**Proceedings of the 7th GACM Colloquium on Computational Mechanics
for Young Scientists from Academia and Industry
October 11-13, 2017 in Stuttgart, Germany**

Modelling functional properties of frost-resistant plant tissues for transfer to construction materials

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Micro Abstract
While frost is a common threat for construction materials, plants have developed strategies to cope with freezing processes. In this contribution, a biologically motivated rigorous modelling approach of a multicomponent aggregate is presented using the framework of the Theory of Porous Media. For a selected numerical example, crucial effects of plants with regard to frost resistance, such as the cell dehydration and the water management, are discussed.

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Introduction and biological background

The exposure to subzero temperatures represents a common threat for conventional construction materials. Since a phase change of the liquid pore water to solid ice implies an increase in volume, the likelihood for the occurrence of damage is particularly high for porous construction materials with a high water saturation. Consequently, damage occurs due to the formation of ice when the local state of stress exceeds the strength of the material, cf. e. g. [12]. In contrast, plants have developed strategies to cope with frost events. Some factors of frost hardiness are of physiological nature. In particular, these are strategies to avoid freezing in the first place, for example lowering the ice nucleation temperature [11]. But also physical processes based on structural properties are a factor of frost hardiness, especially when ice formation cannot be avoided. In that case, the porous structure of the plant plays a crucial role. Ice formation starts at species-specific and tissue-specific locations in the extracellular space, where the phase change of the pore water to solid ice does not threaten the ability of a plant to survive [6]. However, intracellular freezing is always a critical process for plants [13]. The existence of extracellular ice promotes the dehydration of the cells, therewith avoiding ice formation within cells. Thus, besides the porosity-induced heterogeneous and anisotropic permeability properties, governing the water management from the cells to the preferred sites of ice formation, also the hydraulic gradient, which can be derived from the water potential, cf. [8], plays a central role. This contribution introduces a coupled thermo-hygro-mechanical material model based on the Theory of Porous Media (TPM). Therewith, the description of the underlying physical processes of frost hardiness, particularly the phase-change process of the pore water, the water management and the solid deformation can be realised considering their coupled behaviour.

Multiphasic modelling approach

Due to the coupled character of the processes in frost-resistant plants, a modelling approach based on the TPM, cf. e. g. [1, 2], is used. Therein, processes on the microscale are related to a homogenised macroscopic model by a volumetric homogenisation of the microscopic structure within a representative elementary volume (REV), resulting in a model of superimposed and mutually interacting constituents. Based on the works of Eurich et al. [5–7], four constituents are considered for the description of plant tissues. The model proceeds from a thermoelastic solid skeleton, which is formed by the cell bodies containing initially trapped water. Within the pore space, two mobile fluids are present, namely materially compressible air and materially incompressible water, where the latter can be subjected to a phase transition and turns into ice. Phase transitions of a single substance within the framework of the TPM are comprehensively described in the work of Ehlers & Häberle [4] by introducing a singular surface. As outlined in the previous section, plant tissues are porous materials, where porosity occurs on the tissue scale determining the bulk fluid flow, which is mainly caused by evaporation of water on the surface. But also on the cell scale, the material exhibits a porous character, where cell dehydration occurs by water flowing through the pores in the cell wall. Both water transport phenomena are described by adapted Darcy equations. Furthermore, in order to account for the anisotropic and heterogeneous microstructure, material parameters can be assigned for each spatial point individually. In case of the permeability and the thermal conductivity, tensorial material parameters are introduced for the description of anisotropic effects. However, if the morphology of the pore space is altered, the plant tissue may lose its porous character, particularly when the pore content is solid due to a phase transition. This transition of the bulk material from a porous material to a solid material is comprehensively discussed in Eurich et al. [7] by introducing the compaction point as a function of solid deformation and the phase transition of water.

Biological motivation for the application of Darcy's filter law

Controlled water management was recognised as one of the crucial factors for frost hardiness of plant tissues, cf. Mc Cully et al. [9] or Kramer & Boyer [8]. In classical biology references, cf. e. g. Kramer & Boyer [8] or Molz [10], the effective water flow is explained by the introduction of the water potential. Thus, the flow direction of the water is oriented towards the direction of lower water potential. For engineering applications, Darcy's law is established for the description of fluid flow within porous media under the assumptions of negligible frictional forces and quasi-static conditions. According to Ehlers [3], the original formulation by Darcy for the filter velocity was given via

$$n^F \mathbf{w}_F = -\, k^F \operatorname{grad} h, \tag{1}$$

where k^F is the (isotropic) Darcy permeability and h the so-called pressure head (also referred to as piezometric head). By comparing (1) with the concept of the water potential, h can be easily identified as the potential function. As in biology, there are also for engineering applications different contributions to the potential, depending on the modelling approach. Within the rigorous continuum-mechanical framework of the TPM [5], the filter velocity of water in frost-resistant plant tissues is given via

$$n^L \mathbf{w}_L = -\, \frac{\kappa_r^L \mathbf{K}^S}{\mu^{LR}} \, [\operatorname{grad} p^{LR} - \rho^{LR} \mathbf{g} \, - \, \frac{p^C}{s^L} \operatorname{grad} s^L \,]. \tag{2}$$

Therein, κ_r^L is the relative permeability factor, μ^{LR} the effective dynamic viscosity and $\mathbf{K}^S$ the intrinsic permeability tensor of second order. It has been shown in Eurich et al. [6] that this quantity determines significantly the direction of the water flow and is, therefore, characterising the water management crucially. The expression within the brackets is the gradient of the pressure head, where $\operatorname{grad} p^{LR}$ is the contribution that arises from the water pressure, $\rho^{LR}\,\mathbf{g}$ from the gravitational potential and $(p^C/s^L) \operatorname{grad} s^L$ acknowledging the partial saturation within plant tissues and arises, therefore, at the liquid-gaseous interface from the interaction of the involved fluids. In detail, p^{LR} is the effective water pressure, ρ^{LR} the effective density, $\mathbf{g}$ the gravitational acceleration, p^C the capillary pressure and s^L the liquid saturation.

