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A Coupled SPH-DEM Model for Fluid and Solid Mechanics of Apple Parenchyma Cells During Drying

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Abstract

A coupled SPH-DEM based two-dimensional (2-D) micro-scale single cell model is developed to predict basic cell-level shrinkage effects of apple parenchyma cells during air drying. In this newly developed drying model, Smoothed Particle Hydrodynamics (SPH) is used to model the low Reynolds Number fluid motions of the cell protoplasm, and a Discrete Element Method (DEM) is employed to simulate the polymer-like cell wall. Simulations results reasonably agree with published experimental drying results on cellular shrinkage properties such as cellular area, diameter and perimeter. These preliminary results indicate that the model is effective for the modelling and simulation of apple parenchyma cells during air drying.

Introduction

Food drying and its related processing is one of the leading global industries with an ever-increasing competitive market, and -where production cost and environmental concerns are increasingly critical. Drying is used to preserve around 20% of the world's perishable crops [1] and in most industrialised countries, the drying industry accounts for nearly 20% of the total industrial energy consumption [2]. Fresh fruit, vegetables and grains are perishable in nature due to microbial reactions, and these reactions are accelerated by higher water content in the food materials. For example, water content in fruits, vegetables and grains can vary from 20% to 90% by weight [3]. Drying mainly removes water from food materials, down to safe limits, to reduce microbial spoilage. It even helps to lower the storage volume and food mass in comparison to some other food preservation techniques such as freezing and canning [2]. In considering this background, it is clear that optimising the drying process performance is very important, and it is crucial to have a better fundamental understanding of the physical changes which occur during the process. Also, such an understanding will lead to more precise control of the process parameters, leading to the development of new products with enhanced quality at a reduced cost [4-6].

Due to the effect of water removal during the drying process, the structure of these bio materials undergoes deformations which are quantified as drying properties that eventually affect the food quality and the market value of the product. Shrinkage, porosity development and density variations are some of the key quantifiable physical changes, and are of great interest to the food industry. Since plant cells are the fundamental building blocks of all of these food materials, the aforementioned macroscopic property changes can better be optimised with the aid of a proper understanding of the underlying micro mechanics in cellular structures and other drying-related fundamental heat and mass transfer phenomena. There is a lack of the literature on physically sensible and applicable drying models, which account for cellular structural mechanics and drying related physical changes. The aim of this research is to use MeshFree Particle Methods to model, visualise and investigate the fundamental cellular-level mass transfer-driven physical changes during food drying. The approach uses Smoothed Particle Hydrodynamics (SPH) and a Discrete Element Method (DEM) to model the cellular structure and related fluid and solid mechanics in given drying conditions. Due to the Meshfree nature of the model, it can better handle large deformations, multi-phase interactions [7] and can account for sub-cellular details which are key concerns in microscale drying mechanics. The scope of this paper is to present the basic level concepts used in the model, and some of the key results obtained until the present time. In following sections, an overview of the model and simulation techniques used will be presented, and followed by simulation results and comparisons with experimental data in the literature. Finally, directions for future works will be outlined.

Coupled SPH-DEM Cellular Drying Model

To simulate the drying mechanics, firstly a 2-D single fresh cell is modelled using SPH and DEM. Thereafter drying mechanics are incorporated into the model to resemble the moisture removal driven shrinkage observed in actual plant cells. In this study, a plant tissue is approximated to an aggregate of individual cylindrical cells as shown in figure 1.

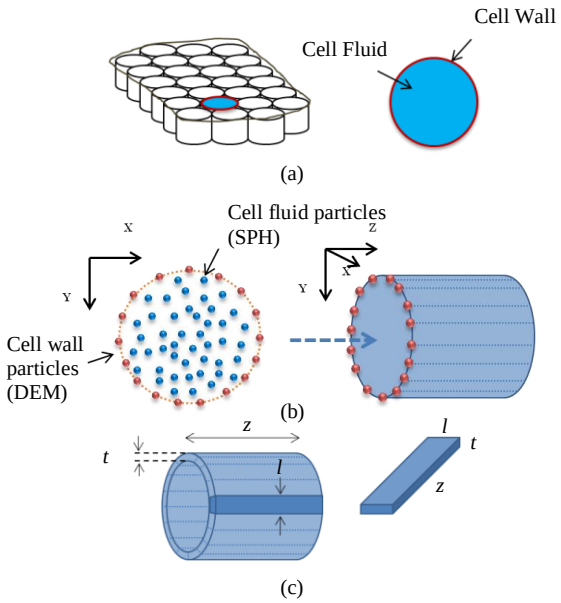
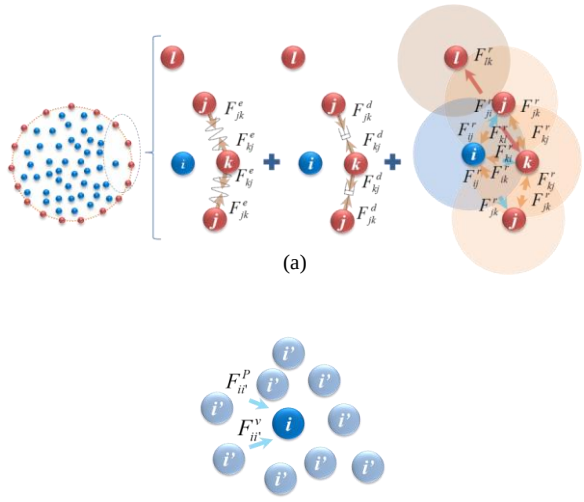


