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Analytical solution and experimental validation of a model for hydration of soybeans with variable mass transfer coefficient

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ABSTRACT

The hydration of soybeans was mathematically modeled using a lumped parameter model from the mass balance for water present in soybeans. The balance reveals that the water flow in the grains occurs through natural convection until the surface, while diffusion is responsible for the inside of the grains. In order to reflect the decrease in mass transfer, K_S, as the concentration of water in the grains increases, the coefficient was assumed to present linear variation according to moisture following the approach by other authors. Such model had been numerically solved before; however, its analytical solution remained unknown. The analytical solution to the model was obtained and compared with both the numerical solution and the analytical solution to an elementary case of K_S (constant) and validated against experimental data on moisture as a function of time for soybeans in cultivar CD 202 at different temperatures. This process confirmed that the analytical solution is correct and able to be applied in the simulation, analysis, optimization and projects of hydration units as well as any processes involving kinetics in accordance with the model studied. The parameters adjusted to both the numerical and the analytical solution were identical and grew exponentially with temperature. Finally, a generalized model was proposed to represent moisture as function of time and temperature using the results obtained in this study.

1. Introduction

A great motivation to process soybeans is to provide more solid production and the development of new food, nutritional, pharmaceutical, cosmetic and industrial products, including coproducts and ingredients for particular applications that use soil-derived components (Guriqbal, 2010). In terms of processing soybeans to produce food, hydration is an important part of the protein extraction process as a pretreatment for the grains to have their texture characteristics altered to facilitate protein extraction (Ciabotti et al., 2009; Coutinho et al., 2010; Nicolin, 2012; Nicolin et al., 2013; Pan and Tangratanavalee, 2003). Therefore, to understand hydration kinetics it is crucial to establish an exact relationship between moisture and hydration time for the grains.

Empirical models are an alternative when mathematically modeling the hydration of grains, with emphasis to models Peleg (1988), Singh and Kulshrestha (1987) and Pilosof et al. (1985) widely applied to describe the hydration of food products. Empirical models are easy to be computationally solved and generally provide a set of data with great adjustments (Saguy et al., 2005), however, they present some disadvantages such as ignoring elementary stages of mass transfer and being direct representations of experimental data. As a result of these disadvantages, empirical models have provided little or no information on transport mechanisms (Bequette, 1998; Pinto and Lage, 2001; Saguy et al., 2005).

Phenomenological models, in turn, consider theoretical assumptions and elementary stages of mass transfer proving more favorable than empirical models regarding the focus on detailed understanding on the studied process (Bequette, 1998). Some authors proposed phenomelogical models for lumped parameters considering spatial variations for variables of interest to describe the hydration of soybeans (Coutinho et al., 2007, 2005) and peas (Omoto et al., 2009). Regarding the hydration of soybeans, in their three studies the authors proposed a model from the same mass balance for water in the grains with accumulating water caused by convective mass transfer around the grain. These models considered different manners of including variations for both the mass transfer coefficient and the grain volume during hydration. The mass transfer coefficient in these studies was regarded as function of concentration of water in the grains to reflect the decrease in such property as the system reaches steady state. Regarding the modeling for hydration of peas, the authors proposed a lumped parameters model from the same mass balance present in studies by Coutinho et al., 2007, 2005. Convective flow and constant mass

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Nomenclature

a	constant of K_S linear (cm/h)
b	constant of K_S linear (cm^4/g h)
A	surface area of grains (m^2)
i	exponential function index
K_1	constant of analytical solution (cm^4/g h)
K_2	constant of analytical solution (h^{-1})
K_S	overall mass transfer coefficient (cm/h)
K_S^C	constant mass transfer coefficient (cm/h)
K_S^L	linear mass transfer coefficient (cm/h)
n	summation index
N	number of experimental values
N_A	water flow (g/cm^2 h)
N_{PC}	number of Omoto model parameters plus one
N_{PL}	number of parameters in the model with K_S linear
p	parameter in temperature exponential function
R	grain size (cm)
t	time (h)
T	temperature (°C)
V	grain volume (m^3)

