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Numerical investigation of microstructural damage during kneading of wheat dough

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ABSTRACT

The focus of this study is the kneading process of wheat dough. As an idealized kneader geometry, the eccentric cylinder benchmark geometry was considered. This work presents the first computational study in which the dough model developed by Tanner's group (R.I. Tanner, F. Qi, S.-C. Dai, Bread dough rheology and recoil: I. Rheology. J. Cereal Sci. 148 (1) (2008) 33–40) was solved for inhomogeneous flow. The values of the model parameter were obtained from small amplitude oscillatory shear, stress relaxation, start-up of simple shear, and compression experiments. To computationally evaluate the damage function, a time evolution equation had to be implemented for the Cauchy–Green strain tensor. The flow problem was numerically solved using a finite volume procedure available in the software OpenFOAM package rheoTool. As a result of the rapid decrease in accumulated strain, filaments of low damage were formed near the outer diverging part of the cylinder, convected downstream and further extended, and eventually broken down. Planar extension had the most destroying effect on the microstructure. In the future, we will investigate three-dimensional free-surface flows in industrial kneading geometries.

1. Introduction

Dough is a complex soft material. At the macroscopic scale, it is a quasi-homogeneous continuous medium. At the microscopic scale, however, dough can be seen as a heterogeneous suspension of starch granules, other long-chain components, and gas bubbles in a viscoelastic gluten matrix. To form a dough, flour, water, yeast and some other minor ingredients are first mixed. Subsequent kneading brings air into the dough and develops the gluten network. Detailed knowledge about the rheological and microstructural changes that occur during kneading and its impact on product quality is currently lacking. Therefore, the industrial kneading process is commonly controlled by using visual and haptic information from trained personnel. Under-kneading provides a dough with insufficient gas retention capacity. Over-kneading leads to smaller water absorption capacity and impairs the dough's ability to rise, making dough very dense and tough. Slightly over-kneading the dough, however, can even improve the end-product quality. Nevertheless, both extremes should be avoided.

Developing a constitutive model for dough is a challenging task due to the complexity of its microstructure. Generalized Newtonian models have been used in several works to describe the rheology of bread dough (Dus & Kokini, 1990; Launay & Buré, 1973; Wang & Kokini, 1995a). The limitation of these scalar models is that they only account for a varying viscosity, but cannot capture transient and elastic effects. Classical viscoelastic models of differential type have also been extensively employed. For instance, Kokini' group (Dhanasekharan, Huang, & Kokini, 1999; Dhanasekharan, Wang, & Kokini, 2001) compared the rheology of wheat flour dough with the predictions of the White–Metzner, Giesekus, and Phan-Thien Tanner (PTT) models. In the case of the latter two models, four relaxation modes were utilized. By specifying the mobility factor to be much larger than 0.5, the Giesekus model reproduced the extension-thinning behavior of the dough at high extension rates. By using a Bird-Carreau dependency for the viscosity and the relaxation time, the White–Metzner showed the overall best performance. The steady shear viscosity and first normal stress coefficient were very well predicted. However, transient shear properties were much better captured by the Giesekus and PTT models. Furthermore, because of its asymptotic behavior, the White–Metzner model was unable to capture the uniaxial extensional viscosity at large extension rates. Bagley (1992) studied the uniaxial compression of wheat flour dough using the upper-convected Maxwell model. By using a single relaxation time, good agreement between the experimental and calculated results could be obtained. However, the rheological parameters had to be varied with the compression rates to get good fits, which reflects the presence of a broad distribution of relaxation times.

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Since the last 20 years, a few models have been specifically developed for dough. With the incorporation of a linear memory function and a damping function, the Wagner model was found to capture the nonlinear relaxation modulus as well as the steady viscosity (Wang & Kokini, 1995b). However, the transient viscosity and the first normal stress coefficient were not well predicted. Phan-Thien, Safari-Ardi, and Morales-Patiño (1997) represented the gluten network by a hyperelastic term whereas the starch globules and other long-chain components that are not part of the permanent network were described by the multi-mode Maxwell constitutive equation. The elastic stress contribution was tempered by a strain function to represent the strain softening behavior and the partial failure of the gluten network. The dynamic moduli as well as the transient simple shear data could be reasonably described. Ng, McKinley, and Padmanabhan (2006) constructed a nonlinear constitutive equation of Lodge rubber-like liquid form by combining combining the linear viscoelastic modulus of the critical gel Winter and Chambon (1986) with finite strain kinematics. The initial power-law response and subsequent strain-hardening during filament stretching could be captured. The most sophisticated rheological model for dough was presented by Tanner, Dai, and Qi (2007,2008). Like in solid mechanics, a damage function was utilized to describe the partial microstructural breakdown. As in Charalambides, Wanigasooriya, and Williams (2002), a Mooney–Rivlin term was included so that the same damage function could be used for all types of deformations. By using a power-law memory function in the Lodge constitutive expression, the dough rheology could be successfully predicted in a variety of tests, including steady shear, small amplitude oscillatory shear, stress relaxation, and uniaxial extension. The numerical treatment of integral constitutive equations is not straightforward (Keunings, 2003). This may be the reason why Tanner's damage model has only been analytically solved for rheometric flows so far.

