

# Estimation of semolina dough rheological parameters by inversion of a finite elements model

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## Abstract

The description of the rheological properties of food material plays an important role in food engineering. Particularly for the optimisation of pasta manufacturing process (extrusion) is needful to know the rheological properties of semolina dough. Unfortunately characterisation of non-Newtonian fluids, such as food doughs, requires a notable time effort, especially in terms of number of tests to be carried out. The present work proposes an alternative method, based on the combination of laboratory measurement, made with a simplified tool, with the inversion of a finite elements numerical model. To determine the rheological parameters, an objective function, defined as the distance between simulation and experimental data, was considered and the well-known Levenberg-Marquardt optimisation algorithm was used. In order to verify the feasibility of the method, the rheological characterisation of the dough was carried also by a traditional procedure. Results shown that the difference between measurements of rheological parameters of the semolina dough made with traditional procedure and inverse methods are very small (maximum percentage error equal to 3.6%). This agreement supports the coherence of the inverse method that, in general, may be used to characterise many non-Newtonian materials.

## Introduction

The rheological characterization of food materials plays an important role in the field of food engineering. The rheological measures of a product in the manufacturing stage can be useful both in quality control and process optimization (Barbosa-Canovas and Ibarz, 2002). For

example the rheological properties of semolina dough are very important for the pasta manufacturing process, particularly for the extrusion optimisation (Fabbri *et al.*, 2007).

Many instruments can be used to measure the rheological properties of the food doughs. The methods can be classified on the basis of the principles used: empirical/imitative or fundamental. The first one are directly relate to the technological behaviour but not to the physical properties of the material. Examples are the imitative measure of the dough carried out with farinographs, amylographs, alveograph and mixograph (D'Egidio *et al.*, 1990; Weipert, 1990; Oliver and Allen, 1992; Khatkar *et al.*, 1996; Peressini *et al.*, 1999; Dobraszczyk and Salmanowicz, 2008; El-Bakry *et al.*, 2010). The fundamental methods are based on the mathematical correlation between strain and stress fields and are performed using rotational rheometers (plate-plate, cone-plate or coaxial cylinder) or non-rotational rheometers (capillary extrusion rheometers). Rotary tools are easy to use, but do not allow operating in flow conditions with high viscosity fluids such as food dough. In this case, the capillary extrusion rheometers fit better, moreover high strain rate are even permitted (more than  $10^4 \text{ s}^{-1}$ ). The working scheme of a tube rheometer is simple: the fluid is extruded through a small size tube and the viscosity is obtained relating drop pressure between the inlet and outlet with the volumetric flow rate. As the section of the extrusion tube is small enough to force the fluid to flow in laminar conditions, for a Newtonian fluids it is possible to determine the viscosity value simply fitting a single measurement of flow ( $Q$ ) and pressure drop ( $P$ ) with the equation of Hagen-Poiseuille. In the case of non-Newtonian fluids the determination is much more complicated. In particular it is necessary to measure the pressure drop at different flow rates (usually three is recognised as minimum value) and than apply some empirical corrections, such as the important Mooney-Rabinowitsch, on wall strain rate (Steffe, 1996). This method requires different assumptions: a negligible fluid compressibility, independence of the rheological properties from time and pressure, constant temperature and absence of radial and tangential components in the velocity field. Since the last hypothesis is difficult to satisfy, a further correction is often necessary to consider the influence of the effects of cross flow at the capillary inlet (Bagley, 1957). According to Bagley it is necessary to repeat the  $P(Q)$  measurements for a series of capillaries with different ratio between and length and radius. The Bagley correction tends to be less important with the increase of the ratio length/radius of extrusion tube, but unfortunately building long and thin tubes involves practical problems about feasibility, thermal insulation, cleaning possibility and cost. Supplemental corrections may increase the precision of the method: correction on  $P$  due to increase of the kinetic energy during the transition between ducts with variable section; correction on  $Q$  to consider the possible sliding effect between the boundary layer and wall, correction due to heating of the fluid by mechanical energy dissipation. As a consequence, the characterisation of non-Newtonian fluids may requires a notable time effort, especially in terms of number of tests to be carried out. The present work proposes an innovative inverse method to estimate the

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rheological parameters of food materials, particularly suited for high viscosity fluids such as food doughs. The method is based on the combination of the inversion of a finite elements numerical model and a very small number of laboratory measurements, made with an apparatus simpler than industrial capillary rheometers.

