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A Particle-Based Micromechanics Approach to Simulate Structural Changes of Plant Cells During Drying

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Abstract
This paper is concerned with applying a particle-based approach to simulate the micro-level cellular structural changes of plant cells during drying. The objective of the investigation was to relate the micro-level structural properties such as cell area, diameter and perimeter to the change of moisture content of the cell. Model assumes a simplified cell which consists of two basic components, cell wall and cell fluid. The cell fluid is assumed to be a Newtonian fluid with higher viscosity compared to water and cell wall is assumed to be a visco-elastic solid boundary located around the cell fluid. Cell fluid is modelled with Smoothed Particle Hydrodynamics (SPH) technique and for the cell wall; a Discrete Element Method (DEM) is used. The developed model is two-dimensional, but accounts for three-dimensional physical properties of real plant cells. Drying phenomena is simulated as fluid mass reductions and the model is used to predict the above mentioned structural properties as a function of cell fluid mass. Model predictions are found to be in fairly good agreement with experimental data in literature and the particle-based approach is demonstrated to be suitable for numerical studies of drying related structural deformations. Also a sensitivity analysis is included to demonstrate the influence of key model parameters to model predictions.

Keywords: Smoothed Particle Hydrodynamics, Mesh-free methods, particle methods, Plant cell models, Food drying, Cell micro mechanics

Introduction
Plant based food products and related processing industries are significantly influencing the current global economy. To preserve most of such plant based food products, drying is used as a key technique and it is believed that more than 20% of worlds perishable crops are being dried for preservation (Grabowski, Marcotte et al. 2003). Also drying is a comparatively advantageous preservation technique compared to other techniques such as freezing and canning due to the reduction of product weight and volume which benefits highly in transportation and storage. Drying processes contribute largely for the industrial energy consumption and it is reported that drying processes consume around 20% of the total industrial energy consumption in developed countries (Jangam and Mujumdar 2010). These highlight the importance of studying the underlying physical mechanisms of the process to improve both the process and the products and even it can lead to new food products with new structures (Bolin and Huxsoll 1987; Bai, Rahman et al. 2002; Aguilera, Chiralt et al. 2003).

The 4th International Conference on Computational Methods (ICCM2012), Gold Coast, Australia
www.ICCM-2012.org
In most of these plant based foods water is contained from 20% to 90% by weight of the bulk material (Jangam 2011). At the same time, all the plant based food structures basically made out of a cellular structure that contains large number of cells. In each of those cells, the cell fluid mainly stores water and during drying processes, water removes mainly from the cell fluid and causes the cellular structure to deform. Many authors have experimentally found out at during a drying process, bulk structural changes are mainly governed by bulk level moisture content of the food material (Suzuki, Kubota et al. 1976; Lozano, Rotstein et al. 1980; Ratti 1994; Moreira, Figueiredo et al. 2000; Bai, Rahman et al. 2002; Mayor and Sereno 2004). It has been further demonstrated that there is a fairly good linear relationship between the cellular structural deformations and the bulk level moisture content. Also, the cellular structural deformation and the bulk level structural deformations are reported to be well interrelated (Lee, Salunkhe et al. 1967; Lozano, Rotstein et al. 1980; Hills and Remigereau 1997; Lewicki 1998; Ramos, Silva et al. 2004; Mayor, Silva et al. 2005). These cellular structural deformations can be characterized by changes of the cell geometrical parameters such as area, diameter and perimeter. In this work, our aim was to numerically study, model and simulate the mechanisms underlying all these drying related cellular structural deformations. Some of the basic research outcomes of this approach were recently presented (Karunasena, Senadeera et al. 2012) and this paper is dedicated to present the further studies of the structural mechanics and sensitivity analysis of the model predictions to key model parameters.

