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Measurement and mathematical modeling of the relative volume of wheat dough during proofing

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ABSTRACT

Dough is a complex system where yeast cells produce carbon dioxide during the leavening process. Mechanistic models were fitted to measurements of the relative volume of wheat dough during proofing obtained from a Rheofermentometer. The measurements are carried out using 2% and 4% of fresh yeast and proofing temperatures of 28, 32 and 35 °C. The free parameters were the viscosity, a specific CO_2 production rate and the number of bubbles. The following assumptions were made: spherical bubbles in the dough liquid, considered to behave as a Newtonian liquid, the applicability of the Bernoulli and ideal gas equations as well as the diffusion theory. The relative volume during proofing was simulated with an average percentage error less than 0.5% and the dependency between volume expansion and calculated CO_2 production rate was obtained with an R^2 of 0.88.

1. Introduction

Proofing of dough is a key step in the production of voluminous baked goods. However dough is a complex system where yeast cells are used in the leavening process to produce carbon dioxide for the typical sponginess and fluffiness of the final product. Variances in the leavening time are common and can possibly lead to non-optimal capacity utilization in bakeries or products with a minor volume. The optimal proofing time can only be determined by specially trained and experienced operators. Often baking improvers are added to standardize dough and thus minimize variances. Supervising this process by calculating the production rate, and possibly predicting the optimal proofing time as early as possible during the fermentation, could strongly assist this process and avoid non optimal leavened dough. A computational assisted method using mathematical process models could also be integrated in computer assisted optimization of bakeries as described by Hecker et al. (Hecker et al., 2013).

One of the first attempts to model the leavening process was presented by de Cindio and Correra (de Cindio and Correra, 1995). They introduced a complex model, including the kneading and baking process. The different metabolic pathways like lactic acid and ethanol production were included to calculate pH and acidity. Later Shah et al. (Shah et al., 1998) presented a more simple model, based on classical one-component (carbon dioxide) diffusion theory for the rising gas bubbles. The model described a single representative bubble with a mean bubble radius. The carbon dioxide concentration available in the dough was considered to be constant at its maximum solubility, but the influence of the viscosity was not considered. Chiotellis and Campbell (Chiotellis and Campbell, 2003b) extended the model from Shah et al. with a Michaelis–Menten-like time-dependent CO_2 production rate, allowing the carbon dioxide concentration in the dough liquid to increase over time. They further extended the model by using a bubble distribution rather than one mean bubble size. Córdoba (Córdoba, 2010) also considered viscous effects and the Michaelis–Menten-like kinetic modification. However, by choosing a Michaelis–Menten constant of zero, it resulted in a constant CO_2 production rate. He also performed model simulations to fit the model to actual measured data using four different dough recipes.

Romano et al. (Romano et al., 2007) described the variation of dough volume as a function of time, using the more often used Gompertz model derived from the description of bacterial growth in pH-controlled batch cultures. Bikard et al. (Bikard et al., 2008) presented a 3D numerical simulation approach, modeling a 1 cm^3 of dough sample using the finite element method.

Many individual properties of dough are already known and have been often described. For example Upadhyay et al. (Upadhyay et al., 2012) described rheological characteristics and the microstructure of dough. Zúñiga and Le-Bail (Zúñiga and Le-Bail, 2009) presented results of heat transfer measurements in the dough,

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showing gradients towards the core. Also pressure inhomogeneity can be observed as described by Grenier et al. (Grenier et al., 2010). In situ methods like the X-ray tomography give insights into the actual bubble growth as described by Babin et al., Bellido et al. and Turbin-Orger et al. (Babin et al., 2006; Bellido et al., 2006; Turbin-Orger et al., 2012). They presented changes of dough porosity during the leavening process (an increase in porosity from 0.1 to 0.7) as well as coalescence phenomena. The phenomenon of coalescence was also discussed by Mills et al. (Mills et al., 2003). They showed the appearance of coalescence after a certain amount of time based on model simulations derived from Shah et al. (Shah et al., 1998). The formation of new bubbles was neglected due to the very high pressure that needs to be overcome according to the Young Laplace law. By introducing an anisotropy factor (ratio of the major to the minor axis of an ellipsoid), Bellido et al. (Bellido et al., 2006) showed that only ellipsoid bubbles were present. They showed that the bubbles size was distributed according to a log-normal distribution with a geometric mean of 50 μm radius. The mean of the bubble radii varied in publications between 16 μm (Upadhyay et al., 2012), 110 μm (Turbin-Orger et al., 2012), 180 μm (Babin et al., 2006) and 300 μm (de Cindio and Correra, 1995).

For the mechanistic mathematical description of the volume evolution during the proofing process, certain assumptions are necessary: only spherical bubbles are present which are evenly distributed in liquid dough and which do not change in number; the Bernoulli, the Henry and the ideal gas law as well as the diffusion theory can be applied; the CO_2 is the only diffusing substance. The temperature is the same all over the dough. One representative bubble is simulated.

