Modelling 3-D cellular microfluidics of different plant cells for the prediction of cellular deformations under external mechanical compression: A SPH-CG-based computational study

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Abstract
Computational modelling of plant cellular materials and relevant mechanics are of interest in numerous research fields. Depending on the complex fluid and solid mechanics involved, there are many numerical modelling approaches applicable in the development of such computational models. This research investigation focuses on computational modelling three-dimensional (3-D) microfluidics of parenchyma cells of three different plant cellular materials: apple, potato and grape with the intention of studying corresponding physical deformations under external mechanical compression which potentially can derive valuable insights about processing of such plant materials. A coupled Smoothed Particle Hydrodynamics (SPH) and Coarse-Grained (CG) approach has been utilised to numerically model the cell fluid and cell wall mechanics, respectively. Quantitative simulation results indicated almost similar cell deformations yielding to top and bottom flat surfaces. In terms of stress-strain behaviour, apple and grape cells revealed stiffer behaviour relative the potato cell. It is evident based on this study that depending on the differences of physical properties of plant cells, their behaviour under compression varies. Findings of this research can be potentially beneficial in further studies towards prediction of 3-D tissue deformation under external mechanical loading.

Keywords
Cellular deformation; Coarse-grained methods; Microfluidics; Plant cell modelling; Smoothed particle hydrodynamics; SPH

Introduction
Plant materials are a common source for many basic human and animal requirements such as food, shelter and energy. In food engineering and other research fields, modelling of plant cellular materials play a vital role, enabling the prediction of food material properties under different physical conditions. Depending on the complex fluid and solid mechanics involved, there are many numerical modelling approaches applicable in this context [1, 2]. However, in the case of large cellular deformations and involved complex physical mechanisms, sources from the literature suggest to use meshfree methods over grid or mesh-based methods such as Finite Element Method (FEM) or Finite Volume Method (FVM) [1, 3-6]. Accordingly, this study focused on modelling three-dimensional (3-D) microfluidics of parenchyma cells of three different food plant materials: apple, potato and grape in order to study their physical deformations under external mechanical compression. In doing so, a coupled meshfree particle-based method was used involving Smoothed Particle Hydrodynamics (SPH) and Coarse-Grained (CG) method. The following sections present the key formulation of the methodology as well as key results and discussion.

Methodology
In this study, the plant cellular models were developed complying with experimentally observed physical properties, using a SPH-based cell fluid model and Coarse-Grained (CG)-based cell wall model [3, 7-12]. The key formulation used here are summarised below [5].

Cell Fluid Model
The cell fluid model was developed based on the assumption of an incompressible Newtonian liquid which demonstrates mechanical properties similar to water. Low-Reynolds-number characteristics were established for the fluid flow through a relatively larger viscosity. Navier-Stokes equations were employed to model its behaviour using SPH [4, 13]. Accordingly, to determine the physical behaviour of the cell fluid, four force fields were adopted as given in Figure 1: pressure forces ($\mathbf{F}_p$), viscous forces ($\mathbf{F}_v$), wall-fluid repulsion forces ($\mathbf{F}_{rw}$) and wall-fluid attraction forces ($\mathbf{F}_{aw}$).

![Figure 1. 3-D SPH-based cell fluid model: pressure forces ($\mathbf{F}_p$), viscous forces ($\mathbf{F}_v$), wall-fluid repulsion forces ($\mathbf{F}_{rw}$) and wall-fluid attraction forces ($\mathbf{F}_{aw}$).](image)

Here, based on the Lagrangian type SPH formulation, which are used to model weakly compressible low-Reynolds number fluid flows [8, 14], the momentum equation approximates the pressure forces ($\mathbf{F}_{p,i}^{\prime}$) and viscous forces ($\mathbf{F}_{v,i}^{\prime}$) as follows.

$$\mathbf{F}_{ij}^{p} = -m_i \sum_{i} m_i \left( \frac{p_i}{\rho_i} + \frac{p_i}{\rho_i} \right) \nabla_j W_{ii'}$$  \hspace{1cm} (1)
\[ F_{ij} = m_i \sum_{i'-j} \left( \frac{r_i + r_{i'}}{\rho_i \rho_{i'}} \right) \frac{1}{r_{ii'}} \frac{\partial W_{ii'}}{\partial r_{ii'}} \]  

Here, \( m \), \( P \), \( \rho \), \( \mu \), \( v \) and \( W \) are the fluid particle mass, cell turgor pressure, density, dynamic viscosity, velocity and the smoothing kernel, respectively. The use of SPH to provides the overall computational framework to robustly model large cell deformations and complicated mechanics relevant to cell rupture and phase change. Even though such mechanics are not discussed in this article, it is the intention of authors to use this framework to study similar broad applications [10]. In such applications, the internal fluid flow can also be modelled.

