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Bottom-up model for understanding the effects of wheat endosperm microstructure on its mechanical strength

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ABSTRACT

Wheat flours are essential ingredients of daily food products like bread, cookies or pastries. Their quality depends on the milling process and mechanical strength of wheat grains. Although it is well known that the strength and rupture of grains are strongly controlled by the endosperm microstructure, the respective roles of the starch and polymer volume fractions and their adhesion are not yet fully understood. This typical biological microstructure can be modeled as a cemented granular material, where the two size populations of starch granules (large:A-type, small:B-type) are the particles, and the protein matrix, which partially fills the space between granules, plays the role of a cement. This structural model of wheat endosperm is used, together with mechanical characteristics of starch and proteins obtained by means of Atomic Force Microscopy (AFM) measurements, to simulate the mechanical behavior and breakage of wheat endosperm in milling process. We find that the porosity outweighs the effect of other parameters for the elastic modulus, which declines as a nearly linear function of porosity. We also show that the tensile strength is an increasing function of the amount and connectivity of starch granules with increasing concentration of stresses along chains of granules. This effect is more significant at low porosity where stress distribution is mainly controlled by the contact network between starch granules. This effect explains why the protein content is not fully correlated to vitreousness, and samples of similar protein content can be different in vitreosity. Finally, we find that the starch-granule adhesion strongly affects the tensile strength whereas the effect of starch volume fraction appears mainly at high interface adhesion, which is the case of hard type wheat grains.

1. Introduction

Wheat flour characteristics such as particle size distribution and starch damage level are important factors for food product quality (Pasha et al., 2010). Such characteristics arise from the mechanical properties of the starchy endosperm, which is made of starch granules embedded in a protein matrix (Evers and Millar, 2002), and the milling process. The observed differences in flour properties are generally attributed to two main wheat grain characteristics: hardness and vitreousness (Haddad et al., 2001; Greffeuille et al., 2006, 2007). Wheat hardness represents the potential of producing fractions from a specific mechanical loading. It is usually estimated from a controlled grinding operation and a measure of particle size distribution (Williams and Sobering, 1986). Hence, from a mechanical viewpoint, wheat hardness reflects the fracture energy of wheat grains in response to mechanical loading during the grinding process (Wang and Jeronimidis, 2008).

Wheat hardness is a genetic-controlled property mainly linked to the Ha locus on the short arm of chromosome 5D (Turnbull and Rahman, 2002) and there is increasing evidence that it expresses itself through differences in starch-protein adhesion (Barlow et al., 1973; Greenwell and Schofield, 1986; Glenn and Johnston, 1992). Furthermore, these differences in adhesion depends on the nature and content of specific proteins, called puroindolines, present at the starch-granule interface (Turnbull and Rahman, 2002; Morris, 2002). The presence of the wild type version of puroindolines

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leads to a soft mechanical behavior due to a low adhesion between starch granules and the protein network, whereas mutation or deletion of one or both of the puroindolines genes results in a hard texture (Hogg et al., 2004; Giroux and Morris, 1998; Beecher et al., 2002).

Grain vitreousness is an optical property related to endosperm translucence and it characterizes the mealy and vitreous states of the starchy endosperm (Anjum and Walker, 1991; Weightmann et al., 2008). It is mainly controlled by the environmental conditions during growing and grain maturation (Parish and Halse, 1969; Oury et al., 2015; Lopez-Ahumada et al., 2010) which affect the grain density via the proportion of voids in the endosperm (Anjum and Walker, 1991; Dobraszczyk et al., 2002). If vitreousness was generally significantly correlated with the protein content (Weightmann et al., 2008; Lopez-Ahumada et al., 2010), this relationship remains under debate as different levels of vitreousness can be observed for grains displaying the same protein content (Greffeuille et al., 2006, 2007).

This means that the volume fraction of starch, which is the main constituent of wheat endosperm whose accumulation during grain development is also affected by growing conditions (Dai et al., 2009; Zhang et al., 2010; Hurkman and Wood, 2011; Ni et al., 2012), may well affect grain vitreousness. Therefore, starch particle content or its size distribution are expected to play a role in vitreousness and hence in the milling behavior of wheat grains. However, this factor has not yet been fully investigated on quantitative grounds.

