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Moisture diffusivity coefficient estimation in solid food by inversion of a numerical model

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ABSTRACT

Knowledge of moisture diffusivity coefficients of water in food is a very important physical parameter for design, modelling and simulation of different food plants and related processes such as baking, drying and ripening. Unfortunately specific moisture diffusivity values are not easily found in literature, particularly for processed foods. The aim of this study was to develop a method, based on the inversion of finite element models, to estimate the moisture diffusivity in different solid food products. An example on salami, biscuit and flat bread is shown. The research work was divided in three phases: experimental determination of the moisture concentration versus time in various food products stored in water saturated atmosphere; development of a numerical model of water transfer inside the food product for the numerical determination of moisture content versus time and parameter estimation of moisture diffusivity, by minimizing the distance between numerical model and experimental results using the Levenberg–Marquardt algorithm.

The estimated moisture diffusivity coefficients resemble those reported in literature for almost similar products (3.857E − 12, 6.804E − 11 and 1.792E − 12 m^2/s for salami, biscuits and flat bread respectively). The obtained values were then used for solving direct models, in unsteady conditions, showing a good agreement with experimental data.

The method may be used on different food materials and it is possible to hypothesize an integrated automatic instrument, useful both for laboratory and industrial purposes.

1. Introduction

In recent years mathematical modelling and computer simulation based on numerical analysis have become the main tools for design, development, optimization and control of various food processes (Baik, Marcotte, Sablani, & Castaigne, 2001). This is due to the availability of high speed computers, inexpensive memory and dedicated software, which help researchers in managing resources in an efficient and cost effective manner, compared to experimental trial and error techniques (Mohamed, 2010). Using numerical models, the average values of physical properties of heterogeneous foods may be replaced by time/space/temperature/moisture-dependent variables. Knowledge of moisture diffusivity coefficients in food is very important for design, modelling and simulation of different food processes such as baking, drying and ripening. Unfortunately specific moisture diffusivity values, are scarce in literature, in particular for processed foods. The physical properties of food vary mainly with composition and temperature. The experimental determination of moisture diffusivity coefficients requires a series of highly time-consuming measurement (da Silva, da Silva, & Mariani, 2009). Moreover parameter determination by using laboratory experiments might not be representative of real conditions. Scientific literature reports a growing interest in the estimation of physical properties by inverse methods. By definition, inverse methods are a general mathematical technique to estimate unknown causes on the basis of the observations of their effects, as opposed to modelling of direct problems whose solution involves finding effects on the basis of a description of their causes (Kahveci & Cihan, 2004). The simple empirical calibration by a "trial and error method" procedure that compares experimental values of a variable with those simulated is the most common inverse method. The main problems of this simple method are the high computational times and the difficulty to evaluate how the model parameters are to be tuned to match the measured data well. Moreover, the end of the calibration process and the uncertainty on the obtained parameters cannot be quantified in a rigorous way. Therefore, this calibration method cannot ensure that the best parameter set is found (Currenti, Del Negro, & Nunnari, 2005; Ritter, Hupet, Munoz-Carpena, Lambot, & Vanclooster, 2003). More structured inverse methods combine forward models with appropriate optimization algorithms (generally iterative) to automatically find the best parameter set that minimizes an objective function (Currenti et al., 2005). In general the solution is found by fitting the numerical solution provided by the model to the measured data, by varying the model parameters. Indeed, the search for optimal parameters consists in finding the minimum of an objective function, defined by the distance between computed and measured values. Within this framework, many different optimization algorithms can be used

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(Hopmans & Simunek, 1999; Levenberg, 1944; Marquardt, 1963; Nelder & Mead, 1965).

In food engineering, the inverse method was used especially to determine thermal properties (Anderson & Singh, 2006; Mariani, Lima, & Coelho, 2008; Martins & Silva, 2004; Mendonça, Celso Filho, & da Silva, 2005; Mohamed, 2009; Mohamed, 2010; Monteau, 2008; Ramsaroop & Persad, 2012; Simpson & Cortes, 2004; Zueco, Alhama, & González Fernández, 2004). On the other hand, to our knowledge, there are only a few studies concerning the determination of moisture diffusivity coefficient in food products by inverse methods (da Conceição Silva, da Silva, Mariani, & Darche, 2012; da Silva et al., 2009; Fabbri, Cevoli, Cocci, & Rocculi, 2011; Silva, da Correa, & Silva, 2010) and only one is based on the inversion of a finite element model. Fabbri et al. (2011) proposed a method, based on just simple laboratory determination of average carbon dioxide concentration and on the inversion of a finite element model, to estimate the carbon dioxide diffusivity in the egg component. In this study, the Nelder–Mead Simplex optimization algorithm was used. da Silva et al. (2009) determined the moisture coefficient during hot air drying of mushrooms (*Agaricus blazei*). Experimental drying kinetics were applied to sliced mushroom at different air temperatures and air velocities in order to find an analytical solution to the mass transfer equation for drying using an inverse problem with two optimization methods: Levenberg–Marquardt and Differential Evolution algorithm. The same optimization techniques were implemented by da Conceição Silva et al. (2012) to estimate the moisture coefficient during osmotic dehydration of the West Indian cherry (acerola) by inverse method. The difference between average moisture contents experimentally determined and calculated by Fick's equation was minimized. Effective moisture diffusivity during the dehydration of acerola was calculated by the inverse method, using the Levenberg–Marquardt algorithm also by Silva et al. (2010).