Wall-fluid repulsion forces \( (F_{rw}) \) and wall-fluid attraction forces \( (F_{aw}) \) were used to model the physical interactions between cell fluid and wall. Lennard-Jones (LJ) force fields were used to define these forces as follows [4].

\[ F_{rw} = \sum_{k} f_{rk} x_{ik} \]  
\[ F_{aw} = \sum_{k} f_{wk} x_{ik} \]

**Cell Wall Model**

In this study, a Coarse-Grained (CG)-based model was used for the cell wall as shown in Figure 2. Each CG element represents characteristics of the relevant cell wall segment. The physical interactions of the cell wall are modelled through six force fields: Stiff forces \( (F^s) \), damping forces \( (F^d) \), wall-fluid repulsion forces \( (F_{rw}) \), wall-fluid attraction forces \( (F_{aw}) \), bending stiffness forces \( (F^b) \) and wall cell contraction forces \( (F^c) \) as presented in Figure 2 [5].

**Cell Compression**

External mechanical compression of the cell was arranged through two horizontal compression plates. At the bottom and top of the cell as shown in Figure 3 [5]. The physical relationship between the cell and compression plates were determined through the plate-wall force \( (F_{pw}) \) as follows.

\[ F_{cw} = -k_{pw} \Delta x_{cw} \]  

Here, \( k_{pw} \) is defined as the corresponding force coefficient and \( \Delta x_{cw} \) the difference between \( r_{cw} \) and the current wall particle-plate distance.

**Computational Implementation**

Considering similar physical size, both the apple and grape cells were simulated with 3082 fluid particles and 2067 wall particles as seen in Table 1. A higher number of particles were used to represent the fluid and wall segments of the potato cell due to the larger average diameter [15, 16]. The model equations relating to drying and compression were numerically calculated with relevant physical and numerical parameters for corresponding biological cells [17] as given in Tables 1 and 2.

**Figure 3. Computational setup for cell compression through the SPH-CG model [4, 5].**

| Model Parameter | Apple | Potato | Grape |
|-----------------|-------|--------|-------|
| Initial cell radius [μm] | 2516 | 3708 | 3082 |
| Initial cell wall thickness [μm] | 6 | 1 | 3 |
| Cell wall shear modulus (G) [MPa] | 18 | 166 | 33 |
| Turgor pressure of fresh cell \( (P_f) \) [kPa] | 200 | 200 | 200 |
| Osmotic potential of fresh cell \( (-\sigma) \) [kPa] | -200 | -200 | -200 |
| Number of fluid particles \( (n_f) \) | 3082 | 2067 | 2067 |
| Number of wall particles \( (n_w) \) | 2516 | 6.8 | 2.0 |
| SPH smoothing length \( (\delta) \) [μm] | 2.0 | 2.0 | 2.0 |
| Compression plate velocity \( (\text{ms}^{-1}) \) | 2.0 | 2.0 | 2.0 |

**Table 1. Physical and numerical parameters used for modelling different cells**

| Model Parameter | Value |
|-----------------|-------|
| Cell fluid viscosity \( (\mu) \) [Pas] | 0.1 |
| Cell wall damping ratio \( (\gamma) \) [Ns/m] | 5 × 10^{-6} |
| Initial fluid density \( (\rho_0) \) [kg/m^3] | 1000 |
| Cell wall permeability \( (L_w) \) [m^2 N^{-1} s] | 2.5 × 10^{-6} |
| Cell wall bending stiffness \( (k_b) \) [Nmrad^{-1}] | 10.0 × 10^{-20} |
| Cell wall contraction force coefficient \( (k_{cw}) \) [Nm^{-1}] | 1.0 × 10^{-4} |
| Cell fluid compression modulus \( (K) \) [MPa] | 20 |
| Time step \( (\Delta t) \) [s] | 1.0 × 10^{-3} |

**Table 2. Physical and numerical parameters used in common for different cells**

Model was programmed as a C++ source code and simulations consisted of two stages: initial inflation stage (model initialisation to steady-state cell shape) and the compression stage. The High-Performance Computing (HPC) facility at the Queensland University of Technology (QUT), Brisbane,
Australia was used for running the simulations and model outcomes were visualised using the OVITO software [18].

