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► **To cite this version:**

Emna Chichti, Rafik Affes, Matthieu George, Valerie Lullien-Pellerin, Farhang Radjai, et al.. Numerical modeling of wheat fractionation role of starch volume fraction. Modeling Granular Media Across Scales - MGMA2014, Jul 2014, Montpellier, France. 2014. hal-01594308

HAL Id: hal-01594308

<https://hal.science/hal-01594308v1>

Submitted on 3 Jun 2020

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Numerical modeling of wheat fractionation Role of starch volume fraction

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Wheat endosperm is a cemented granular material composed of a binary-sized mixture of almost spherical starch granules bounded to one another with an amorphous protein matrix. The milling properties of wheat grains depend on this typical microstructure, largely controlled by the genetic background and the growing conditions. An original Atomic Force Microscopy nano-scratch methodology has been developed [1] to assess the local rheological properties of the protein matrix, the starch granules and their interface. The determined relative stiffness and failure strength, together with information on the phase distribution, were then used to construct 2D numerical samples of wheat endosperm. The granular structure of the sample with different granular packing was computed using a Molecular Dynamics approach. The protein matrix was added in the form of bridges connecting neighboring particles. The samples were then meshed using a triangular lattice of one-dimensional spring elements that were characterized by stiffness and yield force. The rheological properties of each element were set according to the location of its two nodes leading to five different elements: starch, matrix, starch-matrix, starch-starch and voids. The samples were then subjected to an increasing uniaxial tensile stress until failure using an iterative procedure based on conjugate gradient minimization. The Lattice Element Method, developed by Topin [2,3], was used for the simulations and a parametric study was performed where the protein content, the starch granular packing and the starch-protein adhesion, suggested to be responsible of the wheat fragmentation, were varied. The results showed that, depending on the sample porosity, the bulk elastic properties do not follow the mixing law of diluted composites, highlighting the granular backbone effect of percolating particles. A non-linear evolution of the bulk elastic modulus as a function of the sample porosity was also noted, with little effect of the granule solid fraction. Concerning the failure properties, the results showed that the particle volume fraction has a greater influence on the yield stress at high starch-protein adhesion and that for the same porosity, increasing particles volume fraction leads to higher yield stress. Finally, we noted that the yield stress strongly depends on the sample porosity at high starch-protein adhesion and is weakly affected by the porosity at low adhesion, whatever the particle volume fractions.

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[2] V. Topin, J.-Y. Delenne, F. Radjai, L. Brendel, and F. Mabilbe. Strength and failure of cemented granular matter. *European Physical Journal E: Soft Matter*, 23:413–429, 2007.

[3] R. Affes, J.-Y. Delenne, Y. Monerie, F. Radjai, and V. Topin. Tensile strength and fracture of cemented granular aggregates. *European Physical Journal E*, 35:1–15, 2012.