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Microscale modeling of coupled water transport and mechanical deformation of fruit tissue during dehydration

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ABSTRACT

Water loss of fruit typically results in fruit tissue deformation and consequent quality loss. To better understand the mechanism of water loss, a model of water transport between cells and intercellular spaces coupled with cell deformation was developed. Pear (*Pyrus communis* L. cv. Conference) was chosen as a model system as this fruit suffers from shriveling with excessive water loss. A 2D geometric model of cortex tissue was obtained by a virtual fruit tissue generator that is based on cell growth modeling. The transport of water in the intercellular space, the cell wall network and cytoplasm was predicted using transport laws using the chemical potential as the driving force for water exchange between different microstructural compartments. The different water transport properties of the microstructural components were obtained experimentally or from literature. An equivalent microscale model that incorporates the dynamics of mechanical deformation of the cellular structure was implemented. The model predicted the apparent tissue conductivity of pear cortex tissue to be $9.42 \pm 0.40 \times 10^{-15}$ kg m^{-1} s^{-1} Pa^{-1}, in the same range as those measured experimentally. The largest gradients in water content were observed across the cell walls and cell membranes. A sensitivity analysis of membrane permeability and elastic modulus of the wall on the water transport properties and deformation showed that the membrane permeability has the largest influence. The model can be improved further by taking into account 3-D connectivity of cells and intercellular pore spaces. It will then become feasible to evaluate measures to reduce water loss of fruit during storage and distribution using the microscale model in a multiscale modeling framework.

1. Introduction

Fresh fruits are mostly composed of water, the unique universal solvent that is fundamentally important in all life processes. Water loss equates to loss of saleable weight, and thus means a direct loss in revenue, as well as affects overall fruit quality. Measures that minimize water loss after harvest will usually enhance profitability. Loss in weight of only 5% will cause many perishable commodities to appear wilted or shriveled (Wills et al., 1998). Texture is one of the most important quality attributes of fruit and vegetables. Most plant materials contain a significant amount of water and other liquid-soluble materials surrounded by a semi-permeable membrane and cell wall. The texture of fruits and vegetables is dependent on the turgor pressure, and the composition of individual plant cell walls and the middle lamella, which "glues" individual cells together (Barrett et al., 2010). Cell walls are accepted as the main structural component affecting the mechanical properties of fruits and vegetables (Zdunek and Konstankiewicz, 2004; Bourne, 2002; Waldron et al., 2003; Vanstreels et al., 2005). Also the turgor pressure, cell size and shape, volume of vacuole and volume of intercellular spaces, chemical composition have a major influence on tissue strength and macroscopic fruit firmness (Oey et al., 2007).

Shrinkage is one of the major physical changes that occur during the dehydration process. It results from the collapse of cells during water evaporation, which has a negative impact on the quality of dehydrated product. At first, shrinkage causes changes in the shape of the product. These changes are due to the stresses developed while water is removed from the material (Rajchert and Rzace, 2009). Shrinkage during dehydration can be classified in three different types (Gekas, 1992): one-dimensional when the volume change follows the direction of diffusion; (2) isotropic or

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Nomenclature

b	damping factor (–)
c_ψ	water capacity (kg kg_{DM}^{-1} Pa^{-1})
D	diffusion coefficient (m^2 s^{-1})
E	Young's modulus of elasticity (Pa)
F	total force acting upon the node (N)
J	water flux (kg m^{-2})
K_{eff}	water conductivity (kg m^{-1} Pa^{-1} s^{-1})
k	Spring constant (N m^{-1})
l	cell wall length (m)
L	thickness of the simulated tissue (m)
m_i	mass of the vertex (kg)
P_m	permeability of the membrane (m s^{-1})
R	Universal gas constant (8.314) (J mol^{-1} K^{-1})
T	temperature (K)
V_w	molar volume of water (18^*10^{-6}) (m^3 mol^{-1})
v	velocity (m s^{-1})
x	position (m)

Greek symbols

ε	strain (m m^{-1})
ρ_w	density of water (kg m^{-3})
ρ_{DM}	dry matter density (kg_{DM}^{-1} m^{-3})
σ	stress (Pa)
ψ	water potential (Pa)

Subscripts

a	air
c	cell
i	node
m	cell membrane
s	solute
T	total
w	cell wall

three-dimensional; and (3) anisotropic or arbitrary. Volume reduction patterns for fruits and vegetables are often of type 3 and in a less extent of type 2. Shrinkage of apple parenchyma, for example, was found to be highly anisotropic (Mavroudis et al., 1998; Moreira et al., 2000). Cellular shrinkage during dehydration has been observed during osmotic dehydration of parenchymatic pumpkin tissue (Mayor et al., 2008), apple (Lewicki and Porzecka-Pawlak, 2005) and convective drying of grapes (Ramos et al., 2004).