An inverse method 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 minimisation of an objective function, defined by the distance between measured and simulated values (Tarantola and Valette, 1982). Within this aim, many different optimisation algorithms have been developed (Levenberg, 1944; Marquardt, 1963; Nelder and Mead, 1965). Inverse methods have been used to determine food physical properties (Simpson and Cortes, 2004; Zueco *et al.*, 2004; Mohamed, 2008; Monteau, 2008; Da Silva *et al.*, 2009, 2010; Fabbri *et al.*, 2011, 2014), even if the studies concerning the determination of viscosity rheological are very few and not referred to non-Newtonian food materials (Lebaal *et al.* 2005; Guet *et al.*, 2006; Fullana *et al.*, 2007; Kalyon and Tang, 2007; Park *et al.*, 2007; Bandulasena *et al.*, 2007; Nascimento *et al.*, 2010; Bandulasena *et al.*, 2011).

## Materials and methods

The method consists of three steps: i) an experimental determination of  $P_e(Q(t))$  conducted with a simple laboratory extruder on a food dough; ii) development of a numerical model, able to describe the behaviour of the above measuring tool, and numerical determination of  $P_m(Q(t))$ ; iii) model parameter estimation by minimising the distance between numerical and experimental results.

### Experimental determination: $P_e(Q(t))$

A simple extruder, based on the texture analyser (TA-HDi, Stable Micro System, Ltd., Godalming, UK), was set up. The tool consists of a steel cylinder with an internal diameter of 20 mm, inside, which a piston is moved by a displacement, controlled electrical motor. The opposite side of the cylinder terminate with a die characterised by a length of 40 mm and a radius of 5 mm and radius. The load cell used has a full scale of 2.5 kN.

The material used in this experimentation was a dough of semolina, supplied by an industrial pasta producer (1 kg), mixed at 25°C with 0.5 kg of water for 15 min by using a household mixer (Kenwood Major, Hampshire, UK). After mixing the dough was rested in a plastic enclosure for 20 minutes at room temperature. Subsequently about 20 g was inserted in the extrusion cylinder. The extrusion pressure value ( $P_o$ , observed pressure) was measured as ratio between the applied force and the piston cross-section area, while the flow rate  $Q(t)$  was obtained from the extruder speed. The curve  $P_e(Q)$  was determined by imposing a linear law of flow rate  $Q(t)$ , in order to change the flow between 0 and  $3.6 \cdot 10^{-7} \text{ m}^3 \text{ s}^{-1}$  in 2 s. This procedure is based on the hypothesis of fluid perfectly incompressible, that is a condition inherited by the aqueous nature of the involved fluid combined with the low fluid velocities.

The measurements were repeated in triplicate and the  $P_e(Q(t))$  curves were fitted by using a power law equation.

### Numerical model: $P_m(Q(t))$

A numerical model based on finite elements technique was developed using ADINA (ADINA R&D, Inc., Watertown, MA, 2002) (Kumar and Swartzel, 1993; Puri and Ananteswaran, 1993; Bathe, 1996).

The model replicates the geometrical and physical conditions of the extrusion experiment reported in the above paragraph. The computational domain was divided in 4000 elements with linear shape function that generated 2175 vertex. The initial mesh was refined up to a level

for which the calculus improvements were not significant. As the geometry changes during time, as a consequence of the piston movement, a continuous re-meshing scheme is applied. During the re-meshing the total nodes number does not change significantly.

The rheological behaviour of the material (dough) is described by the following power law:

$$\tau = k\dot{\gamma}^n \quad (1)$$

where  $\tau$  (Pa) is the shear stress,  $\dot{\gamma}$  (1/s) is the shear rate, while  $k$  ( $\text{Pas}^n$ ) and  $n$  are the consistency index and the flow index of the material, respectively.

The die outlet pressure was imposed as equal to atmospheric pressure, while the relative speed between dough and wall was considered equal to zero. The same piston movement law of the experimental determination was imposed.

The dough density of  $1200 \text{ kgm}^{-3}$  was used, as reported by Baik *et al.* (2001).

The calculated  $P_m(Q)$  curve, parameterised on rheological model was defined following:

$$P_m = f(k, n, Q(t)) \quad (2)$$

### Adaptation of the numerical model to experimental data

Estimation of the  $n$  and  $k$  parameters was made minimising the distance between numerical ( $P_m(Q)$ ) and experimental ( $P_e(Q)$ ) results.

