Modelling the Mixing of Wheat Flour Dough

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Abstract Wheat is grown to make, among other things, pasta, bread, noodles and biscuits. In fact, about 40% of exported Australian wheat goes to make noodles, while a small amount of Durum is exported to Italy to make pasta. The functionality of such products depends not only on the properties of the wheat, but also on how it is mixed with various ingredients to produce the dough which is baked, boiled or dried. The paper examines how modelling can be viewed as a linking of mathematics to data by considering some of the recent experiments performed at the Grain Quality Research Laboratory, CSIRO Plant Industry, aimed at developing mathematical models of the mixing process in a Mixograph^{TM}. Among other things, the goal is to characterize quantitatively and explicitly the role played by the proteins and starches in guaranteeing quality. The hope is that this will act as a guide for plant breeders in the development of new wheat varieties, as well as improving the design of industrial dough mixers.

1. THE ART OF MODELLING: LINKING MATHEMATICS TO DATA

An early and crucial step in any modelling or simulation endeavour is the formulation of the mathematical model describing the process under investigation. But, how does one construct the mathematical model? It is not difficult to write down involved mathematical equations. The challenge is to choose the mathematics so that the model yields practical and useful insights about the problem under examination.

The strategy often employed by the applied and industrial mathematician is to first identify the question which one is aiming to resolve, as it determines the type of information required to construct an answer (cf. Anderssen *et al.* (1997)). One then aims to identify the type of data which can be measured because, in one way or another, they contain such information. Only at this stage is one in a position to formulate mathematical models which define how the required information is related to the data and how the answer can be quantified in terms of that model.

For a particular question, there is no unique set of data which is the only source of information from which an answer can be constructed. The process is much more one of identifying how to obtain suitable data using the available experimental equipment, or of identifying the type of data which have a strong link to the required information. The former is a matter of economics, where one aims to maximize the utility of available resources, while the latter is one of aiming to minimize the complexity of the mathematical modelling involved.

The goal of the present paper is to examine the validity of this point of view within the context of modelling the mixing of wheat flour dough.

2. WHEAT, FLOUR AND DOUGH

The questions which can be ask about the mixing of wheat flour dough relate to all stages of the process which transforms wheat into flour and then into dough. Many relate to the fact that, when compared with other cereals, wheat is special because the dough that it makes, when wheat flour is mixed with water and other ingredients, has the following properties:

(a) Dough is a viscoelastic material, which controls the sizes of the gas bubbles which form during fermentation.

(b) The dough has superior gas retention properties, since the rate of diffusion of gasses through dough is very small.

(c) When cooked, the dough forms a solid foam.

In this context, some of the questions of interest include:

- What controls the viscoelasticity of the dough?
- What is the value of the diffusion coefficient for carbon dioxide in dough?
- What is the nature of the gelatilization occuring in the dough during cooking?

The examinations of each of these questions will involve quite separate modelling considerations, and each of these considerations will, in turn, spawn new questions. For example, the viscoelasticity of dough is known to be controlled by its proteins. For both synthetic and biological polymers, there is overwhelming experimental evidence that their basic physical properties are controlled by their highest molecular weight components. For wheat proteins, the highest molecular weight components are the glutenin molecules. The quality of the bread, pasta or noodles, made from a given dough, is therefore controlled, in a major way, by its glutenin proteins. Genetic studies determine how the wheat chromosomes control the linking of the monomers to form the higher molecular weight glutenin macromolecules.

Each step in this logic involves a different modelling consideration. For example, the molecular weight distribution (MWD) of the proteins must be determined experimentally in order to estimate the relative proportions and sizes of the glutenin molecules in different wheat varieties. Various methods are available for determining the MWD of polymers including

- Centrifuge Methods.
- Size Exclusion HPLC.
- Field Flow Fractionation (FFF).
- Rheological Mixing Rules.

Each of these procedures involves a different mathematical model. Each of these models reflects how closely the MWD is related to the measured data. The MWD is only poorly determined by the centrifuge method, and this procedure has been replaced by alternative procedures, such as FFF, where there is a more direct link between the MWD and the measured data. FFF is popular because it accurately measures the hydrodynamic diameters of the molecular weight components, and because a simple mathematical formula defines the molecular weights in terms of the hydrodynamic diameters. Rheological mixing rules are not so popular, as the structure of the mathematical models which relates the MWD to the measured relaxation modulus is controversial.

In summary, there are various points of view from which one can explore the modelling of the mixing of wheat flour dough. In the remainder of this paper, attention will focus on the actual mixing of the dough in Mixograph^{TM} experiments performed at the Grain Quality Research Laboratory, CSIRO Plant Industry.

3. MODELLING THE MIXING

In a traditional examination of the material properties and behaviour of a wheat flour dough, the three basic steps are (Anderssen *et al.* (1996)):

1. Identify the rheological characteristics of the dough encapsulated in the particular application under consideration. For example, if the performance of commercial mixers in a biscuit factory is the focus of the study, the underlying rheology can vary from strongly elongational in block-and-sprag types (used to make crackers and milk coffee) to predominantly shear in split-durimal types (used to make shortbreads). Where possible, rheological experimentation and modelling in the laboratory should aim to match the nature of the commercial mixing under examination.
2. Design the experiments to be performed so that they answer the types of questions under consideration about the dough. For example, if the interest relates to the efficient manufacture of pasta, then it is necessary to design the experiments to be performed on a suitable extruder.
3. The choice of the mathematical model which encapsulates, possibly via a link concept (Anderssen (1993)), the input-output nature of the experiment performed to obtain the data. For example, if the effect of additives in bread dough is being examined, then the elongational viscosity of the dough represents an appropriate measure for assessing the differences (Meissner and Hostettler (1994)).