Numerical example

According to Eurich et al. [5], the governing equations of the plant model are the momentum and the energy balance of the overall aggregate and the mass balances of the pore fluids, to solve the primary variables solid displacement $\mathbf{u}_S$, temperature θ and fluid pressures p^{LR} and p^{GR}, respectively. In order to account for the strongly coupled character of the underlying processes, a monolithic solution scheme has been applied using mixed finite elements with quadratic approximations for the solid displacement and linear approximations for the other unknowns using the Finite-Element tool PANDAS (Porous media Adaptive Nonlinear finite element solver based on Differential Algebraic Systems, http://www.get-pandas.com).

At the example of the so-called winter horsetail, the coupled processes are studied. The cross-section has a characteristic shape, with a large gas-filled compartment in its centre and smaller gas bubbles distributed in the cross-section. For an idealised cross-section, the temperature distribution can be calculated as shown in Figure 1, when a temperature drop on the outer surface is prescribed as during a frost experiment. As the temperature is in the gas-filled compartments for some time higher than in the surrounding tissue, water accumulates at the edges due to condensation of humidity in the air. As condensation is not included in the theoretical model, the simulation accounts for a simplified model, where a film of pure water is assumed to be initially present at the inner edge, the gas constituent is assumed to be solely air. Therefore, when the temperature at the inner edge falls below the freezing point at $273.15\,K$, the water starts to freeze, as shown in Figure 2. Note, that the reduced ice nucleation temperature of the trapped water within the tissue is taken into account in the simulation. The ice formation at the inner edge leads, in turn, to a dehydration of the tissue cells, effectively caused by a decrease of the pressure head, as motivated in the preceding section.

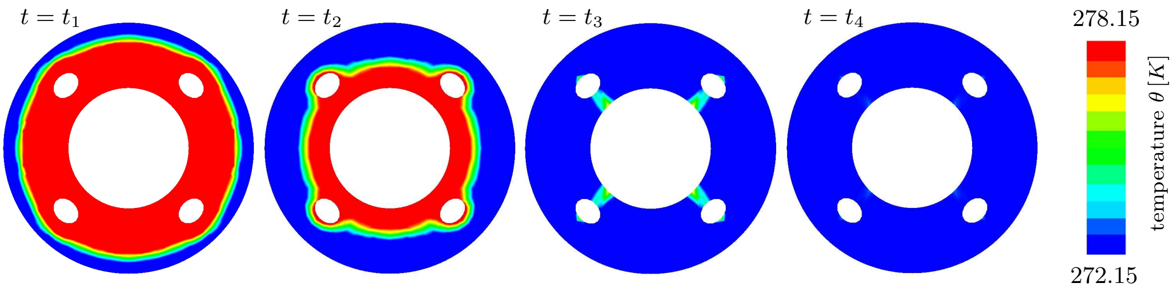

Figure 1. Temperature distribution in a winter horsetail cross-section during a freezing experiment for selected time steps.

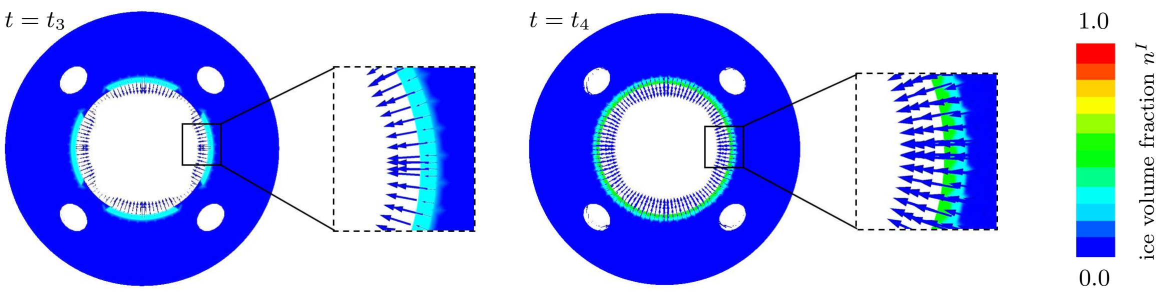

Figure 2. Evolution of the ice volume fraction n^I in a winter horsetail cross-section with resulting water efflux. Note, that there is no ice formation during time steps $t = t_1$ and $t = t_2$.

Conclusions

This contribution discusses the crucial factors with regard to frost hardiness of plant tissues with a focus on physical processes. The introduced TPM-based modelling approach enables a biologically motivated description of the coupled thermo-hygro-mechanical processes. The numerical example shows the dehydration of the cells due to ice formation on inner surfaces of the cross-section and its effect on the water flow management. The understanding in particular of the underlying physical processes of plant tissues with regard to frost hardiness is the first milestone for the development of smart construction materials in the future.

Acknowledgements

This work has been funded by the German Research Foundation (DFG) as part of the Transregional Collaborative Research Centre (SFB/Transregio) 141 "Biological Design and Integrative Structures"/A01.

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