The problem domain involves several complex phenomena. Firstly, food materials undergo excessive deformations during drying due to the influence of intense heat and mass transfer within the process. Secondly, cellular structure is a multi-phase system that contains solid, liquid and gas phases. For example, cell walls can be considered as mainly made out of solid phase, cell cytoplasm can be approximated to a fluid phase medium and intercellular spaces can be assumed as mainly consisting of the gaseous phase. Thirdly, cellular structure is a discrete problem domain consisting of cells, middle lamella and intercellular spaces. Fourthly, the deformations are influenced by both micro and macro level mechanisms and therefore multi-scale approaches are needed to fully define the deformation phenomena. Considering all these different phenomena, conventional grid based techniques such as Finite Element Methods (FEM) and Finite Different Methods (FDM) seems to be not so applicable to model the cellular structure due to their grid-related fundamental limitations. But, recently developed Mesh-free methods seem to be more appropriate to treat this kind of a problem domain (Liu and Liu 2003).

Recently several researchers (Liedekerke, Ghysels et al. 2009; Liedekerke, Ghysels et al. 2010; Van Liedekerke, Ghysels et al. 2011) have developed quite comprehensive SPH – DEM coupled cell models to study the basic mechanical responses of cells to external loading such as compression, tension and shear. Further, they have extended the models to three-dimensional (3-D) single cell models and even simulated cell wall breakages at compression (Van Liedekerke, Tijskens et al. 2010). Also multi-scaling techniques have been proposed for these basic mechanical studies of plant tissues (Ghysels, Samaey et al. 2010; Ghysels, Samaey et al. 2010). The cell model used in the research work presented in this paper is basically two dimensional (2-D) and follows the SPH-DEM models of above authors but with further improvements to cater drying related mechanisms. This paper is organized in such a way that the overall methodology used for the modelling and simulations are given in detail in the next section. There after the simulation results are presented and discussed. Finally the insights implying from the results are presented along with planned future work.
Methodology

Cell model

In this study, a plant tissue is approximated to an aggregate of individual cylindrical cells as shown in Fig. 1. For each individual cell, the top surface can be used as a 2-D model of the actual cell mechanics, if the Z direction deformations are assumed to be uniform and the XY plane stresses and Z directional velocity components are neglected. The model is composed of two basic components, the cell wall and the cell fluid. When considering the cell wall, it is experimentally demonstrated that it usually composed of a fibrous structure with visco-elastic properties and can undergo plastic deformations (Köhler and Spatz 2002). Many researchers (Liedekerke, Ghysels et al. 2010; Van Liedekerke, Tijskens et al. 2010; Van Liedekerke, Ghysels et al. 2011) have used a neo-Hookean solid material (Wu, Spence et al. 1985; Chaplain 1993; Zhu and Melrose 2003) in a Discrete Element Method (DEM) (Loodts, Tijskens et al. 2006; Pathmanathan, Cooper et al. 2009) for their cell wall models demonstrating fairly good agreements with tensile and compressive experimental results. This work basically uses a similar wall model that incorporates stiff forces, damping forces and repulsion forces. But, in addition to these, for better representation of the cellular drying related deformations, two new features are introduced. They are the cell wall-cell fluid attractions and cell wall bending stiffness, which will be explained in next paragraphs.

Above mentioned cell wall related all the forces are put together in a discrete manner in to solid phase wall elements as seen in Fig. 1. These wall elements are then considered as a circular chain of linked wall particles, where each particle bears properties of each wall element and wall deformations are defined as inter-particle displacements and displacement rates of wall particles. As illustrated in Fig. 2, each wall particle is driven by six types of forces; stiff forces \( F^e \), damping forces \( F^d \), repulsion forces \( F^{rf} \) and \( F^{rw} \), attraction forces \( F^a \) and forces due to bending stiffness of the wall \( F^b \). \( F^e \) forces account for the cell wall stiffness to resist extension and compression of the cell wall elements and calculated based on relative displacements of adjacent wall particles. \( F^d \) forces account for viscous characteristics of the cell wall and are calculated based on relative velocities of adjacent wall particles. \( F^{rf} \) forces are the repulsion forces between fluid and wall particles which help to ensure the fluid particles are maintained within the cell wall by avoiding any undesirable fluid penetrations. \( F^{rw} \) forces are used to limit any unrealistic cell wall particle inter-penetrations and are calculated based on relative distances between non-bonded wall particles. Next, we introduce \( F^a \) attraction forces to the wall model to limit wall-fluid separations around the cell wall to maintain fluid particles attached sufficiently to the wall in dried conditions. Also, we introduce \( F^b \) to account for cell wall bending stiffness observed in real plant cell walls. Thus, as seen in the Fig. 2, the total force on wall particle \( k \) can be derived using neighbouring fluid particles \( i \), bonded wall particles \( j \), non-bonded wall particles \( l \) and is shown in Eq. (1).