The eccentric cylinder geometry is often used as a benchmark problem for testing numerical methods and viscoelastic constitutive models. The advantage of this geometry is that it has smooth boundaries. However, eccentric cylinder flow is still complex in that it involves a combination of simple shear, planar extension, and rigid body rotation. The eccentric cylinder geometry is also of industrial interest because of its high distributive and disperse mixing characteristics. Beris, Armstrong, and Brown (1987) were the first to report successful viscoelastic calculations for the upper-convected Maxwell model at large Deborah numbers. Baloch, Grant, and Webster (2002) solved the linear and exponential versions of the PTT model. They studied the impact of the model parameters on the flow kinematics, stress fields, local rate of work, and power consumption. Davies and Li (1994) solved the White–Metzner (WM) model to investigate the effects of temperature and pressure. Germann and coworkers solved the extended White–Metzner model (Germann, Dressler, & Windhab, 2011) and a polymer blend model (Germann & Windhab, 2012).

The goal of the this work was to study the flow of wheat dough between two eccentric cylinders using Tanner's damage model. The eccentric cylinder geometry was selected as it represents an idealization of a kneader. For the simulation, we employed the differential formulation of Tanner's damage model. An effective method for numerically evaluating the damage function in an inhomogeneous flow field was developed. The remainder of this article is organized as follows. An overview of the dough model employed in the numerical simulations is given in Section 2. The experimental protocol and parameter fitting are provided in Section 3. We describe the flow problem and discuss the numerical solution methodology in Section 4. The computational results are discussed in Section 5. The final conclusions of this study are drawn in Section 6.

2. Dough model

2.1. Integral version

Tanner's damage model relates the stress tensor, $\boldsymbol{\sigma}$, to the composite strain tensor, $\mathbf{S}$, by an integral over all past history of deformation (Tanner, Qi, & Dai, 2008)

$$\boldsymbol{\sigma} = f(\varepsilon_H)\int_{-\infty}^{t} m(t-t')\mathbf{S}(t')\mathrm{d}t', \tag{1}$$

where f and m are the damage and memory functions, respectively. The damage function is assumed to depend on the Hencky strain, ε_H. Typically, it is unity for very small strains (no damage) and decreases sharply as the strain is further increased. In our work, we employ the following functional dependency:

$$f(\varepsilon_H) = \{A_1 + A_2\,\varepsilon_H + A_3\,\varepsilon_H^2\}e^{-(A_4\,\varepsilon_H)^{A_5}}, \tag{2}$$

where A_1, A_2, …, A_5 are nondimensional fitting parameters. The memory function is assumed to have a power-law form, which is extensively used in the context of gel-like materials (Winter & Chambon, 1986), as (Tanner, Qi, et al., 2008)

$$m(t) = pG(1)t^{-(p+1)}, \tag{3}$$

where p is a constant depending on the dough type. The quantity $G(1)$ corresponds to the numeral value of the elastic modulus at the time instant $t = 1$ s and has dimensions Pa s^p. In most Lodge-type integral models, the strain is expressed in terms of the Finger tensor, $\mathbf{C}^{-1}$. However, Tanner, Dai, et al. (2008) found that a linear combination of the Cauchy-Green strain tensor, $\mathbf{C}$, and its inverse, $\mathbf{C}^{-1}$, performs better. Consequently, the strain tensor in Eq. (1) is defined as (Tanner, Qi, et al., 2008)

$$\mathbf{S} = \frac{1}{1+a}(\mathbf{C}^{-1} - a\mathbf{C}), \tag{4}$$

where the constant a controls the magnitude of the deformation in extension and compression.

All parameters of the dough model can be found from a set of standard rheological tests including small amplitude oscillatory shear (SAOS), stress relaxation, start-up of simple shear, and compression (Tanner, Qi, & Dai, 2011). The limiting behavior of the model in these standard flows will be discussed next.

2.1.1. Small amplitude oscillatory shear

Small amplitude oscillatory shear measurements conducted at various frequencies ω within the linear viscoelastic region can be used to find the model parameters p and $G(1)$. For this type of flow, we have $f \approx 1$. The storage and loss moduli, $G'(\omega)$ and $G''(\omega)$, respectively, are given in terms of the oscillation frequency according to the following power-law relation (Tanner, Qi, et al., 2008):

$$G'(\omega) = G'(1)\omega^p, \tag{5}$$

$$G''(\omega) = G''(1)\omega^p, \tag{6}$$

where p determines the slope in a double logarithmic plot and $G'(1)$ corresponds to $G'(\omega)$ at $\omega = 1$ rad s^{-1}. Furthermore, the parameter $G(1)$ can be obtained from (Pipkin, 1986; Tanner, Qi, et al., 2008)

$$G(1) = \frac{2G'(1)\Gamma(1+p)}{p\pi}\sin\frac{p\pi}{2}, \tag{7}$$

where $\Gamma(x)$ indicates the gamma function.