Results and Discussion

As presented in Figure 4, it is evident the SPH-CG approach is capable of modelling the three different cells considered in this study, incorporating the respective physical properties and accommodating large boundary deformations due to external compression. It is observed that the spherical fresh cells eventually get flattened at the top and bottom regions as they interact with the plates. Further, Figure 5 shows the overall stress-strain variation of the three cells when going through compression stage. Relevant experimental results on apple tissue compression has also been compared with the model predictions [19]. In tandem, it is observed that both apple and grape cells are harder than potato cells, which is mainly due to the larger size of the potato cells and the thinner cell walls. Also, the single cell simulations have shown higher cell wall stresses compared to tissue simulations, which may be mainly due to the absence of intercellular force fields in this model, compared to the tissue composed of many cells bonded by pectin materials in a honeycombed structure. An enhanced validation for the modelling framework seems achievable through developing tissue models and incorporation of plastic behaviour into the cell wall model [5].

![Figure 4](image.png)

**Figure 4.** SPH-CG model predictions for compression of different plant cells: (a) apple; (b) potato; (c) grape

From Figure 6, the variation of the cell strain (ratio of the vertical height before and after) indicate several insights. Firstly, apple and grape cells show almost identical behaviour when compared with the potato cell, which is larger in size. At each compression time instance, the strain experienced by the apple and grape cells are higher than the potato cell, mainly due to the higher cell wall shear modulus or stiffness as seen in Table 1. Even though the cell wall shear modulus of the grape cell is about twice that of the apple cell, cell wall thickness is around half of apple cell’s value. Therefore, the overall cellular behaviour has become quite similar. This is mainly due to the effects of wall stiff force ($F^W$), which mainly governs the cell wall mechanical response [4, 10]. It can be deduced this mechanical behaviour has a correlation with the product of shear modulus and cell wall thickness.

For all cell types, there is an initial non-linear strain behaviour against time, followed by a linear trend in the strain. This can be mainly attributed to the inertial effects of top compression plate making the first contact with the top region of the cell during the compression phase [5]. There is an initial lag period ($56–64$ $\mu$s) of momentum transmission. This momentum and subsequent force transmission period could be given as the key reason behind the non-linear strain variation. Following this initial lag phase, the cell deforms steadily in alignment with the plate movement which corresponds to the linear strain variation observed in Figure 6 (time $> 64$ $\mu$s). A similar trend is observed for stress-time relationship as presented in Figure 7, however with more sensitivity to cell deformation than the wall strain, which is damped out by cell wall damping forces $F^d$ [4, 5]. In literature, there is evidence of comparable behaviours being observed in previous cell modelling investigations [10].

![Figure 5](image.png)

**Figure 5:** Stress-strain variation for different plant cells during compression with comparisons to experimental findings [19]

![Figure 6](image.png)

**Figure 6:** Strain variation against time for different plant cells

Conclusion

This study focused on modelling three-dimensional (3-D) microfluidics of parenchyma cells of three different food plant materials: apple, potato and grape using a SPH-CG coupled approach in order to study their physical deformations under external mechanical compression. Quantitative simulation results indicated quite similar cell deformations yielding to top and bottom flat surfaces in each of the cells. In stress-strain
behaviour, apple and grape cells indicated stiffer behaviour compared to the larger potato cell. However, both trends were showing stiffer nature compared to the tissue compression experimental results due to the non-existence of inter-cellular bonds and corresponding damping effects. The cell strain variation shows an initial non-linear behaviour with time followed by a linear trend, indicating gradual tensioning of the cell walls. However, stress variation with time indicated more sensitive increments to cellular deformations. In both cases, the gradients were such that both apple and grape cell show a stiffer behaviour compared to potato. So, it is evident based on this study that depending on the differences of physical properties of plant cells, their behaviour under compression varies. Findings of this research will be much useful in further studies on the topic towards prediction of 3-D tissue deformation under external forces [20, 21], which is much applicable in the field of food engineering (e.g. food drying, food processing etc.)

![Stress variation against time for different plant cells](image)

Figure 7: Stress variation against time for different plant cells

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