Figure 1. (a) Plant tissue is approximated as an aggregate of cylindrical cells and the top surface of each cylindrical can be considered as a 2-D representation of the cell, (b) Cell wall and cell fluid in 2-D cell model, (c) A discrete element of the cell wall.



(a)

(b)

Figure 2. (a) DEM-based cell wall model where each particle driven by stiff forces, damping forces and repulsion forces (shaded regions represent influence range of each particle), (b) In SPH-based cell fluid model, each fluid particle is driven by pressure forces, viscous forces and repulsion or attraction forces from wall.

In each cell, the top surface can be used as a 2-D model of the actual cell mechanics if the Z directional deformations are assumed to be uniform and the XY plane stresses and Z directional velocity components are neglected (see figure 1). The model is composed of two basic components, the cell fluid and the cell wall.

Cell walls have a fibrous structures in nature with time-dependent properties including elastic, visco-elastic and plastic behaviours [8]. Accordingly, researchers [9-12] have used a neo-Hookean solid material [13] for their cell models by incorporating a DEM-based [14, 15] discrete wall element scheme (see figure 1(c)) which has been incorporated in to this work. These wall elements can be represented 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 figure 2(a), each wall particle is driven by three types of forces; stiff forces $\boldsymbol{F^e}$, damping forces $\boldsymbol{F^d}$and repulsion or attraction forces $\boldsymbol{F^r}$. $\boldsymbol{F^e}$ forces account for the cell wall stiffness and calculated based on relative displacements of adjacent wall particles. $\boldsymbol{F^d}$ forces account for viscous characteristics of the cell wall and calculated based on relative velocities of adjacent wall particles. $\boldsymbol{F^r}$ forces have three purposes; one is to ensure the fluid particles are maintained within the cell wall by avoiding any undesirable fluid penetrations. Secondly, to avoid any wall-fluid separations with respective to the initial relative positions. Here $\boldsymbol{F^r}$ forces are calculated based on relative distances between fluid-wall particles. Thirdly, $\boldsymbol{F^r}$ forces are used to avoid any unrealistic cell wall particle inter-penetrations and is calculated based on relative distances between non-bonded wall particles. All these $\boldsymbol{F^r}$ forces are defined as Lenard-Jones (LJ) type interactions where if the gap between two interacting particles changes, they are repulsed or attracted to restore their initial relative positions. The boundary conditions are defined using these interaction forces. Thus, as seen in the figure 2(a), the force on wall particle k can be derived using fluid particles i, neighbouring wall particles j, non-bonded wall particles l as shown in equation (1). The detailed formulations were based on the cell wall models developed by several previous researchers [10-12].

$$\boldsymbol{F_k = F^e{}_{kj} + F^d{}_{kj} + F^r{}_{ki} + F^r{}_{kl}} \quad (1)$$

Plant cells usually have higher water content in their protoplasm which can contribute approximately 80% - 90% of the cell mass [16, 17]. On this basis, the cell fluid properties can be approximated to water, and modelled as a Newtonian liquid with low Reynolds number flows. SPH has been used to model the cell fluid quite promisingly [10-12] and it has been demonstrated further that the technique can even handle extreme conditions such as cell wall breakage [9]. Also SPH can handle extreme deformations, multiphase flow and problems involving various scales [18]. Therefore, SPH is used in this work to model the cell fluid. As seen in figure 2(b), each fluid particle in the cell fluid is driven by three types of forces; pressure forces $\boldsymbol{F^p}$, viscous forces $\boldsymbol{F^v}$ and repulsion or attraction forces $\boldsymbol{F^r}$. $\boldsymbol{F^p}$ and $\boldsymbol{F^v}$ forces represent cell turgor pressure and viscous effects, and are calculated with SPH using the neighbouring fluid particle properties. $\boldsymbol{F^r}$ forces represent the repulsions or attractions from the cell wall as the neighbouring fluid particles tries to reach or leave the cell wall and are calculated based on relative particle distances. Accordingly, as seen in figure 2, forces on the fluid particle i can be derived using other fluid particles i' and neighbouring wall particles j as shown in equation (2). In here also the detailed formulations were based on the cell fluid models developed by several previous researchers [10-12].