Figure 1. 2-D cell model
Figure 2. Forces acting on a given cell wall particle $k$

\[
F_k = F_{e_{kj}} + F_{d_{kj}} + F_{rf_{ki}} + F_{rw_{kl}} + F_{a_{ki}} + F_{b_k} \tag{1}
\]

According to previous researchers (Liedekerke, Ghysels et al. 2010) stiff force on wall particle $k$ due to bonded wall particles $j$ can be calculated for each individual wall element using Eq. (2).

\[
F_{e_{kj}} = G z_0 t_0 \left( \lambda_{\theta} - \frac{1}{\alpha^2 \lambda_{\theta}^5} \right) \tag{2}
\]

Here $G$ is the shear modulus ($\approx E/3$) where $E$ is the Young’s modulus of the wall material, $z_0$ is the initial cell height, $t_0$ is the initial cell wall thickness, $\lambda_{\theta} = l/l_0$ is the extension ratio of each cell wall element where $l$ is the length of the wall elements at any given instance and $l_0$ is the initial undeformed length of the wall element. The parameter $\alpha$ is calculated using Eq. (3) with $\beta = 0.5$ for cylindrical cells.

\[
\alpha = \frac{\beta + \sqrt{\beta^2 - 4(\beta - 1)/\lambda_{\theta}^5}}{2} \tag{3}
\]

Cell wall damping forces $F_{d_{kj}}$ are defined as in Eq. (4), where $\gamma$ is the wall damping constant and $v_{kj}$ is the relative velocity of wall particle pairs.

\[
F_{d_{kj}} = -\gamma v_{kj} \tag{4}
\]

Repulsion forces on any wall particle from fluid particles $F_{rf_{ki}}$ are defined as in Eq. (5), where $f_{ki}$ is defined according to Lenard-Jones (LJ) force type as given in Eq. (6) and they act between each interacting particle pairs and are equal in magnitude and opposite in direction.

\[
F_{rf_{ki}} = f_{rf_{ki}} x_{ki} \tag{5}
\]

\[
f_{rf_{ki}} = \begin{cases} 
\frac{f_{rf} \left( \frac{r_0}{r_{ki}} \right)^8 - \left( \frac{r_0}{r_{ki}} \right)^4}{\left( \frac{r_0}{r_{ki}} \right)^2} & \frac{r_0}{r_{ki}} \geq 1 \\
0 & \frac{r_0}{r_{ki}} < 1 
\end{cases} \tag{6}
\]
In Eq. (5), \( x_{ki} \) is the position vector of wall particle \( k \) relative to particle \( i \). In Eq. (6), \( r_0 \) is the initial gap between the two particles, \( r_{ki} \) is the gap at any time of interest and \( f_{0}^{rf} \) is the strength of the LJ contact. This method ensures that if fluid particles come closer to the wall, they are repulsed back towards their usual position. The non-bonded wall-wall repulsion forces \( F_{rw_{ki}} \) are also defined in the same manner using a LJ contact strength \( f_{0}^{rw} \).

As mentioned above, this research work introduces fluid-wall attraction forces \( F_{w_{ki}}^{a} \) to ensure fluid continues to sufficiently kept attached to the wall during the drying process. It is defined in the same LJ force type described above, using a LJ contact strength \( f_{0}^{a} \) and only acts between neighbouring wall and fluid particles once they try to separate each other exceeding the initial relative positions. Next, to account for stiffer plant cell walls which resist local bending effects, a bending stiffness is also introduced in this work within the cell wall model. Many of the previous researchers who have modelled red blood cells (Hosseini and Feng 2009; Pan and Wang 2009; Shi, Pan et al. 2012) have implemented wall bending stiffness in their particle based models by considering the changes of local curvature of the wall and defining bending moments which are finally resolved in to equal and opposite forces acting on adjacent wall particles. In this work, a similar concept is used and bending moments were simply calculated and transformed to forces acting on wall particles using the formula given in Eq. (7). Here, \( k_{b} \) represents the bending stiffness, \( l \) is the length of the particular wall element of interest, \( \theta \) is the external angle as shown in Fig. (2) and \( \Delta \theta \) is the change of the \( \theta \) angle. It should be noted that these bending forces act in pairs on each wall element through each of the two respective wall particles such that they are equal in magnitude and opposite in direction. Further, it should be noted that these forces are defined so that they act perpendicular to the respective wall element.

