_{G})'_{G}. \end{aligned}$$
(A.8)

**Thermodynamical restrictions:** The inclusion of the derivatives of the *Helmholtz* free energies (A.8) into the entropy inequality (A.5) yields

$$\mathbf{T}_{E}^{S} \cdot \mathbf{D}_{S} - \rho^{S} \frac{\partial \psi^{S}}{\partial \theta} \theta'_{S} - \rho^{S} \frac{\partial \psi^{S}}{\partial \operatorname{grad} \theta} \cdot (\operatorname{grad} \theta)'_{S} - \rho^{S} \frac{\partial \psi^{S}}{\partial \mathbf{C}_{S}} \cdot (\mathbf{C}_{S})'_{S} - \rho^{S} \frac{\partial \psi^{S}}{\partial \mathbf{C}_{S}} \cdot (\operatorname{Grad}_{S} \mathbf{C}_{S})'_{S} - \rho^{S} \eta^{S}_{E} \theta'_{S} + \\ + \mathbf{T}_{E}^{L} \cdot \mathbf{D}_{L} - \rho^{L} \frac{\partial \psi^{L}}{\partial \theta} \theta'_{L} - \rho^{L} \frac{\partial \psi^{L}}{\partial \operatorname{grad} \theta} \cdot (\operatorname{grad} \theta)'_{L} - \rho^{L} \frac{\partial \psi^{L}}{\partial \mathbf{D}_{L}} (\mathbf{D}_{L})'_{L} - \rho^{L} \eta^{L}_{E} \theta'_{L} + \\ - \rho^{L} \frac{\partial \psi^{L}}{\partial \operatorname{grad} s^{L}} \cdot (\operatorname{grad} s^{L})'_{L} - \rho^{L} \frac{\partial \psi^{G}}{\partial \mathbf{w}_{L}} \cdot (\mathbf{w}_{L})'_{L} - \rho^{L} \frac{\partial \psi^{L}}{\partial \mathbf{D}_{L}} \cdot (\mathbf{D}_{L})'_{L} - \rho^{L} \eta^{L}_{E} \theta'_{L} + \\ + \mathbf{T}_{E}^{G} \cdot \mathbf{D}_{G} - \rho^{G} \frac{\partial \psi^{G}}{\partial \theta} \theta'_{G} - \rho^{G} \frac{\partial \psi^{G}}{\partial \operatorname{grad} \theta} \cdot (\operatorname{grad} \theta)'_{G} - \rho^{G} \frac{\partial \psi^{G}}{\partial \rho^{GR}} (\rho^{GR})'_{G} - \\ - \rho^{G} \frac{\partial \psi^{G}}{\partial \operatorname{grad} \rho^{GR}} \cdot (\operatorname{grad} \rho^{GR})'_{G} - \rho^{G} \frac{\partial \psi^{G}}{\partial \mathbf{w}_{G}} \cdot (\mathbf{w}_{G})'_{G} - \rho^{G} \frac{\partial \psi^{G}}{\partial \mathbf{D}_{G}} \cdot (\mathbf{D}_{G})'_{G} - \rho^{G} \eta^{G} \theta'_{G} - \\ - \hat{p}_{E}^{L} \cdot \mathbf{w}_{L} - \hat{\rho}^{S} \mathbf{x}_{S} \cdot \mathbf{w}_{L} - \hat{\mathbf{p}}_{E}^{G} \cdot \mathbf{w}_{G} - \\ - \frac{1}{\theta} (\mathbf{q}^{S} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \operatorname{grad} \theta + \mathcal{P} \frac{n^{G}}{\rho^{GR}} (\rho^{GR})'_{G} - \\ - \hat{\rho}^{S} (\psi^{S} + \frac{1}{2} \mathbf{x}_{S} \cdot \mathbf{x}_{S} - \psi^{L} - \frac{1}{2} \mathbf{x}_{L} \cdot \mathbf{x}_{L} + \frac{\mathcal{P}}{\rho^{SR}} - \frac{\mathcal{P}}{\rho^{LR}}) \ge 0.$$

Since (A.9) has to be fulfilled for arbitrary values of the derivatives  $(\operatorname{grad} \theta)'_S$ ,  $(\operatorname{Grad}_S \mathbf{C}_S)'_S$ ,  $(\operatorname{grad} \theta)'_L$ ,  $(\operatorname{grad} s^L)'_L$ ,  $(\mathbf{w}_L)'_L$ ,  $(\mathbf{D}_L)'_L$ ,  $(\operatorname{grad} \theta)'_G$ ,  $(\operatorname{grad} \rho^{GR})'_G$ ,  $(\mathbf{w}_G)'_G$  and  $(\mathbf{D}_G)'_G$ , the factors in front of these variables have to vanish for the equilibrium case, such that