The aim of this study was to develop a method, based on the inversion of finite element models, to estimate the moisture diffusivity in different food products. As an example of the technique, salami, biscuit and flat bread samples were used. Work was divided in three phases: (I) experimental determination of the moisture concentration versus time in various food products stored in a water saturated atmosphere; (II) development of a numerical model of the water transfer in the food product and numerical determination of moisture content versus time; (III) parameter estimation of moisture diffusivity for the different food products, minimizing the distance between numerical model and experimental results.

2. Materials and methods

2.1. Phase I — experimental determination of the average moisture concentration ($\overline{C}_{\exp}$)

Measurements were carried out on three different products: salami, biscuit and flat bread. All products were purchased from a local supermarket.

Salami (Clai S.C.A., Imola, Italy) made up of pork meat, salt, dextrose, spices and herbs. For the experimentation ten cylinders of salami, 10 mm diameter and 10 mm height were taken from various slices by using a corer.

Biscuits (Eurospin S.p.A, San Martino Buon Albergo VR, Italy) were characterized by a circular shape with a 55 mm diameter, and height of 10 mm, with a center hole of 10 mm. Ingredients were wheat flour, sugar, vegetable fat, yogurt, skimmed milk powder, raising agents, salt and flavorings. Whole biscuits were used for the experimentation.

The flat bread analyzed is a typical Italian product, named "piadina", with a diameter of about 200 mm and a thickness of about 3 mm (Gastone S.R.L., Ravenna, Italy). Ingredients were wheat flour, water, salt, and pork fat (shortening). For the study, ten square samples (10 × 10 mm) were taken from the center of ten flat breads.

Initial moisture content of all products was determined by gravimetric method using the standard methods (salami: AOAC 950.46, 1990; biscuit: AOAC 934.01, 2000; flat bread: AACC 44–15A, 1995).

Each sample derived from different products, was placed inside a glass enclosure containing a small jar filled with distilled water, to saturate the air with humidity. By means of a candle, anaerobiosis was created, in order to limit the growth of mold on the surface of samples, a risk associated with the high humidity of the environment.

During storage at 20 °C, samples were removed from the glass enclosure and weighed for determining the moisture content daily, until constant weight. Candles were always lit before closing. By measuring the absorbed water weight, the moisture concentration ($\overline{C}_{\exp}$, mol/m^3) was calculated.

2.2. Phase II - numerical determination of average moisture concentration $\left(\overline{C}_{num}\right)$

Diffusion models were developed using Comsol Multiphysics 4.2a (COMSOL Inc., Burlington, MA), a commercial partial differential equations solver based on finite element technique.

The geometric models replied the real dimensions and shapes of the samples used for the measurements. In particular the models are two-dimensional and axisymmetric for salami and biscuit, while three-dimensional for flat bread. The mass transfer is governed by Fick's law, according to which the mass flux is proportional to the concentration gradient through the mass diffusivity (D):

$$\frac{\partial C_{num}}{\partial t} = D\left(\frac{\partial^2 C_{num}}{\partial x^2} + \frac{\partial^2 C_{num}}{\partial y^2} + \frac{\partial^2 C_{num}}{\partial z^2}\right) \quad (1)$$

where C_{num} is calculated moisture concentration at time t (s) and at space coordinates x, y and z (m).

Initial and boundary conditions are:

- initial moisture concentrations ($C_{0\text{-}num}$) were assumed as uniformly distributed and was experimentally determined (salami: 24460 mol/m^3; biscuit: 490 mol/m^3; flat bread: 22862 mol/m^3).
- moisture diffusivities (D) were considered independent from time and space;
- boundary moisture concentrations were set up assuming that the exterior layers of samples, in contact with the water saturated air, are saturated immediately.

The food saturation concentrations, were determined considering the concentrations reached at equilibrium during the experimental tests (salami: 53254 mol/m^3; biscuit: 8040 mol/m^3; flat bread: 51067 mol/m^3).

The choosing of an affordable Diriclet boundary condition, allowed by the air saturation experimental condition, permits to avoid the estimation of a further parameter, represented by the natural convection mass transfer coefficient.

The mesh of three models was made by 452, 585 and 5638 elements, respectively for salami, biscuit and flat bread (Fig. 1). Particularly the mesh of salami and biscuit models was characterized respectively by 276 triangles and 176 quadrilateral and by 313 triangles and 272 quadrilaterals. The flat bread model was 3D therefore the mesh was composed of 3174 tetrahedra, 2464 prisms, 616 triangles and 304 quadrilaterals.

2.3. Phase III — parameter estimation of moisture diffusivity, minimizing the distance between numerical $\left(\overline{C}_{num}\right)$ and experimental results $\left(\overline{C}_{\exp}\right)$

The distance between simulation and experimental data was considered as an objective function (OF), and defined as following:

$$OF(D) = \int \left[\overline{C}_{\exp}(t) - \overline{C}_{num}(t, D)\right]^2 dt \approx \sum_i \left[\overline{C}_{\exp}(t_i) - \overline{C}_{num}(t, D)\right]^2 \quad (2)$$