\[
F_{w_{ki}}^{b} = \frac{k_{b}}{l} \tan \left( \frac{\Delta \theta}{2} \right)
\]  

(7)

Up to now, details of the cell wall model was given and this point onwards cell fluid model is presented. Plant cells can contain water up to approximately 80% - 90% of the cell mass (Pitt 1982; Hills and Remigereau 1997). On this basis, the cell fluid is modelled as a liquid with properties approximated to water, and modelled as a Newtonian fluid with low Reynolds number flow characteristics. For plant cell models, SPH has been used to model the cell fluid quite promisingly by several previous researchers (Liedekerke, Ghysels et al. 2009; Liedekerke, Ghysels et al. 2010; Van Liedekerke, Ghysels et al. 2011) and it has been demonstrated further that the technique can even handle extreme conditions such as cell breakage due to extreme external loading conditions (Van Liedekerke, Tijskens et al. 2010). These provide clues of SPH applicability for cellular modelling as outlined in the introductory section. Therefore, SPH was used in this work to model the cell fluid and it was further used to model the cellular drying mechanisms which will be discussed in upcoming paragraphs.

Figure 3. Forces acting on a given fluid particle \( i \)
\[ F_i = F_p^i + F_v^i + F_r^i + F_a^i \]

As seen in figure 2(b) and Eq. (8) each fluid particle in the cell fluid is driven by four types of forces; pressure forces \( F_p \), viscous forces \( F_v \), repulsion forces \( F_r \) and attraction forces \( F_a \). \( F_p \) and \( F_v \) are representing cell turgor pressure effects and fluid viscous effects. As shown in Eq. (9) and Eq. (10), for any given fluid particle \( i \), these forces are calculated using the properties of neighbouring fluid particles \( i' \), according to fundamental Lagrangian type SPH equations typically used to model low Reynold’s number incompressible fluid flows (Morris, Fox et al. 1997; Liedekerke, Ghysels et al. 2010).

\[ F_p^{ii'} = -m_i \sum_{i'} m_{i'} \left( \frac{p_{i'}^r + p_{i'}^s}{\rho_{i'}^2} \right) \nabla \rho_{ii'} \]  

\[ F_v^{ii'} = m_i \sum_{i'} m_{i'} (\mu_i + \mu_{i'}) \rho_{ii'} \left( \frac{1}{\rho_{ii'}} \right) \left( \frac{1}{r_{ii'}} \right) \]  

Where \( m, P, \rho, \mu, z \) and \( W \) are fluid particle mass, cell turgor pressure, density, dynamic viscosity, cell height and SPH smoothing function. For the smoothing function \( W \), a more stable quartic smoothing function (Liu and Liu 2003) was used in this work which is given in Eq. (11).

\[ W_{ij} = \frac{15}{7\pi h^2} \begin{cases} 2 - \frac{9}{8} R^2 + \frac{19}{24} R^3 - \frac{5}{32} R^4 & 0 \leq R \leq 2 \\ 0 & R > 2 \end{cases} \]  

Where \( h \) and \( R \) are the smoothing length used in SPH formulations and \( R = \frac{r_{ii'}}{h} \). To update the pressure of the particles as the system evolves with time, an equation of state is used as in Eq. (12), which is in accordance with the previous works by other researchers (Liedekerke, Ghysels et al. 2010).

\[ P_i = P_0 + K \left[ \left( \frac{\rho}{\rho_0} \right)^7 - 1 \right] \]  

