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Rheological parameters estimation of non-Newtonian food fluids by finite elements model inversion

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ABSTRACT

The knowledge of fluid food rheological properties plays an important role in process engineering. Unfortunately, characterization of non-Newtonian fluids requires a notable effort in terms of time and resources. As a consequence, the aim of this research was to set up an method, based on the combination of the inversion of a simple finite element model and a laboratory measurement, carried on with a simplified tool. Although the method has a more general applicability, for illustrative purpose, it is here mainly shown with reference to power-law rheological model and two different materials (tara gum mixture and dough of water and flour). To measure the rheological parameters, the square of distance between simulated and experimental data was considered as an objective function, and some well-known optimization algorithms were tested. In order to verify the feasibility of the method, the experimental rheological characterization of the considered materials were carried out using a rotational rheometer. The calculated rheological parameter values were comparable with those obtained by traditional procedure (mean percentage error 6.47 ± 5.57). The most efficient optimization algorithm, in terms of iterations number, computational speed and minimum of the objective function, was the Levenberg–Marquardt one, but even other tested algorithms drove to similar final results (maximum difference of 18% between the optimized k and n values). The results demonstrated also that the precision of the calculated rheological parameters does not depend on the initial parameter values.

In the light of the obtained results, the method could represent a feasible technique and well suited for various rheological models and viscosity range of food materials. Moreover, the method could be susceptible to some development by an industrial point of view being possible to hypothesize the development of an integrated automatic instrument, equipped with finite element software, useful both for laboratory and industrial purposes.

1. Introduction

Rheology is the science that studies the flow and deformations of solids and fluids under the influence of mechanical stress. The description and the modeling of the rheological properties of food fluid plays an important role in process engineering. In the food manufacturing stage, the rheological measures of a product can be useful both in quality control and process optimization (Barbosa-Canovas and Ibarz, 2002). Many methods and instruments have been used to measure the rheological properties. The various techniques described in the literature may be classified on the basis of the used principles: empirical/imitative or fundamental. The results of empirical and imitative tests do not directly relate to the physical properties of the material, but to the technological behavior, typically. These determinations are simple, fast and suitable for standardized on-line tests. Examples are the classical imitative measure of the dough carried out by means farinographs, amylographs, alveograph and mixograph (El-Bakry et al., 2010; Dobraszczyk and Salmanowicz, 2008; Peressini et al., 1999; Khatkar et al., 1996; Oliver and Allen, 1992; D'Egidio et al., 1990; Weipert, 1990).

The fundamental rheological measurements are instead based on the application of a controlled strain field and on the measure of the relative level of stress. The strain and stress fields are then correlated by a mathematical model. The measurement of fundamental rheological parameters is performed by using instruments such as rotational rheometers (coaxial cylinder, cone-plate or plate–plate) or non-rotational rheometers. Rotary tools are

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widespread, but do not allow to operate in flow conditions with high viscosity fluids. For these fluids, the capillary extrusion rheometers fit better, and moreover high strain rate are permitted. However, for the non-Newtonian materials, a significant amount of experimental data is required (Nascimento et al., 2010). Usually, it is necessary to measure the pressure drop at different flow rates and length/radius ratio of extrusion tube and apply some empirical corrections, such as the important Mooney–Rabinowitsch on wall strain rate (Steffe, 1996), or Bagley on the effects of cross flow at the capillary inlet (Bagley, 1957).

Scientific literature reports a growing interest in the estimation of physical properties by inverse methods. An inverse method generally combines a numerical model with an algorithm for parameter estimation, in order to search the best set of model parameters. The search of optimal parameters consists in finding the (hopefully global) minimum of an objective function defined by the distance between measured and simulated values (Tarantola and Valette, 1982). A trial and error method which simulate the experimental test for different parameter values, can be used, even if it may require a long time to assess a good solution. However, a more systematic approach requires to couple a numerical finite element model with an optimization module with the aim to identify the best set of parameters (Gavrus et al., 1996). Within this framework, some well-known optimization algorithms may be used such as those developed by Levenberg (1944), Marquardt (1963) and Nelder and Mead (1965).

In food engineering, inverse methods have been usually used to determine thermal properties (Mohamed, 2010; Monteau, 2008; Simpson and Cortes, 2004; Zueco et al., 2004) and mass transfer coefficients (Fabbri et al., 2014; da Conceição Silva et al., 2012; Fabbri et al., 2011; Da Silva et al., 2010; Silva et al., 2010; Da Silva et al., 2009). The studies concerning the determination of rheological properties by inverse methods, are especially devoted to the evaluation of elastic and plastic materials properties (Mesa-Munera et al., 2012; Zhang et al., 2010; Tsvkarnoto, 2009; Wang and Hirai, 2009; Lin et al., 2009; Bosisio et al., 2007; Cooreman et al., 2007; Wang et al., 2005; Fratini et al., 1996; Gelin and Ghouati, 1995, 1994; Schnur and Zabaras, 1992). The studies related to the determination of viscosity by inverse method are very few (Bandulasena et al., 2011; Nascimento et al., 2010; Bandulasena et al. 2007; Park et al., 2007; Kalyon and Tang, 2007; Fullana et al., 2007; Guet et al., 2006; Lebaal et al., 2005) and none of them is referred to non-Newtonian food materials.