The distance between simulation and experimental data, considered as the objective function (OF), is defined as:

$$OF(n, k) = \int_0^{T_F} [P_m(k, n, Q(t)) - P_e(Q(t))]^2 dt \quad (3)$$

where  $T_F=2$  s

The integral is solved numerically by discretisation, subdividing the integration domain  $\Delta t$  in  $N$  points:

$$OF(n, k) = \Delta t \sum_{i=1}^N [P_m(k, n, Q(t_i)) - P_e(Q(t_i))]^2 = F^T \cdot F \quad (4)$$

According to the common minimum squared errors criteria, the optimal value of  $n$  and  $k$  is the one which corresponds to the minimum of OF. This was searched with a global optimisation algorithm. Particularly, in this study, the Levenberg-Marquardt was used (Levenberg, 1944; Marquardt, 1963).

The problem is solved by the repeated application of the following procedure:

i) set initial values of  $n$  and  $k$ ;  $d=0$

ii)  $t_d = d \cdot \Delta t$  (5)

iii) calculated (by FEM simulation)  $P_m(k, n, Q(t_d))$  and  $F$

iv) determine  $J$

v) solve the linear system  $(J^T J + \lambda I) \Delta Z = -J^T F$  by Cholesky method obtaining  $\Delta Z^d$  (6)

vi) for each iteration the parameters vector is updated:  $Z^{d+1} = Z^d + \Delta Z$  (7)

vii)  $d \leftarrow d+1$  (8)

viii) go to 2 until  $\left\| \frac{\Delta Z}{Z} \right\| \leq \epsilon$  (9)

where:

$\lambda$ : a scalar, called damping coefficient. In this implementation the following law was used:

$$\lambda(d) = \lambda_0 \cdot 3^{(1-d)} \quad (10)$$

$$\lambda_0 = 100$$

$d$ : iteration index

$I$ : identity matrix

$Z$ : incremental vector of parameters to be estimate  $Z = [k, n]^T$

$\Delta Z$ : incremental vector of parameters to be estimate  $\Delta Z = [\Delta k, \Delta n]^T$

$J$ : Jacobian matrix with  $i \in \{1, \dots, N\}$  and  $J \in \{1, 2\}$ :

$$J_{ij} = \left[ \frac{\partial P_m(Q(t, j))}{\partial Z_j} \right] \quad (11)$$

$$\varepsilon = 1\%$$

For computational efficiency reasons, the partial derivatives of jacobian matrix are simply approximated to their incremental ratio, referring to a parameters values variation of 1%.

The initial trial parameter values were arbitrarily selected. Initial  $k$  value was fixed to 8.5 kPas<sup>n</sup> based on a rough Newtonian estimation (Friso and Bolcato, 2004) while, initial  $n$  value, ranging between 0 and 1, was set equal to 0.5.

### Verification of the method feasibility

In order to verify the method feasibility, a rheological characterisation of the same material used in the above sections, by using a traditional procedure, was carried on.

The experimental determinations for the traditional procedure, replicated three times, were carried out with the same extruder proposed in the above sections, but by using 12 different dies characterised by the combination of four lengths (20, 30, 40 and 50 mm) and three radius (2.5, 3, 4 mm) (Figure 1). A linear piston motion law, in order to change the flow between 0 and  $3.6 \cdot 10^{-7} \text{ m}^3\text{s}^{-1}$  in 2 s was imposed.

The observed values of rheological parameters ( $k_o$  and  $n_o$ ) were obtained applying the classical Hagen-Poiseuille equation plus the Mooney-Robinowitsch (Steffe, 1996) and Bagley (1975) corrections following the procedure described by Steffe (1996).

The  $k_o$  and  $n_o$  parameters values, obtained by traditional procedure, were compared with those obtained by the inverse method proposed in this research.

## Results and discussion

The curve  $P_o(Q)$  determined during the experimental phase and by using a simple extruder is reported in Figure 2. For a flow rate of about  $4 \cdot 10^{-7} \text{ m}^3\text{s}^{-1}$ , the pressure reaches a value of about  $3.5 \cdot 10^6 \text{ Pa}$ . The curve was fitted by a power law with a determination coefficient equal to 0.90 ( $P = 7.5 \cdot 10^8 Q^{0.3705}$ ).

As concerning the finite elements model, the pressure (Pa), viscosity (Pas) and speed fields ( $\text{ms}^{-1}$ ) can be evaluated for different  $n$  and  $k$  values. These physical fields, at the time of about 0.5 s from starting, are reported in Figure 3 as example, calculated with  $n$  and  $k$  values obtained by the inverse method. The physical quantities are represented by colour scales and it can be seen that the pressure and speed inside the cylinder are uniform, while they show higher gradients inside the die.