$$\boldsymbol{F_i = F^p{}_{ii'} + F^v{}_{ii'} + F^r{}_{ij}} \quad (2)$$

Table 1 shows the key physical properties used for the model of a fresh apple cell in this study. The SPH and DEM formulations were programmed in C++, and simulations were performed on a multi-processor computer. To develop the C++ code, a FORTRAN source code [18] 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 [18]. The cell wall is modelled with 100 particles and with additional 100 virtual particles to avoid unnecessary fluid penetrations [10]. Deploying a higher number of particles is recommended for better accuracy of the SPH approximations of the cell fluid. But due to the computational cost, this preliminary study used 500 cell fluid particles initially located on a square grid. In the SPH formulations a quartic smoothing kernel [18] is used for better accuracy, stability and computational efficiency. The cell model was validated by sufficiently reproducing theoretical hoop direction wall forces by model predictions [10].

Model Parameter	Value	Reference
Initial cell diameter	150 μm	[16]
Initial cell height	100 µm	set
Shear modulus (cell wall)	80 MPa	[11, 19]
Cell wall initial thickness	6 µm	[20]
Initial cell fluid mass	1.77×10^{-9}kg	set
Cell wall mass (10% of cell fluid mass)	1.77×10^{-10}kg	set
Cell wall damping ratio	1×10^{-6} Nm^{-1}s	[11]
Cell fluid viscosity	1×10^{-2} $Pa\ s^{-1}$	[10, 11]
SPH smoothing length	1.2 × fluid grid spacing	[10, 21]
Fresh cell turgor pressure	300 kPa	set
Initial cell osmotic potential	−300 kPa	[10, 12]
Cell wall permeability	10^{-12} m^2N^{-1}s	[22]
Cell fluid compression modulus	20 MPa	set

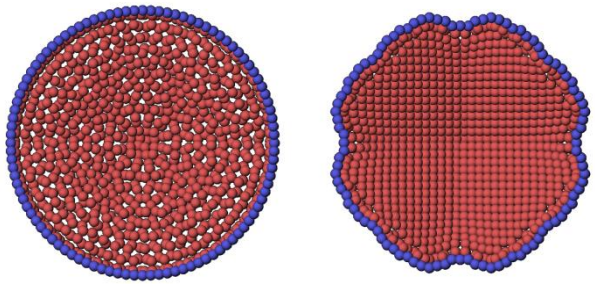
Table 1. Key parameters used to model the fresh apple cell

Results and Discussion

In food dehydration, moisture is removed from the cells and this mainly influences cellular shrinkage which critically governs the final dried food structure. This 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 almost a linear relationship between the volume of removed water and the bulk volumetric shrinkage during drying [23-27]. Also, it has been observed that the apple cell diameter, perimeter and area reduce with the moisture content almost lineally throughout the drying cycle and it is directly related with bulk shrinkage [28]. Therefore the moisture content can be used to predict cellular scale shrinkage and eventually the bulk scale shrinkage. Following this hypothesis, this work uses the above-mentioned SPH-DEM cell model to predict the cellular level shrinkage of an apple cell during drying by altering the cell fluid mass.