The present paper proposes a novel technique to estimate the rheological parameters of food fluid materials. The method is based on the combination of the inversion of a finite elements model and a very simple laboratory equipment. Work was divided into three phases: (I) experimental determination of the pressure vs flow rate, conducted with a simple laboratory extruder; (II) development of a numerical model, able to describe the behavior of the above measuring tool, and numerical determination of the pressure vs flow rate; (III) parameter estimation by minimizing the distance between numerical model and experimental results. Although the method has a more general applicability, herein is mainly illustrated with reference to two different food materials (tara gum mixture and dough of water and wheat flour).

2. Materials and methods

2.1. Phase I-experimental determinations of $P_o(Q(t))$

For the experimental determinations, two type of materials were used. The first one was a mixture of water and tara gum hydrocolloid at 2%, characterized by low viscosity, whereas the second one, was a dough made with water and white flour, characterized by high viscosity.

For the hydrocolloid mixture, 2 g of tara gum purchased from a local confectionary company, were dispersed in 100 ml of distilled water and mixed by a magnetic stirrer (ARE heating magnetic stirrer, VELP Scientifica, Usmate (MB) Italy). Tara gum is partially soluble in cool water and so it was treated, for 60 min, at room temperature (25 °C) and then heated at 80–89 °C, for 30 min, to make easier the total dispersion. Before the extrusion test, the hydrocolloid mixture was equilibrated at room temperature for 3 min.

For the dough, 1 kg of wheat flour (Molino Spadoni, Coccolia, Italy) was mixed with 0.6 kg of water for 15 min at 25 °C, by using a household mixer (Kenwood Major, Hampshire, UK). After mixing, the dough was rested in a plastic enclosure for 20 min at room temperature.

A simple extruder, based on the texture analyzer (TA-HDi, Stable Micro System, Ltd., Godalming, UK), was set up. The tool was composed of an aluminum alloy pipe with an internal diameter of 20 mm and a length of 70 mm and of a piston moving inside the pipe. The opposite side of the cylinder ended with a die characterized by a length (L) of 40 mm and a radius (R) of 2.5 mm (Fig. 1). During the test, the piston was moving following a linear speed law in order to pass from 0 to 1 mm/s in 10 s and from 0 mm/s to 0.8 mm/s in 10 s, for the tara gum mixture and the dough, respectively. The extrusion pressure value (P_o, observed pressure) was measured as ratio between the force applied by texture analyzer (N) and the piston cross-section area (m^3). While the flow rate vs time curve $Q(t)$ was obtained from the piston motion law. For each material, the measure was carried out in triplicate. The $P_o(Q(t))$ curves were averaged and fitted by using a power law (aQ^b) and a sigmoidal model ($(ab + cQ^d)/(b + Q^d)$). All the elaborations were performed with a confidence limit of 95% by using Statistica 7.0, (StatSoft. Inc. Tulsa).

2.2. Phase II-numerical determination of $P_c(Q(t))$

A numerical model based on the finite elements technique was developed by using Comsol Multiphysics 5 (COMSOL Inc.,

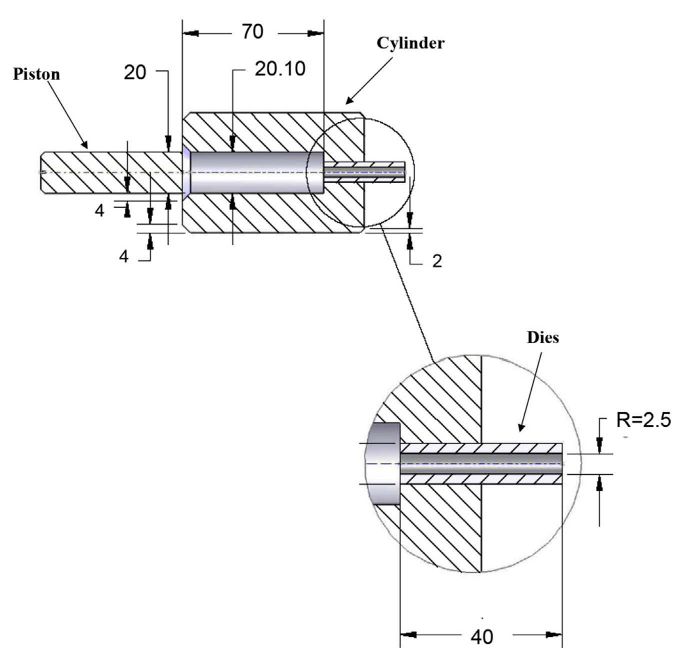

Fig. 1. Schematic representation of the simple tool used during the experimental determination of $P_o(Q(t))$.