Where \( P_0 \) is the initial cell turgor pressure, \( K \) is the fluid compression modulus; a parameter to ensure the fluid behaves in the SPH scheme in a sufficiently incompressible manner. To update the density of a fluid particle \( i \), following equation is used which is derived from the basic SPH continuity equation (Liedekerke, Ghysels et al. 2010).

\[ \frac{d\rho_i}{dt} = \frac{1}{z} \frac{d\rho_i^*}{dt} - \frac{\rho_i^*}{z^2} \frac{dz}{dt} + \frac{\rho_i}{m_i} \frac{dm_i}{dt} \]  

Where \( \rho_i^* \) is the density of particle \( i \) in 2-D which is defined as \( \rho_i^* = h\rho_i \). The first term in Eq. (13) accounts for the slight density changes of the cell fluid due to cell deformation in 2D. The second term adds a correction to the density evolution by compensating for the height change of the cell.
The third term accounts for the change of the water content of the cell due to the cell wall permeability. This term is of great importance in case of drying because the moisture escape from the cell fluid happens through the cell wall and cell wall permeability plays a big role in that. The derivatives used in these three terms can be defined as follows (Liedekerke, Ghysels et al. 2010):

\[
\frac{d\rho_t}{dt} = m_i \sum_{iv} v_{iiv} \cdot \nabla W_{iiv}
\]

\[
\frac{dz}{dt} = \frac{z(t=t_0) - z(t=t_0+t)}{\Delta t}
\]

\[
\frac{dm_i}{dt} = -\frac{A_c L_p \rho_i}{N_f} (P_i + \Pi)
\]

In Eq. (15), \(z(t=t_0)\) and \(z(t=t_0+t)\) are height of cell at the previous time step and the next time step and \(\Delta t\) is the size of the time step. In Eq. (16), \(A_c\), \(L_p\), \(N_f\) and \(\Pi\) represent total surface area of the cylindrical cell at a given time, cell wall permeability, total number to fluid particles used to model the cell fluid and the osmotic potential of the cell at a given condition.

The final two terms in Eq. (8) are the repulsion and attractive forces acting on a given fluid particle due to the other wall particle of the each interacting wall-fluid particle pairs and are defined in LJ force type as in Eq. (17) and Eq. (18).

\[
F^{rw}_{ik} = \sum_k f^{rw}_{ik} x_{ik}
\]

\[
F^{a}_{ik} = \sum_k f^{a}_{ik} x_{ik}
\]

### Simulation of drying mechanisms

In food drying, moisture is removed from the cellular structure and causes cellular structural shrinkage and leads to the final dried food structure. This phenomenon is one of the key criteria in determining the drying cycle time, where the drying process is continued until a particular moisture amount is removed, which causes a corresponding level of shrinkage. Further, it has been experimentally demonstrated that there is a direct relationship between the volume of removed water and the bulk volumetric shrinkage during drying (Suzuki, Kubota et al. 1976; Lozano, Rotstein et al. 1980; Ratti 1994; Moreira, Figueiredo et al. 2000; Mayor and Sereno 2004). Also, it is reported that for the apple fruit cells, the cell diameter, perimeter and area reduce with the moisture content almost lineally throughout the drying cycle and it is directly related with bulk shrinkage (Mayor, Silva et al. 2005). Therefore the moisture content can be used to predict cellular shrinkage and eventually the bulk level shrinkage. Following this hypothesis, the above-mentioned SPH-DEM cell model was used to predict the cellular level shrinkage of an apple cell during drying.
In the simulations, cell fluid mass is made to vary in steps and this allows the cell to settle by changing its size by contracting or expanding the cell wall to attain force balance in the particle scheme. To vary the cell fluid mass in each case, the moisture content and osmotic potential are artificially initiated to different values with initial turgor pressure set to 0 kPa. Higher moisture content values with higher osmotic potentials are used to simulate turgid conditions of the cell and lower moisture contents with lower osmotic potential are used to artificially make the cell to become flaccid and are used in this work to represent dried conditions. This follows the fundamentally accepted phenomena of dehydration related turgor loss and cellular shrinkage. In each case, the cell is allowed to inflate by exchanging water through the semi-permeable cell membrane until cell wall forces balance with the steady state cell fluid forces. To reduce the simulation time taken to achieve steady state conditions in each case, the cell wall permeability is artificially set to a larger value (such as $5 \times 10^{-6}$ m²N⁻¹s) than the realistic value given in the Table 1. Using this approach, shrinkage simulations of a lengthy drying process (which could last for many hours) can be achieved by simulating a set of intermediate states using comparatively very small real time simulations (well below 1 s). Due to the use of a very small time step (such as $5 \times 10^{-9}$ s) in the simulations for the stability requirements, it should be noted that simulating a real process as it is, that lasts for many seconds or more, is computationally formidable.