$$\frac{\partial \psi^{S}}{\partial \operatorname{grad} \theta} = \mathbf{0}, \qquad \frac{\partial \psi^{S}}{\partial \operatorname{Grad}_{S} \mathbf{C}_{S}} = \overset{3}{\mathbf{0}}, 
\frac{\partial \psi^{L}}{\partial \operatorname{grad} \theta} = \mathbf{0}, \qquad \frac{\partial \psi^{S}}{\partial \operatorname{grad} s^{L}} = \mathbf{0}, 
\frac{\partial \psi^{L}}{\partial \mathbf{w}_{L}} = \mathbf{0}, \qquad \frac{\partial \psi^{L}}{\partial \mathbf{D}_{L}} = \mathbf{0}, 
\frac{\partial \psi^{G}}{\partial \operatorname{grad} \theta} = \mathbf{0}, \qquad \frac{\partial \psi^{G}}{\partial \operatorname{grad} \rho^{GR}} = \mathbf{0}, 
\frac{\partial \psi^{G}}{\partial \mathbf{w}_{G}} = \mathbf{0}, \qquad \frac{\partial \psi^{G}}{\partial \mathbf{D}_{G}} = \mathbf{0}.$$
(A.10)

Consequently, the *Helmholtz* free energies  $\psi^{\alpha}$  depend on the following process variables

$$\psi^S = \psi^S(\theta, \mathbf{C}_S, \mathcal{M}^S), \quad \psi^L = \psi^L(\theta, s^L), \quad \psi^G = \psi^G(\theta, \rho^{GR}).$$
 (A.11)

Furthermore, the derivative of the liquid saturation with respect to the motion of the liquid is included by making use of the mass balances and the quotient rule of calculus

via

$$(s^{L})'_{L} = -\frac{\hat{\rho}^{S}}{n^{F}\rho^{LR}} - s^{L}\mathbf{I}\cdot\mathbf{D}_{L} - \frac{s^{L}}{\rho^{LR}}\frac{\partial\rho^{LR}}{\partial\theta}\theta'_{L} + \frac{s^{L}\hat{\rho}^{S}}{n^{F}\rho^{SR}} - \frac{s^{L}n^{S}}{n^{F}}\mathbf{I}\cdot\mathbf{D}_{S} - \frac{s^{L}n^{S}}{n^{F}\rho^{SR}}\frac{\partial\rho^{SR}}{\partial\theta}\theta'_{S} + \frac{s^{L}}{n^{F}}\operatorname{grad} n^{S}\cdot\mathbf{w}_{L}.$$
(A.12)

Equation (A.12) is inserted into the entropy inequality (A.9) to state its final form

$$\begin{split} \underbrace{[\mathbf{T}_{E}^{S} + n^{S}(s^{L})^{2}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\mathbf{I}}_{\mathbf{T}_{E\,\mathrm{mech}}^{S}} - 2\rho^{S}\mathbf{F}_{S}\frac{\partial\psi^{S}}{\partial\mathbf{C}_{S}}\mathbf{F}_{S}^{T}]\cdot\mathbf{D}_{S} - \\ - \rho^{S}[\eta_{E}^{S} - (s^{L})^{2}\frac{\rho^{LR}}{(\rho^{SR})^{2}}\frac{\partial\psi^{L}}{\partial s^{L}}\frac{\partial\rho^{SR}}{\partial \theta}} + \frac{\partial\psi^{S}}{\partial \theta}]\theta'_{S} + \\ + \underbrace{(\mathbf{T}_{E}^{L} + n^{L}s^{L}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\mathbf{I})\cdot\mathbf{D}_{L} - \rho^{L}(\eta_{E}^{L} - s^{L}\frac{1}{\rho^{LR}}\frac{\partial\psi^{L}}{\partial s^{L}}\frac{\partial\rho^{LR}}{\partial \theta}} + \frac{\partial\psi^{L}}{\partial \theta})\theta'_{L} + \\ + \mathbf{T}_{E}^{G}\cdot\mathbf{D}_{G} - \rho^{G}(\eta^{G} + \frac{\partial\psi^{G}}{\partial \theta})\theta'_{G} + (\mathcal{P}\frac{n^{G}}{\rho^{GR}} - \rho^{G}\frac{\partial\psi^{G}}{\partial\rho^{GR}})(\rho^{GR})'_{G} - \\ - \underbrace{[\hat{\mathbf{p}}_{E}^{L} + (s^{L})^{2}\rho^{LR}\frac{\partial\psi^{L}}{\partial s^{L}}\operatorname{grad} n^{S} + \hat{\rho}^{S}\overset{'}{\mathbf{x}_{S}}]\cdot\mathbf{w}_{L} - \\ - \hat{\mathbf{p}}_{E}^{G}\cdot\mathbf{w}_{G} - \frac{1}{\theta}(\mathbf{q}^{S} + \mathbf{q}^{L} + \mathbf{q}^{G})\cdot\operatorname{grad}\theta - \\ - \hat{\rho}^{S}[\psi^{S} + \frac{1}{2}\overset{'}{\mathbf{x}_{S}}\cdot\overset{'}{\mathbf{x}_{S}} - \psi^{L} - \frac{1}{2}\overset{'}{\mathbf{x}_{L}}\cdot\overset{'}{\mathbf{x}_{L}} + \mathcal{P}\frac{1}{\rho^{SR}} - \mathcal{P}\frac{1}{\rho^{LR}} + \\ + (s^{L})^{2}\frac{\rho^{LR}}{\rho^{SR}}\frac{\partial\psi^{L}}{\partial s^{L}} - s^{L}\frac{\partial\psi^{L}}{\partial s^{L}}] \geq 0. \end{split}$$
(A.13)