In this paper, we analyze the role of starch and protein volume fractions with respect to the mechanical properties of wheat endosperm by means of numerical simulations. The mechanical model is a particulate system in which the starch granules are embedded in a porous protein matrix. Two different methods have been applied to simulate this model. In (Delenne et al., 2008), the authors used the Discrete Element Method (DEM) in which the protein matrix is introduced only through its cohesive action between starch granules (Cundall and Strack, 1979). This approach accounts for the effect of internal damage on the elastic and failure properties of endosperm. More recently, the Lattice Element Method (LEM) was used for a detailed parametric study of wheat endosperm (Topin et al., 2007; Affes et al., 2012). In this method, both starch granules and protein are represented as continuous material phases. The authors investigated the influence of particle-matrix adhesion and protein content on strength and failure properties of the endosperm. Three distinct crack regimes were established, and the importance of starch-protein adhesion and protein content for crack propagation and fraction properties were quantitatively analyzed.

The LEM has the advantage of allowing for a realistic representation of the endosperm texture. But it needs as its input parameters the elastic constants of the starch granules and protein matrix, as well as the adhesion at the interfaces between starch granules and between the matrix and starch granules. In the previous studies (Topin et al., 2008), the mechanical properties of starch and protein phases were derived from the work of (Barlow et al., 1973; Glenn and Johnston, 1992), where micro-indentation tests were performed on wheat grain sections or individual polymers included in a resin. The resulting mechanical properties of starch and proteins appeared to be weakly contrasted and were thus considered to be identical. However, recent work of (Chichti et al., 2013) based on Atomic Force Microscopy (AFM) measurements, revealed that the mechanical properties of the phases differed from those used by (Topin et al., 2008).

In this paper, we use a 2*D* Lattice Element Method together with our AFM measurements of phase properties, in order to analyze the effects of starch and protein volume fractions with respect to shear strength and effective elastic behavior of wheat endosperm. After a brief description of the numerical model and methodology used to prepare the samples, we analyze the effective behavior for a set of samples created with different values of the starch and protein volume fractions and their interface adhesion. We compare our results with the existing data and conclude with the salient results of this work.

2. Numerical model of wheat endosperm

2.1. Lattice element method

The wheat endosperm can be described as a cohesive granular aggregate composed of starch granules inter-connected by a protein matrix (Fig. 1(a) and b). This typical microstructure is thus a multi-phase material with three bulk phases of starch, matrix and voids and their interfaces. For the simulations of this multi-phase representation of wheat endosperm, we used the Lattice Element Method (LEM), which has already been successfully used as a model for wheat endosperm fractionation in 2D (Topin et al., 2008, 2009a) and applied to investigate the fracture properties of cemented granular materials in 3D (Affes et al., 2012). This approach has also been extensively used in statistical physics of disordered media (Roux, 1990; Schlangen and Garboczi, 1996, 1997; Van Mier et al., 1997).

The LEM consists in discretizing all phases on a regular or irregular lattice. By allowing the mechanical information to be transmitted along a finite number of space directions, this representation allows for efficient simulation of a large number of different phases. Each node of the lattice belong to a phase and the mechanical properties such as elasticity, elasticity limit and plastic strains are carried by the links between nodes. When the two nodes of a link belong to the same phase, the link represents a 'bulk phase' whereas the links with nodes belonging to different phases carry the 'interface' properties between the phases. The mechanical behavior is thus fully implemented by 1) the distribution of nodes in space (or the type of lattice), 2) the mechanical information carried by a link.

The endosperm sample is composed of three bulk phases φ: starch s, protein p and void space v. We assume a quasi-brittle elastic behavior of starch and protein, as usually observed in mechanical tests for reasonably low moisture content (Haddad et al., 1999; Delwiche, 2000).

This implies that the links should be modeled as linear springs uniquely characterized by their stiffness k^{φ} and breaking threshold f_c^{φ}. Hence, each link between nodes i and j transmits only a single radial force f^{ij} related to the node displacements by

$$f^{ij} = k^{ij}\left(\ell^{ij} - \ell_0\right) \tag{1}$$

where ℓ_0 is the equilibrium element length and ℓ^{ij} is the element length. When the radial force f^{ij} reaches its breaking threshold f_c, the element is broken and its stiffness vanishes. As we shall see, this elemental linear behavior leads to a quasi-brittle behavior with linear elastic properties at the lattice scale with properties depending on the volume fractions of different phases (Fig. 1(c)). The starch-starch (ss) and starch/protein (sp) interfaces may have different values of stiffness and breaking threshold. The bulk links of the void phase and its interface with other phases have, by definition, zero stiffness.

In the following, we will express the element characteristics in stress units. Therefore, the yield stress σ^{φ} of an element belonging to the phase φ and its elastic modulus E^{φ} are defined as