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A coupled SPH-DEM model for micro-scale structural deformations of plant cells during drying ☆

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ABSTRACT

A single plant cell was modeled with smoothed particle hydrodynamics (SPH) and a discrete element method (DEM) to study the basic micromechanics that govern the cellular structural deformations during drying. This two-dimensional particle-based model consists of two components: a cell fluid model and a cell wall model. The cell fluid was approximated to a highly viscous Newtonian fluid and modeled with SPH. The cell wall was treated as a stiff semi-permeable solid membrane with visco-elastic properties and modeled as a neo-Hookean solid material using a DEM. Compared to existing meshfree particle-based plant cell models, we have specifically introduced cell wall–fluid attraction forces and cell wall bending stiffness effects to address the critical shrinkage characteristics of the plant cells during drying. Also, a moisture domain-based novel approach was used to simulate drying mechanisms within the particle scheme. The model performance was found to be mainly influenced by the particle resolution, initial gap between the outermost fluid particles and wall particles and number of particles in the SPH influence domain. A higher order smoothing kernel was used with adaptive smoothing length to improve the stability and accuracy of the model. Cell deformations at different states of cell dryness were qualitatively and quantitatively compared with microscopic experimental findings on apple cells and a fairly good agreement was observed with some exceptions. The wall–fluid attraction forces and cell wall bending stiffness were found to be significantly improving the model predictions. A detailed sensitivity analysis was also done to further investigate the influence of wall–fluid attraction forces, cell wall bending stiffness, cell wall stiffness and the particle resolution. This novel meshfree based modeling approach is highly applicable for cellular level deformation studies of plant food materials during drying, which characterize large deformations.

1. Introduction

Drying is used as a key food preservation technique for around 20% of the world's perishable crops [1]. Plant food materials can contain up to 90% of water by weight [2] and due to such higher moisture contents levels, they are highly susceptible to biological spoilage. During drying, water is removed down to lower limits and it helps to significantly reduce

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Nomenclature

A	cell top surface area (m^2)
A_0	cell top surface area at fresh condition (m^2)
A/A_0	normalized cell area
A_c	total surface area of the cylindrical cell (m^2)
C	cell compactness
C_0	cell compactness at fresh condition
C/C_0	normalized cell compactness
D	cell ferret diameter (m)
D_0	cell initial diameter at fresh condition (m)
D/D_0	normalized cell ferret diameter
E	Young's modulus of the cell wall material (MPa)
EL	cell elongation
EL_0	cell elongation at fresh condition
EL/EL_0	normalized cell elongation
F^e	cell wall stiff forces (N)
F^d	cell wall damping forces (N)
F^{rf}	wall–fluid repulsion forces (N)
F^{rw}	wall–wall repulsion forces (N)
F^a	wall–fluid attraction forces (N)
F^b	forces due to bending stiffness of the wall (N)
F^p	cell fluid pressure forces (N)
F^v	cell fluid viscous forces (N)
G	shear modulus of the cell wall material (MPa)
K	cell fluid compression modulus (MPa)
L	length of any given discrete wall element (m)
L_0	initial length of any given discrete wall element (m)
L_p	cell wall permeability ($m^2\ N^{-1}\ s$)
P	cell perimeter (m)
P_0	cell perimeter at fresh condition (m)
P/P_0	normalized cell perimeter
P_a	pressure of any particle a (Pa)
P_T	initial cell turgor pressure (Pa)
R	cell roundness
R_0	cell roundness at fresh condition
R/R_0	normalized cell perimeter
S	ratio between particle distance and smoothing length (r_{ab}/h)
T_0	initial cell wall thickness (m)
T	cell wall thickness (m)
W	smoothing kernel
X	X – coordinate axis
X	dry basis moisture content at any dried condition ($kg_{water}/kg_{dry\,solid}$)
X_0	dry basis moisture content at fresh condition
X/X_0	dry basis normalized moisture content
Y	Y – coordinate axis
Z	cell height (m)
Z	Z – coordinate axis
Z_0	initial cell height (m)
Z_t	cell height at the previous time step (m)
$Z_{t+\Delta t}$	cell height at the current time step (m)
f_0^{rf}	strength of the LJ repulsion forces between fluid and wall particles ($N\ m^{-1}$)
f_0^{rw}	strength of the LJ repulsion forces between non-bonded wall particles ($N\ m^{-1}$)
f_0^a	strength of the LJ attraction forces between fluid and wall particles ($N\ m^{-1}$)
h	smoothing length (m)
h_0	initial smoothing length (m)
k_b	bending stiffness of cell wall ($N\ m\ rad^{-1}$)
m_a	mass of any particle a (kg)
n_f	cell fluid particle number
n_w	cell wall particle number
r	cell radius (m)