Greek symbols

ρ_A	concentration of water (g/cm^3)
$\rho^i_{A\,\mathrm{calc}}$	concentrations with model calculations (g/cm^3)
ρ^m_{A0}	mean initial concentration of generalized analytical solution (g/cm^3)
$\rho^i_{A\,\mathrm{exp}}$	experimental concentrations (g/cm^3)
ρ_{A0}	initial concentration of water (g/cm^3)
ρ_{eq}	steady-state concentration of water (g/cm^3)
ρ^m_{eq}	steady-state concentration of generalized analytical solution (g/cm^3)
ϕ	objective function (g^2/cm^6)
ϕ_C	Omoto model objective function, K_S constant (g^2/cm^6)
ϕ^g_C	Omoto model overall objective function (soma dos erros quadráticos global) (g^2/cm^6)
ϕ_L	objective function of model with K_S linear (g^2/cm^6)
ϕ^g_L	overall objective function of model with K_S linear (overall sum of squared errors) (g^2/cm^6)

transfer coefficient were both considered. For this study, the authors considered the constant volume of pea grains obtaining an analytical solution for the proposed model.

In this context, the objective of this study was the proposition of a phenomenological model for lumped parameters with mass transfer coefficient dependent on the concentration of water in the grains. Such consideration reflects another factor involving the decrease in mass transfer coefficient values when the moisture in the grains reaches steady state beyond the driving force for the hydration. The model was analytically solved and the analytical solution obtained was compared with the numerical solution to the model and later validated through experimental data on the hydration of soybeans from cultivar CD 202. Furthermore, the model proposed and its analytical solution were compared with the model presented by Omoto et al. (2009), who considered the (K_S) constant mass transfer coefficient. The model parameters with K_S linear and K_S constant were adjusted through the method of least squares. The same parameter values were obtained for both the numerical solution and the analytical solution presented in this study. The parameters presented exponential growth as function of temperature. For the model obtained in this study, a generalization was conducted to include the parameters exponential growth with temperature. The model with K_S linear was considered more satisfactory according to what verified through the Akaike testing (comparison between two models) and the quadratic residues lower than what presented in K_S constant.

2. Material and methods

2.1. Establishing experimental data

Experimental data on moisture as function of time were obtained using soybeans from cultivar CD 202 provided by the Mourãoense Agriculture Livestock Cooperative Ltd (COAMO). Initially, roughly 300 g of soybeans were weighed followed by the preparation of thermostatic bath (Marconi MA184) to control the hydration temperature. The hydration temperatures used were 10, 20, 30, 40 and 50 °C. As the thermostatic bath reached the desired temperature, 1.5 l of sodium benzoate solution (0.2% m/m) were prepared for the immersion of the grains used in the water of hydration to inhibit the proliferation of microorganisms. Subsequently, the sodium benzoate solution was inserted in a recipient in contact with the thermostatic bath for the solution to reach the desired temperature. After reaching the desired hydration temperature, the soybeans were inserted in the bath initiating time counting. Predetermined times provided soybean samples with excessive surface moisture removed using paper towel. The samples were then weighed and inserted in a kiln (Fanem 315 SE) for 24 h at 105 °C to obtain the moisture for each sample (Lutz, 1985).

The experimental grain radius was determined by measuring the diameter of 20 soybean grains using a pachymeter before the grains were subjected to immersion. The mean diameter was calculated as the average of the twenty measurements and the average radius was directed obtained by the average diameter.

2.2. Numerical solution and parameter adjustment

A MATLAB routine for the numerical solution to the model was developed to verify the validity of the obtained analytical solution. The numerical integration for the model applied the "ode45" MATLAB routine based on the Runge–Kutta method (4.5) (Dormand and Prince, 1980). The most satisfactory model parameter values were obtained through the method of least squares using the minimization of a quadratic objective function, Eq. (1). The Levenberg–Marquardt method was applied in parameter optimization (Levenberg, 1944; Marquardt, 1963), by the MATLAB function "nlinfit".

$$\phi = \sum_{n=1}^{N} \left(\rho^i_{A\,\mathrm{calc}} - \rho^i_{A\,\mathrm{exp}} \right)^2 \tag{1}$$

2.3. Analytical solution to the model

The proposed model was obtained through overall mass balance for the soybeans regarded as lumped parameters system and spherical (Coutinho et al., 2007, 2005; Omoto et al., 2009). This balance considered that the convective mass transfer was the predominant cause of the accumulating water inside the grains. The convective flow is given by $N_A = K_S(\rho_{eq} - \rho_A)$. The grain in this equation is considered spherical with constant volume during the entire hydration process. Spatial distribution of moisture inside