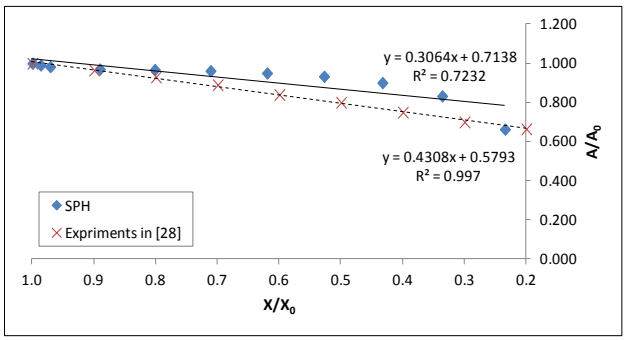
To simulate this, cell fluid mass is made to vary in steps and this allows the cell to settle by changing its size by contracting or expanding the cell wall to attain force balance in the particle scheme. To vary the cell fluid mass in each case, the moisture content and osmotic potential are artificially initiated to different values with initial turgor pressure set to 0 kPa. Higher moisture content values with higher osmotic potential values 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 collapse. 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. Figure 3(a) shows an inflated fresh cell and figure 3(b) shows a cell with reduced moisture content resembling a dried cell. To reduce the simulation time taken to achieve the steady state condition in each case, the cell wall permeability is artificially set to a larger value (5×10^{-6} $m^2N^{-1}s$) than the realistic value given in the table 1. Using this approach, shrinkage simulations of a lengthy drying process (which can 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 5×10^{-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 moisture content value X (proportional to the cell fluid mass), to facilitate easy comparison, the normalised moisture content X/X_0 is calculated by dividing the steady state cell fluid mass values by the fresh or turgid state (at 300 kPa) mass value. To monitor the shrinkage, various geometrical properties such as cell diameter, perimeter and area were considered. These parameters were also normalised by dividing each parameter by its initial value corresponding to the fresh cell. The obtained parameters were: normalised area A/A_0, normalised diameter D/D_0 and normalised perimeter P/P_0. These model predictions were compared with experimental values [28] and a reasonably good agreement could be observed (see figure 4). Linear curves were fitted in each case to compare the model predictions with experimental findings. It is observed from both the figure 3 and figure 4, that the cell tends to shrink while maintaining the wall initial length. Also, at extremely dried conditions the cell wall is becoming quiet warped, and the cell shape deviates considerably from the initial circular shape. This causes cell area and diameter to change rapidly in a nonlinear trend at lower moisture content conditions.

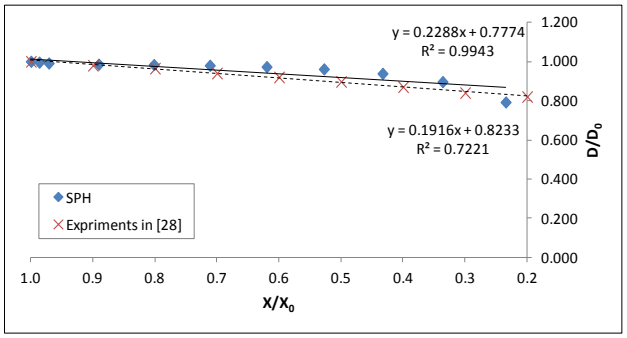


(a) (b)

Figure 3. Visualised SPH-DEM cell model (a) a fresh cell, (b) a dried cell



(a)



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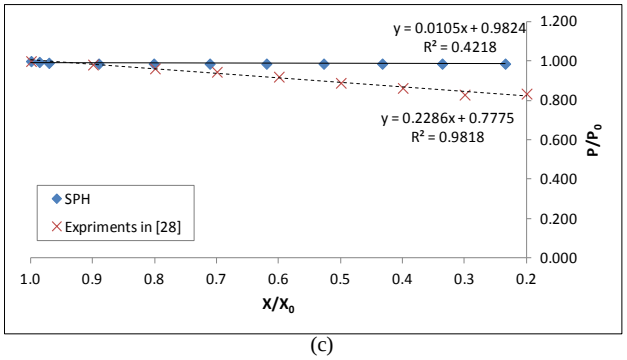

(c)

Figure 4. Comparison of model predictions with the experimental results in [28]: (a) Normalized cell area, (b) Normalized cell diameter, (c) Normalized cell perimeter

Conclusion and Outlook

A 2-D single cell was modelled using SPH and DEM to predict cellular shrinkage as a function of the moisture content. Due to the fundamental capabilities of SPH as a Meshfree technique, the model is claimed to be capable of handling food drying-related

extreme cellular structural deformations, phase change phenomena and mechanisms of various scales; from cellular level to bulk level. The proposed model consists of two main components: cell wall and cell fluid. The cell wall was modelled with discrete elements having visco-elastic properties and the cell fluid was modelled with SPH. To simulate drying mechanisms as a function of the moisture content, cell fluid mass was allowed to change and physical changes were quantified using cell area, diameter and perimeter values.

Based on the preliminary results obtained in simulations, it can be concluded that the model is capable of predicting the cellular shrinkage in 2-D single cell scale as a function of moisture content. The model performances are to be further improved with a finer fluid particle distribution, finetuning the model parameters to reduce fluctuations, and incorporating more realistic cell wall models and boundary conditions. Further, the model is to be extended to a 2-D multi-cell based tissue model and eventually to a three-dimensional multi-tissue model to represent realistic bulk material and related drying mechanisms. In the proposed tissue models, multiscale techniques will be used to reduce the computational time.

Acknowledgements

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