To evaluate the feasibility of the proposed method, the  $k$  and  $n$  values determined by inverse method have been compared with those obtained by the traditional procedure ( $k_o=19.21 \pm 2.11 \text{ kPas}^n$ ;  $n_o=$

$0.353 \pm 0.018$ ). The calculated  $k$  and  $n$  values as function of the iteration numbers, and the distance (percentage error in brackets) from the values obtained by traditional procedure, are reported in Table 1. The calculation was stopped when an almost constant value for  $k$  and  $n$  was reached. To obtain a good agreement between the observed a calculated data, only 7 iterations were necessary. At the last iteration the percentage error for the  $k$  parameter is equal to 3.6%, while for the  $n$  parameter is 2.0%.

The agreement between measurements made with the two procedures positively supports the coherence of the inverse method, even if it is not obvious to understand which of the two results is closer to physical reality.

The evolution of  $k$  and  $n$  parameters, as function of the iteration number, is reported also in Figure 4. It can be seen that  $k$  and  $n$  values

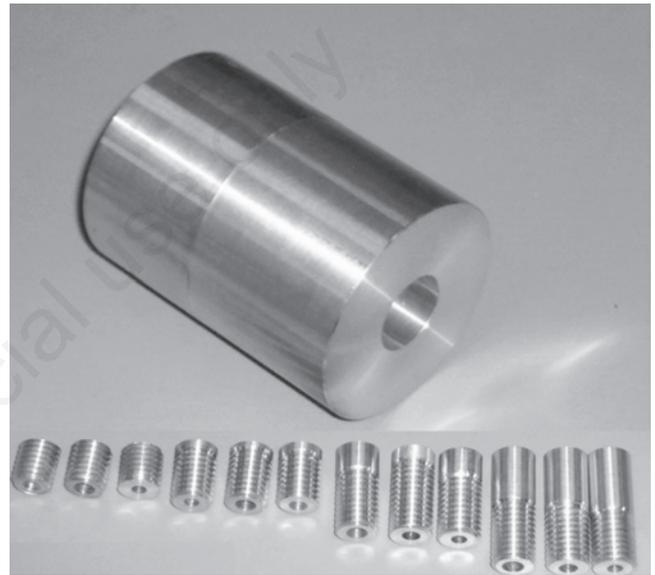


Figure 1. Simple extruder with dies characterised by different combinations of length and radius.

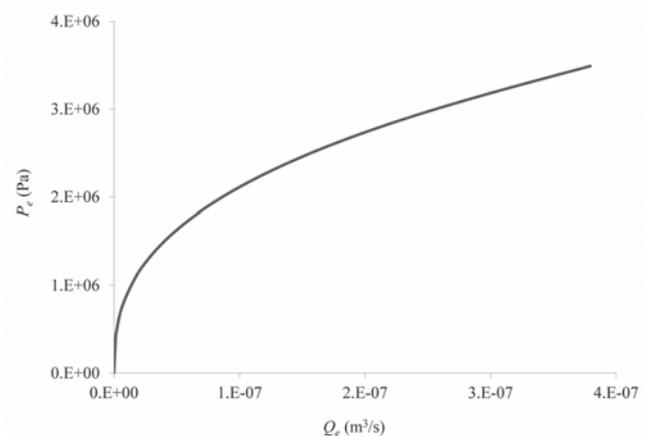


Figure 2. Pressure vs flow rate experimentally determined.

vary quite fast at the beginning of the optimisation, until the 5<sup>th</sup> iteration and after remain rather stable. The calculated  $P_m(Q)$  curve changes as function of the  $n$  and  $k$  values and so with different iteration numbers (Figure 5). The curve tends to approach to experimental one, and from the Figure 5, it can be see that after six iterations the experimental and calculated curves are very similar.

As regard the computational effort, it must be considered that for every iteration three run of the numerical model are necessary. Every run, on an old Intel Pentium III 1 GHz CPU, required about two minutes. As a result, with the inverse method, it was possible to calculate the rheological parameters in about half an hour. This time is negligible if compared with that necessary for samples preparation, measurement executions and data analysis, according to the traditional method.

### Conclusions

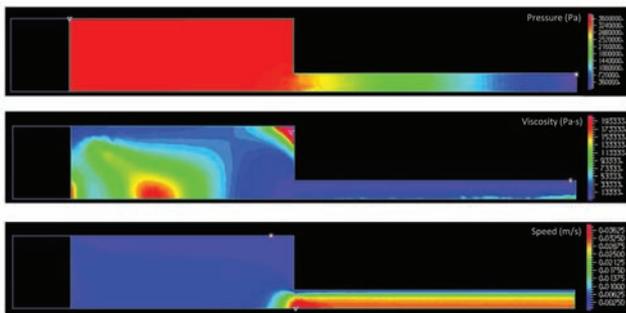
The good agreement between measurements of rheological parameters of the semolina dough made with traditional procedure and

inverse methods supports the coherence of the inverse method that, in general, could be used to characterise many non-Newtonian materials.