As the statistician George Box once taught: "Since all models are wrong the scientist cannot obtain a "correct" one...yet he can derive results which match, to a useful approximation, those found in the real world" (Box, 1976), hence the obvious inadequacies of the model were accepted. Certain modifications to the model used by Córdoba (Córdoba, 2010) are introduced such as a factor for the specific CO_2 production rate as well as the yeast concentration. The model is fitted to measurements, using experiments at different temperatures and different amounts of yeast to show the prediction accuracy of the modified model. The measurements are carried out in a specialized proofing chamber called Rheofermentometer, restricting the dough to develop its volume only in one dimension and giving precise results for the actual dough volume. The model is proposed as a possible monitoring system to supervise the dough leavening process through the indirect measurement of the specific CO_2 production rate.

2. Material and methods

The dough was produced with commercial wheat flour (196.82 g, Schapfenmühle, type 550: 0.51–0.63% mineral supplements in dry matter, 11.87% moisture content), water (119.18 g), salt (4 g) and commercial yeast (4 g and 8 g, Omas Ur Hefe, Fala, Germany, four 41 g units taken from one batch and stored in a fridge at 7 °C for 2 days) in a mixer (N50, Hobart GmbH, Germany).

Mixing time and water temperature were kept constant at 4 min and 32 °C, the temperature of the prepared dough ranged between 23.8 °C and 27.8 °C depending on the room temperature. After mixing, 200 g of the dough was hand rounded on a worktop, until the dough formed a ball. Subsequently the dough was incubated for 80 min in a Rheofermentometer (Chopin, France) at temperatures of 28, 32 and 35 °C, charged with 1 kg weight.

The six different experimental conditions were repeated four times; therefore 24 individual experiments were performed in total.

3. Calculations

3.1. Model calculations

The differential equation system for the dough modeling is based on the work of Córdoba (Córdoba, 2010). However, only first order differential equations were used. The increasing bubble radius over time is described by Eq. (1).

$$\frac{dR}{dt} = \frac{3nR_gT}{16\pi R^2\eta} - \frac{pR}{4\eta} - \frac{\gamma}{2\eta} \tag{1}$$

R is the bubble radius, n the amount of substance in the bubble, R_g the gas constant, T the temperature, η the viscosity, p the pressure in the liquid dough, and γ the surface tension. The change of CO_2 concentration in the liquid dough is presented in Eq. (2). As distinguished from Córdoba (Córdoba, 2010) where the CO_2 production rate was modeled by a Michaelis–Menten-like kinetic, here it is described by the product of a specific CO_2 production rate q_{CO_2} and the yeast biomass X. The decrease of the CO_2 concentration in the liquid dough (last term of Eq. (2)) is obtained by the total amount of CO_2 diffusing in the overall N_b existing bubbles per unit volume of gas-free dough. The exchange area was determined from the sphere radius R.

$$\frac{dC_D}{dt} = q_{CO_2}X - 4N_bD\pi R(C_D - C^*) \tag{2}$$

D is the diffusion coefficient, C_D the carbon dioxide concentration in the dough, C^* the carbon dioxide concentration, which is in equilibrium with its partial pressure in the bubble. Eq. (3) represents the increase of the amount of substance in a bubble due to its concentration difference in the liquid and the gas phase.

$$\frac{dn}{dt} = 4D\pi R(C_D - C^*) \tag{3}$$

According to Shah et al. (Shah et al., 1998) Henrys law can be applied in the form of Eq. (4).

$$C^* = \frac{p}{H}\left(1 - \left(\frac{R_0}{R}\right)^3\right) + \frac{8\gamma}{HR}\left(1 - \left(\frac{R_0}{R}\right)^2\right) \tag{4}$$

The temperature dependence of the Henry's constant was used as described by Chiotellis and Campbell (Chiotellis and Campbell, 2003a) for a carbon dioxide-in-dough system (Eq. (5)).

$$H = 60{,}000\ \frac{\mathrm{J}}{\mathrm{kmol}\cdot K}\cdot T + 900{,}000\ \frac{\mathrm{J}}{\mathrm{kmol}} \tag{5}$$

The temperature dependence of mass diffusion coefficient D was considered according to the Chemical Engineers Handbook (Reid, 1974) as

$$D = 1.77 * 10^{-9}\cdot X_w \cdot \frac{T}{298K}\ \frac{\mathrm{m}^2}{\mathrm{s}} \tag{6}$$

with a water fraction of $X_w = 0.4$.

The specific CO_2 production rate, viscosity and the number of bubbles were used as free parameters. Table 1 gives an overview of the parameters and variables used in the model equations as well as the units and their common values.

To solve the differential equation system the initial conditions were:

$$R(t=0) = R_0,$$

$$C_D(t=0) = 0,$$

$$C^*(t=0) = 0,$$