With respect to modeling mechanical deformation of fruit tissue, most models are based on continuum mechanics. It is often assumed that the biologic material behaves as a nonlinear viscoelastic continuum. Recent work has allowed better understanding and modeling the nonlinear shrinkage of fruit tissue at the macroscale (Aregawi et al., 2013; Defraeye et al., 2013). Most microscopic works on the deformation are based on single cell analysis. Feng and Yang (1973) considered the problem of the deformation and the consequential stresses in an inflated, non-linear elastic, gas-filled spherical membrane compressed between two frictionless rigid plates. Lardner and Pujara (1980) extended this model further by considering the sphere to be filled with an incompressible liquid rather than gas. Their model was able to predict accurately the deformation of sea urchin eggs, as previously reported by Yoneda (1973). Liu et al. (1996) improved the computational algorithm, and applied the model to data on microcapsules. None of these studies allowed for water loss from the sphere. Smith et al. (1998) created a finite element model in which volume loss was included, and applied this to compression data from yeast cells (Smith et al., 2000). Using a finite element method, it was possible in principle to consider any cell wall material constitutive equation, although in practice Smith et al. (2000) only considered the linear elastic case. The more recent work is by Dintwa et al. (2011) who developed a finite element model to simulate the compression of a single suspension-cultured tomato cell, using data from Wang et al. (2004). The model could serve as a basic building block for more complex models for tissue deformation under mechanical loading. The model was limited to mechanical loading and not to the deformation due to water loss and also was applied for single cell and not for a real tissue. We have recently developed a cell growth algorithm that generates representative *in silico* fruit tissue geometries from increasing cell turgor in and cell wall generation by the individual cells in a tissue (Abera et al., 2013a). Using this algorithm in the reversed sense, it becomes possible to perform simulations of the deformation mechanics of tissue as a result of hydrostatic stress occurring during water loss.

We previously also modeled water diffusion in pear fruit tissue samples taking into account the cellular structure of the tissue (Fanta et al., 2013). Shrinkage was, however, taken into account in a static manner by considering different equilibrium states at different water contents, using a global shrinkage coefficient the model lacks to incorporate dynamic deformation due to water loss. Using the cell mechanics algorithm, however, the simulation of the deformation of individual cells in the tissue is possible.

The aim of the present work was to combine and apply the microscale transient water transport model with the cell mechanics model for predicting cell and tissue deformation due to water loss in the actual microstructural architecture of the tissue. The model was also used to calculate the apparent water conductivity of the tissue. Pear fruit (*Pyrus communis* L. cv. conference) was used as a model system. Pears quickly deform resulting in shriveling as a consequence of water loss during low temperature storage (Nguyen et al., 2006).

2. Model formulation

2.1. Microscale model of water transport coupled with deformation

2.1.1. Microscale water transport model

Cortex tissue of pear consists of an agglomerate of cells and intercellular spaces of different shapes and sizes (Verboven et al., 2008). To take into account this microstructure, we have introduced the microscopic layout into the modeling as the computational geometry of the model.

The transport of water in the intercellular space, the cell wall network and cytoplasm were modeled using diffusion laws and irreversible thermodynamics (Noble, 1991). The full derivation of the diffusion equation for the tissue compartment (cell, cell wall and intercellular space) can be found in our previous work (Fanta et al., 2013). For the cells, the unsteady-state model of water transport reads:

$$\left(\rho_{\mathrm{DM},c} + x_c \frac{\partial \rho_{\mathrm{DM},c}}{\partial x_c}\right) c_{\psi,c} \frac{\partial \psi_c}{\partial t} = \nabla \cdot D_c \left(\frac{\rho_{\mathrm{DM},c} c_{\psi,c}}{1 + x_c}\right) \nabla \psi_c \tag{1}$$

where $\rho_{DM,c}$ is the dry matter density of the cell (kg_{DM}^{-1} m^{-3}), x_c the dry matter base water content (kg kg_{DM}^{-1}), D_c the water diffusion