Being an equilibrium part of (A.13), the Lagrangean multiplier reads

$$\mathcal{P} = (\rho^{GR})^2 \frac{\partial \psi^G}{\partial \rho^{GR}} =: p^{GR}, \qquad (A.14)$$

and can be identified as the excess gas pressure, as defined in (4.35).

The fluid stresses  $\mathbf{T}^{\beta}$  contain equilibrium and non-equilibrium parts, where the non-equilibrium parts vanish, viz.:

$$\mathbf{T}_{E}^{G} = \mathbf{0} \quad \text{and} \quad \mathbf{T}_{E\,\text{dis}}^{L} = \mathbf{0}.$$
 (A.15)

Thus, the equilibrium fluid stresses read as in (4.37), respectively, viz.:

$$\mathbf{T}^{G} = -n^{G} p^{GR} \mathbf{I},$$
  

$$\mathbf{T}^{L} = -n^{L} (p^{GR} + s^{L} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}}) \mathbf{I} =: -n^{L} p^{LR} \mathbf{I}.$$
(A.16)

Based on (A.16)<sub>2</sub>, a comparison of the gas pressure  $p^{GR}$  and the liquid pressure  $p^{LR}$  yields

$$p^{LR} = p^{GR} + s^L \rho^{LR} \frac{\partial \psi^L}{\partial s^L}.$$
 (A.17)

The evaluation of the stress of the solid skeleton is based on the first line of (A.13) yielding

$$\mathbf{T}_{E\,\mathrm{mech}}^{S} = \mathbf{T}_{E}^{S} + n^{S} (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} \mathbf{I}.$$
 (A.18)

The partial stress  $\mathbf{T}^{S}$  is derived based on  $(A.4)_{1}$  and (A.18), and is given via

$$\mathbf{T}^{S} = -n^{S} [p^{GR} + (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}}] \mathbf{I} + \mathbf{T}^{S}_{E \operatorname{mech}} = -n^{S} p^{FR} \mathbf{I} + \mathbf{T}^{S}_{E \operatorname{mech}},$$
(A.19)

where

$$p^{FR} := s^L p^{LR} + s^G p^{GR},$$
  

$$\mathbf{T}^S_{E \,\mathrm{mech}} = 2\rho^S \mathbf{F}_S \frac{\partial \psi^S}{\partial \mathbf{C}_S} \mathbf{F}^T_S.$$
(A.20)

The stress  $\mathbf{T}_{E\,\text{mech}}^S$  is found based on  $(A.20)_2$ . These equations are excactly the same as for the quaternary model in (4.38)-(4.41).

Finally, the thermodynamical restrictions for the entropies can be found in case of thermodynamical equilibrium. Thus, the entropy of the solid skeleton reads

$$\eta_{E\,\mathrm{mech}}^{S} = \eta_{E}^{S} - (s^{L})^{2} \frac{\rho^{LR}}{(\rho^{SR})^{2}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{SR}}{\partial \theta} =$$

$$= \eta^{S} - p^{GR} \frac{1}{(\rho^{SR})^{2}} \frac{\partial \rho^{SR}}{\partial \theta} - (s^{L})^{2} \frac{\rho^{LR}}{(\rho^{SR})^{2}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{SR}}{\partial \theta} =$$

$$= \eta^{S} - \frac{p^{FR}}{(\rho^{SR})^{2}} \frac{\partial \rho^{SR}}{\partial \theta} =$$

$$= -\frac{\partial \psi^{S}}{\partial \theta},$$
(A.21)

for the liquid water it is given via

$$\eta_{E \,\mathrm{mech}}^{L} = \eta_{E}^{L} - s^{L} \frac{1}{\rho^{LR}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{LR}}{\partial \theta} =$$