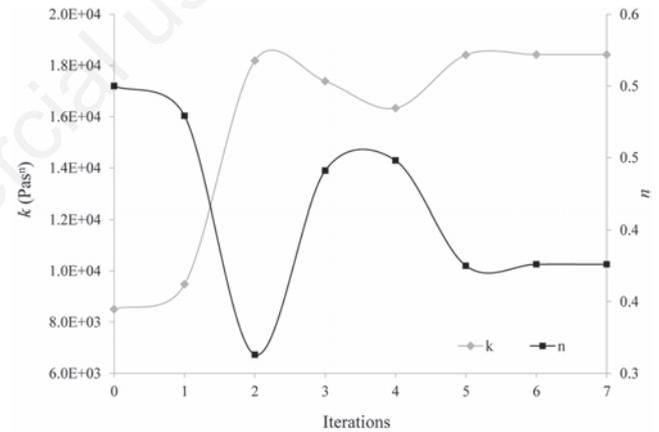
The strong points of the proposed technique are: i) the possibility to use testing tools more simple to build, compared to commercial tube rheometers. In fact a capillary tube is not necessary, but it could be sufficient a simple calibrated die in a thin wall; ii) the possibility to consider, without empirical corrections, the friction between fluid and the wall of the extrusion cylinder, the pressure drop at the inlet, the temperature increase due to mechanical dissipation and the pressure variation due to kinetic energy increase; iii) the possibility (without any additional difficulty for the user) to estimate parameters of rheological models more complex than the simple power law; iv) the possibility to obtain the results with just 1-3 measurement sessions, against the hundreds required by traditional method for non-Newtonian materials. The proposed method has still consistent space for improvement with regards to the choice of optimisation algorithms. The combined application of numerical simulation techniques, inverse methods and physical measurements of integral nature looks extensible to the design of efficient measurement devices even in different physics field (electromagnetic, chemical, thermal, mechanics). Finally, it has to be under-

**Table 1. Rheological parameters values as function of the iteration number. Percentage error between the data obtained by the inverse method and traditional procedure, are reported in brackets.**

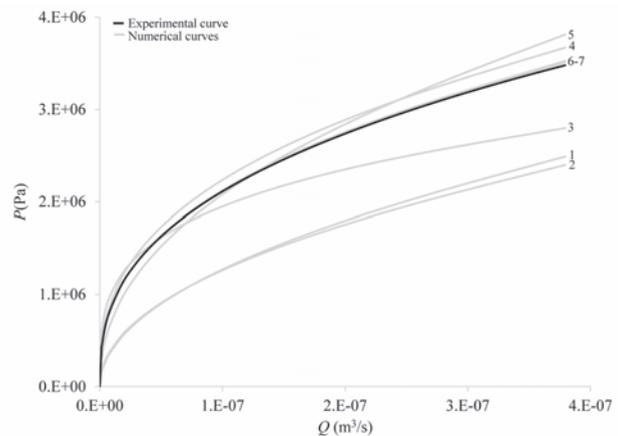
Number of iterations	$k$ (Pas <sup>n</sup> )		$n$	
0	8500.00	(55.6)	0.500	(35.7)
1	9472.85	(50.5)	0.479	(30.0)
2	18,187.78	(4.9)	0.313	(15.1)
3	17,383.15	(9.1)	0.441	(19.7)
4	16,334.01	(14.6)	0.448	(21.6)
5	18,413.94	(3.7)	0.375	(1.8)
6	18,427.81	(3.6)	0.376	(2.0)
7	18,427.84	(3.6)	0.376	(2.0)



**Figure 3. Example of pressure, viscosity and speed fields obtained by FEM simulation for  $k=18427.84$  Pas<sup>n</sup> and  $n=0.376$ . The upper half of the section of the cylindrical pipe is shown.**



**Figure 4. Evolution of  $n$  and  $k$  during the optimisation process.**



**Figure 5. Experimental (black line) and calculated (grey lines)  $P(Q)$  curves for different number of iterations.**

lined how the proposed approach can be used not only for materials characterisation but also even for estimation of characteristic parameters of non-homogeneous bodies of complex shape.

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