After the cell settles with a particular moisture content value $X$ (proportional to the cell fluid mass), to monitor the shrinkage, various geometrical properties such as cell area, diameter and perimeter were considered. To facilitate easy comparison, normalised moisture content $X/X_0$ is calculated by dividing the steady state cell fluid mass values by the fresh or turgid state (at 200 kPa) mass value. The geometric parameters were also normalised by dividing each parameter by its initial value corresponding to the fresh cell. These obtained parameters were: normalised area $A/A_0$, normalised diameter $D/D_0$ and normalised perimeter $P/P_0$.

**Computational setup**

Table 1 shows key parameters used to model a fresh apple cell in this study. The cell model formulations were programmed in C++, and simulations were performed on a multi-processor computer. To develop the C++ code, a FORTRAN source code (Liu and Liu 2003) was referred and incorporated. Time integration of the equations of motion of particles were achieved using a Leapfrog integrator with a time step sufficiently small to ensure the stability of the particle scheme (Liu and Liu 2003). The cell wall was modelled with 100 particles and with additional 100 virtual particles to avoid unnecessary fluid penetrations (Liedekerke, Ghysels et al. 2010). To have the same gap between all the particles in the model, the cell was fully filled with cell fluid particles initially positioned on a square grid-like arrangement and for the given cell diameter and for the given number of wall particles, around 500 fluid particles were required for this.

**Table 1. Key parameters used for the cell model**

<table>
<thead>
<tr>
<th>Model Parameter</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>Initial cell diameter</td>
<td>150 μm</td>
<td>(Hills and Remigereau 1997)</td>
</tr>
<tr>
<td>Initial cell height ($z_0$)</td>
<td>100 μm</td>
<td>Assumed</td>
</tr>
<tr>
<td>Cell wall shear modulus ($\bar{G}$)</td>
<td>18 MPa</td>
<td>(Wu and Pitts 1999)</td>
</tr>
<tr>
<td>Cell wall bending stiffness ($k_p$)</td>
<td>$5.0 \times 10^{-13}$ Nm/rad</td>
<td>Assumed</td>
</tr>
<tr>
<td>Cell wall initial thickness ($t_0$)</td>
<td>6 μm</td>
<td>(Wu and Pitts 1999)</td>
</tr>
</tbody>
</table>
Initial cell fluid mass | $1.77 \times 10^{-9}$kg | Calculated based on cell fluid volume and density
---|---|---
Cell wall mass (10% of cell fluid mass) | $1.77 \times 10^{-10}$kg | (Liedekerke, Ghysels et al. 2010)
Cell wall damping ratio ($\gamma$) | $1 \times 10^{-6}\text{ Nm}^{-1}\text{s}$ | (Van Liedekerke, Ghysels et al. 2011)
Cell fluid viscosity ($\mu$) | $1 \times 10^{-1}\text{ Pa s}$ | (Liedekerke, Ghysels et al. 2010; Van Liedekerke, Ghysels et al. 2011)
SPH smoothing length ($h$) | $1.2 \times$ initial fluid particle spacing | (Liu and Liu 2003; Liedekerke, Ghysels et al. 2010)
Fresh cell turgor pressure ($P_0$) | 200 kPa | (Wang, Wang et al. 2004)
Fresh cell osmotic potential ($\Pi$) | $-200$ kPa | (Liedekerke, Ghysels et al. 2009; Liedekerke, Ghysels et al. 2010) Assumed to be equal to ($-P_0$)
Cell wall permeability | $10^{-12}\text{ m}^2\text{N}^{-1}\text{s}$ | (Taiz and Zeiger 2002)
Cell fluid compression modulus | 20 MPa | Assumed