In the implementation of this traditional approach, the current accepted strategy is to first prepare the dough, to then perform a suitable rheological experiment on the dough, and to finally formulate a mathematical model to interpert the observed data. However, in such situations, the dough is being treated separately from the process by which it has been manipulated and produced, as if it were not a "living system" (Meissner and Hostettler, 1994, p. 18).

The alternative approach is to model the actual mixing process in terms of some constitutive relationship which simulates the changing rheology of the dough during mixing. The major advantage of such an approach is that the rheology of the dough is simulated as a part of the overall modelling of the mixing.

The first step in a long-term project to examine the feasibility and merit of performing such a study of the "elongate-and-rupture" mixing action of a Mixograph^{TM} is discussed in Anderssen *et al.* (1996). In essence, a Mixograph^{TM} record is a series of extension tests. Normally, this is done as two separate steps where the dough is first mixed and then a sample of it is tested in an extension tester. On the other hand, this process is occuring continuously in the actual "elongate-and-rupture" occuring in a Mixograph^{TM} as the dough is mixed. The significance of this fact is discussed in Anderssen *et al.* (1997).

3.1 The GQRL's Electronic Mixograph^{TM}

A standard 35-gram Mixograph^{TM} has been modified to measure the "elongate-and-rupture" action in much greater detail by (a) adding a Hall-effect sensor to monitor the time of revolution of the mixer's head, and (b) replacing the spring by a strain gauge to measure the resistance to the mixing electronically every 2.5 milli-seconds. For these measurements, the Mixograph^{TM} arm is constrained to remain at its mid-scale position.

The goal has been to study the changing rheology of the dough in terms of the traces recorded by the GQRL's Mixograph^{TM}. This has involved

(a) the formulation of a mathematical model for the relative motion between the fixed and moving pins (Buchholz (1990));

(b) the decision to define and measure "mixing time" (which, when specified as minutes and seconds, is only known relative to the speed of the mixer) as the "number of revolutions of the mixer" (since the commencement of the mixing);

(c) an investigation of the dependence, on mixing speed, of the number of revolutions of the mixer to attain peak dough development (using methods previously described in Gras *et al.* (1990) to identify the position of the peak in the dough development); and

(d) an examination of the time of revolution of the mixer as a function of the number of the revolution since the start of the mixing.

4. THE IMPACT OF CURRENT EXPERIMENTS ON THE MATHEMATICAL MODELLING

On the basis of experiments performed todate, insight has been obtained about the nature of the constraints which should be invoked when formulating mathematical models of the mixing process. As explained in Anderssen *et al.* (1998), the evolving rheology of dough will be determined not only by its current configuration, but also by the nature, size and duration of the forces to which it has been subjected. There is a counterpart with steel which, over short periods, behaves like an elastic solid, while, over longer periods, behaves like an elasto-plastic material. The importance of this observation dates from the seminal work of Bauschinger of 1886, who established that the stress-strain behaviour of steel during a monotonic tension or compression test was not necessarily the same as that obtained during repetitive loading (Mughrabi (1996)).

Though the mixing of wheat flour dough is more complex, it clearly involves a repetitive loading process, and, consequently, intuition about the mathematical modelling of the mixing of the dough will be contained in the modelling and decision-making already developed for fatigue analysis of metals.

Fatigue analysis has a long history dating for the seminal work of Endo (Murakami (1991)) on his rainflow counting procedure. As explained by various authors (Dowling (1972), Fuchs and Stephens (1980; Chapter 10)), the essential steps in industrial fatigue analysis are:

1. **Construction of the Experimental Failure Curve.** On the material which is under investigation, perform constant-amplitude repetitive-loading experiments in order to estimate the amplitude of the loading as a function of the number of oscillations of the loading which achieves some appropriate measure of failure such as median failure life.
2. **Reinterpretation of an Actual Loading Curve as a Series of Constant-Amplitude Repetitive-Loadings.** For an actual representative loading scenario, applied to some component in the structure of interest, where the amplitude of the variable loading is continually changing (but the component does not reach failure), reinterpret the loading record, for an appropriate counting procedure such as rainflow counting, as groups of constant-amplitude repetitive-loading experiments.

3. **Estimate the Fatigue Life of the Structure.** According to some appropriate failure rule, such as the Palmgren-Miner linear damage rule, combine the information in the previous two steps to estimate the fatigue life of the component under investigation.

Rainflow counting is widely applied to do the counting in Step 2, because it yields reliable and consistent agreement with reality. Through the use of hysteresis concepts, rainflow counting can be placed on a rigorous and formal footing (Brokate *et al.* (1996)). This leads naturally to the idea that hysteresis concepts will be essential in the modelling on the mixing of wheat flour dough. Other considerations also lead to a recognition of the potential importance of hysteresis concepts, such a the irreversibility of the processes involved.

In the formulation of mathematical models of physical processes which involve hysteresis, such as the mixing of wheat flour dough, the first two crucial steps are

(a) the identification of the nature of the hysteresis process occuring (i.e. Preisach or Duhem-Madelung), and

(b) an assessment of the extent to which the process is rate-independent.

Both these requirements generate the need for appropriate experiments which monitor the mixing of wheat flour dough. This illustrates the close link between experiments and modelling in the study of industrial processes. In recent experiments performed on the GQRL Mixograph^{TM}, these two issues have been resolved for the mixing of wheat flour dough. In fact, it has been shown (Anderssen *et al.* (1998)) that the appropriate hysteresis model is Duhem-Madelung and that, for a wide range of flours, the number of revolutions of the Mixograph^{TM} at which peak dough development occurs is rate independent (i.e. is independent of the speed at which the mixer rotates).

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