$$= \eta^{L} - p^{GR} \frac{1}{(\rho^{LR})^{2}} \frac{\partial \rho^{LR}}{\partial \theta} - s^{L} \frac{1}{\rho^{LR}} \frac{\partial \psi^{L}}{\partial s^{L}} \frac{\partial \rho^{LR}}{\partial \theta} =$$

$$= \eta^{L} - \frac{p^{LR}}{(\rho^{LR})^{2}} \frac{\partial \rho^{LR}}{\partial \theta} =$$

$$= -\frac{\partial \psi^{L}}{\partial \theta}$$
(A.22)

and, finally, for the gaseous constituent via

$$\eta^G = -\frac{\partial \psi^G}{\partial \theta}.\tag{A.23}$$

Note that the evaluation of (A.21)-(A.23) reveals the same functions as for the quaternary model in (4.45), (4.47) and (4.48), respectively. Since the terms introduced thus far do not represent interaction terms, but solely constituent-specific quantities, phase separation requires the result to be the same as for the quaternary model. Only interaction terms are allowed to depend on process variables of another constituent.

In terms of the non-equilibrium parts of (A.13), the dissipative expression of the liquid momentum production reads

$$\hat{\mathbf{p}}_{E\,\text{dis}}^{L} = \hat{\mathbf{p}}_{E}^{L} + (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} \operatorname{grad} n^{S} + \hat{\rho}^{S} \mathbf{\dot{x}}_{S} =$$

$$= \hat{\mathbf{p}}^{L} - p^{GR} \operatorname{grad} n^{L} + (s^{L})^{2} \rho^{LR} \frac{\partial \psi^{L}}{\partial s^{L}} \operatorname{grad} n^{S} + \hat{\rho}^{S} \mathbf{\dot{x}}_{S} =$$

$$= \hat{\mathbf{p}}^{L} - p^{GR} \operatorname{grad} n^{L} - s^{L} p^{C} \operatorname{grad} n^{S} + \hat{\rho}^{S} \mathbf{\dot{x}}_{S} .$$
(A.24)

It is evident that the terms, which are in (4.49) associated to the ice momentum production and to the gradient of the ice volume fraction, are missing in (A.24). The non-equilibrium terms of (A.13) can be summarised as the dissipation inequality

$$\mathcal{D} = -\hat{\mathbf{p}}_{E\,\text{dis}}^{L} \cdot \mathbf{w}_{L} - \hat{\mathbf{p}}_{E}^{G} \cdot \mathbf{w}_{G} - \frac{1}{\theta} (\mathbf{q}^{S} + \mathbf{q}^{L} + \mathbf{q}^{G}) \cdot \text{grad}\,\theta - \\ -\hat{\rho}^{S} \left(\psi^{S} + \frac{p^{FR}}{\rho^{SR}} + \frac{1}{2} \,\mathbf{x}_{S}^{\prime} \cdot \mathbf{x}_{S}^{\prime} - \psi^{L} - \frac{p^{LR}}{\rho^{LR}} - \frac{1}{2} \,\mathbf{x}_{L}^{\prime} \cdot \mathbf{x}_{L}^{\prime}\right) \ge 0.$$
(A.25)

In order to fulfil dissipation inequality (A.25) for arbitrary processes, the following assumptions are made

$$\hat{\mathbf{p}}_{E\,\mathrm{dis}}^{L} \propto -\mathbf{w}_{L}, \quad \hat{\mathbf{p}}_{E}^{G} \propto -\mathbf{w}_{G}, \quad \mathbf{q}^{\alpha} \propto -\mathrm{grad}\,\theta.$$
 (A.26)

Furthermore, with regard to the mass interaction, the constraint reads

$$\hat{\rho}^{S} \propto -(\psi^{S} + \frac{p^{FR}}{\rho^{SR}} + \frac{1}{2} \, \mathbf{\dot{x}}_{S} \cdot \mathbf{\dot{x}}_{S} - \psi^{L} - \frac{p^{LR}}{\rho^{LR}} - \frac{1}{2} \, \mathbf{\dot{x}}_{L} \cdot \mathbf{\dot{x}}_{L}). \tag{A.27}$$

Based on (A.26) and (A.27), the material laws have to be proposed. Finally, the evaluation of the entropy inequality of the ternary model shows that the quaternary model is donward compatible. Therefore, the constitutive equations for the quantities  $\hat{\mathbf{p}}_{E\,\text{dis}}^{L}$ ,  $\hat{\mathbf{p}}_{E}^{G}$ ,  $\mathbf{q}^{\alpha}$  and  $\hat{\rho}^{S}$ in (A.26) and (A.27), respectively, can be found in (4.93)<sub>1</sub>, (4.93)<sub>2</sub>, (4.116)<sub>1</sub> and (4.150), and are the same as for the quaternary model.

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ISBN 978-3-937399-38-6 (D93 - Dissertation, Universität Stuttgart)