**Results and Discussion**

*Simulation of a fresh turgid cell*

The cell was initiated with the physical property values given in the Table 1 and due to the cell wall permeability and initial imbalance of forces in the model, the cell always tends to absorb some more liquid through the cell wall according to Eq. (16) and causes the turgor pressure to increase and the cell wall to stretch. This inflation happens till force balance occurs between cell wall and cell fluid. At the steady state condition, model consistency was evaluated by comparing model-computed wall tension and theoretical wall tension of a cylindrical vessel pressurized to initial turgor pressure value. It was found that the model prediction error was within 8% of the theoretical value and this is well in the acceptable range of results of previous authors (Liedekerke, Ghysels et al. 2010).

*Simulation of cellular shrinkage in drying conditions*

In the simulations, it was assumed that a cell undergoes two basic stages of moisture removal; first stage of moisture removal where as moisture removes, a continuous turgor pressure drop is observed. This stage exists up to a point where the turgor pressure equals to the atmospheric pressure ($P = 0$ kPa). In the second stage of moisture removal, the cell turgor pressure remains equal to atmospheric pressure but moisture is forced to leave the cell. In real drying processes also, this kind of a forced drying stage exists at the mid and latter part of the drying cycle. In the simulations, first stage of drying was achieved by initiating the cell with 0 kPa turgor pressure and allowing the cell to inflate to different turgor pressures according to Eq. (16). A higher final turgor pressure represents a fresh cell and lower turgor pressures represent dried cells. In the second stage related simulations, again the Eq. (16) was used, but both the initial turgor pressure and osmotic potential was artificially set to 0 kPa. Also the cell initial moisture content was set to different values
resembling the targeted final moisture content of the dried cell. In all these first and second stage simulations, the cell is allowed to evolve until it becomes steady state where the cell wall and fluid cease motion. After each simulation, the cell structure was observed as seen in Fig. 4. Also the $A/A_0$, $D/D_0$ and $P/P_0$ values were measured and are presented in Fig. 5.

![Figure 4. Simulation of structural changes of a single cell at different drying conditions](image)

From Fig. 4, it can be clearly seen that the cell tends to shrink as a function of moisture content and the cell loses its circular shape at extremely dried conditions due to cell wall deformations. From Fig. 5, it can be further seen that cell area and diameter predictions fairly agree with experimental results. But, in case of perimeter values, it shows some decreasing trend in the initial phase of drying and thereafter remains unchanged. This implies that the cell model basically tends to release the wall tension caused by the cell turgor pressure during the drying process. At the end of the first stage of drying, since the turgor pressure remains unchanged around 0 kPa, the wall length also seems to remain unchanged throughout. This phenomena can be related to the actual cell wall structure which is found to be a rigid fibrous structure and its deformations are found to be mainly caused by the turgor pressure (Nilsson, Hertz et al. 1958; Wu, Spence et al. 1985; Lin and Pitt 1986; Crapiste, Whitaker et al. 1988-a; Gao and Pitt 1991; Wang, Wang et al. 2004; Taiz and Zeiger 2010). Also the perimeter change phenomena may have some tissue-related mechanics and a tissue model would have to be developed to check the perimeter variation. Because, for this study, the experimental results that were referred for comparison, were basically tissue-based experiments that were eventually used to get the average individual cell perimeter values. Further this highlights the necessity of more intense experiments to specifically measure the cell perimeter changes during drying.

![Figure 5. Changes of normalized area, diameter and perimeter of a single as a function of normalized moisture content](image)
Model sensitivity to key physical properties

Figure 6. Sensitivity of the model to cell wall Young’s modulus

Figure 7. Sensitivity of the model to cell fluid viscosity

As seen in Fig. 6 and Fig.7 several numerical experiments were conducted to check the model sensitivity to some of the key physical properties such as cell wall to Young’s modulus and cell fluid viscosity. It should be noted that only cell area and diameter were considered for this study as the perimeter variation was not so significant. Different cells from different plant varieties usually have their own cell wall Young’s modulus values based on the fibrous structure. Even for the same variety, cell wall Young’s modulus can vary from sample to sample, due to the biological variability. In this background, studying the effects of different Young’s modulus is very important and as seen in Fig. 6 it was found that the model predictions show a very small change of cellular shrinkage to the variation of the cell wall Young’s modulus. This may be explained by the fact that, Young’s modulus usually effects to the initial stage of drying where a positive turgor pressure exists. Based on the simulation results presented in the above sections, it was found that a positive turgor pressure exists only until about 0.9 normalized moisture content. Thereafter, the cellular shrinkage is mainly governed by the forced fluid volume reduction and in those conditions mostly the cell wall is hardly under considerable tension. So the effect of the Young’s modulus seems to be not so significant to influence the cellular shrinkage.
Next, the effect of the fluid viscosity was studied which resembles one of the key cellular cytoplasm characteristics of different plant varieties. By studying the shrinkage patterns of different cell fluid viscosities implies the model capability to predict shrinkage of different plant food varieties. For ease of comparison of viscosities, \( \frac{\mu}{\mu_0} \) ratio was used where \( \mu \) is the cell fluid actual viscosity and \( \mu_0 \) is the viscosity of water (1 × 10^{-3} Pa s). As seen from Fig. 7, it is clear that moderately higher viscosity values (\( \frac{\mu}{\mu_0} \approx 10 - 100 \)) provide better simultaneous predictions of area and diameter than too higher or too lower cell fluid viscosities. These moderate viscosity values seem to be agreeing with the findings of the previous researchers on basic cellular mechanical property simulations of plant cells (Liedekerke, Ghysels et al. 2010; Van Liedekerke, Ghysels et al. 2011).

**Conclusion**

In this paper a mesh-free particle based approach was presented to model and simulate cellular level structural changes of plant foods in 2-D. The model focuses on a single plant cell and was modelled in two parts; cell wall and cell fluid. Considering the fibrous structure of the cell wall, it was modelled as a neo-Hookean solid material using a DEM approach. The cell fluid was approximated to a Newtonian fluid with a moderately higher viscosity compared to water and was modelled using SPH. To simulate the cellular shrinkage, only the mass transfer effects were allowed to occur through the cell wall. The model even accounts for sub-cellular details and cellular level shrinkage was studied with reference to normalized cell area, diameter and perimeter.

Considering the normalized cell area and the normalized diameter measurements, reasonable agreement was observed with an experimental study in literature. Considering the perimeter predictions, it was found that the model shows some shrinkage behaviour only in the initial stage of the drying process where a positive turgor pressure exists. At extremely dried conditions cell wall seems to show a warped shape and allows cell area and diameter to decrease but keeping the perimeter almost unchanged. Further, to study the model sensitivity to key cellular physical properties such as cell wall Young’s modulus and cell fluid viscosity, several numerical experiments were conducted. It was found that the cellular shrinkage is not much influenced by the cell wall Young’s modulus. But cell fluid viscosity was found to be significantly influencing the shrinkage prediction and moderately higher viscosity values seem to be preferred for better accurate predictions.

In concluding, it can be argued that this 2-D single-cell drying model can provide useful insights to understand the mechanisms of cellular structural deformations in the plant foods during drying conditions. The mesh-free based approach used in this model can fundamentally handle extreme deformation, multi-phase nature of the problem and it incorporates mechanisms of different scales. Also the approach allows new physics to be incorporated in to the model. All these characteristics ensure that the approach used could be extended to further studies of cellular food drying. As an outlook, the model could be extended to a 2-D tissue model which can be created using cell aggregation. In such advanced models, more interesting features are to be incorporated such as properties and effects of intercellular space and middle lamella. Even a 3-D bulk cellular drying model could be developed which could provide more realistic insights to better explain the real phenomena in cellular drying mechanisms.
Acknowledgements

This research was conducted with the financial assistance and high performance computing facilities provided by the Queensland University of Technology - Brisbane, Australia. The studies were also financially supported by International Postgraduate Research Scholarship (IPRS) and Australian Postgraduate Award (APA) scholarship.

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