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EFFECT OF PHASE CHANGE CRITERION ON THE PREDICTION OF TEMPERATURE EVOLUTION DURING FOOD DRYING

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Abstract. *In this work, a moisture dependent phase change criterion was considered in Luikov´s heat and mass transfer equations and the drying process of a biological product was investigated. Laboratory experiments were conducted to measure the temperature and the moisture content of sweet potato samples during drying. A finite element formulation was used to solve the coupled system of equations. The inverse problem methodology was applied to estimate the parameters of the proposed functional relationship by minimizing the deviation of experimental data and numerical predictions. Numerical simulation showed good agreement with the measured temperature and moisture values. By including a variable phase change criterion it was possible to reproduce the trends of behaviour of temperatures profiles during drying of sweet potato, suggesting that evaporation inside the sample depends on the local moisture content.*

1 INTRODUCTION

The simultaneous transfer of heat and mass in drying processes in porous media can be described by means of the equations developed by Luikov[1].

Luikov´s heat and mass transfer equations depend on the phase change criterion ε. This coefficient fixes the ratio of vapour diffusion coefficient to the coefficient of total moisture diffusion and it has a value between zero and one.

The drying process may be divided in several periods. At the beginning, since the moisture content is high, there is a continuous supply of liquid water that evaporates at the surface ($\varepsilon \cong 0$) and the temperature evolves from the initial value to the wet-bulb temperature. This stage is known as the initial constant drying rate period, in which the surface contains free water and the material remains at the wet-bulb temperature. External resistance to moisture transfer at the product-air interface controls the process and all heat transferred is used for evaporation of water at the surface. Most of food products do not exhibit this period but a pseudo constant period with a lower drying rate compared to that of pure water is observed. The second stage is the falling rate-drying period. The point at which the falling rate period starts is usually called the critical moisture content. During this period the moisture content at the surface decreases and the temperature increases above the wet-bulb temperature. Evaporation moves progressively from the surface into the material. Depending on drying conditions and material properties, both internal and external resistance can be important. As moisture content decreases, the internal resistance increases and may become the prevailing step while the product temperature approaches the dry bulb temperature. In this case a second falling rate period may be observed. The controlling mechanism is the rate at which moisture moves within the product, mainly by water vapor diffusion ($\varepsilon \cong 1$). The moisture content asymptotically reaches the equilibrium value at the relative humidity and temperature of the air.

Luikov's coupled system of differential equations have been applied to investigate the drying of many products, considering in most cases a constant value for the phase change criterion. Irudayaraj[2] *et al.* studied the thin layer drying of soybean, barley and corn kernels assuming $\varepsilon = 0.7$ and surface evaporation ($\varepsilon = 0$). Haghighi and Segerlind[3] solved the problem of drying soybean considering that moisture totally evaporates inside the kernel ($\varepsilon = 1$). Haghighi[4] *et al*. considered moisture evaporation of the surface in thin layer drying of barley. Irudayaraj and Wu[5] presented a parametric analysis of Luikov`s three-way coupled model (heat, mass and pressure) for Norway spruce and identified the phase change criterion as a key parameter in the transfer process. Thomas[6] *et al*. applied Luikov's system to timber drying assuming moisture and temperature thermophysical properties and a linear moisture dependency in the phase change criterion.

In this work, a finite element formulation is adopted and Luikov´s heat and mass transfer equations are used to study the drying process of an anisotropic biological product like sweet potato. The effect of the phase change criterion ε on the prediction of product temperature was analyzed. The phase change criterion is allowed to vary as function of moisture content and by applying the inverse method the parameter of several proposed functional relationship are estimated.

2 MATHEMATICAL MODEL

The system of differential equations developed by Luikov[1] for the temperature T and the moisture content X can be written in the following general form:

$$c\,\rho\,\frac{\partial T}{\partial t} = \nabla.\left(-J_q\right) + \varepsilon\,\rho_0\,L_V\,\frac{\partial X}{\partial t} \tag{1}$$

$$\rho_0\,\frac{\partial X}{\partial t} = \nabla.\left(-J_m\right) \tag{2}$$

The last term of eqn. (1) accounts for a phase change of the water that flows in the solid.

For anisotropic materials, the flows of heat and mass are expressed by:

$$J_{qx_i} = -\sum_j \lambda_{ij}\,\frac{\partial T}{\partial x_j} \quad \Rightarrow \quad \mathbf{J_q} = -\,\overline{\overline{\lambda}} \cdot \nabla T \tag{3}$$

$$J_{mx_i} = -\sum_j a_{mij}\,\rho_0\,\frac{\partial X}{\partial x_j} \quad \Rightarrow \quad \mathbf{J_m} = -\,\overline{\overline{a_m\,\rho_0}} \cdot \nabla X \tag{4}$$

where the terms corresponding to the cross effect of heat and mass transfer (Duffor and Soret effects) were eliminated since λ_{mq} and λ_{qm} are negligible in this case[7].

The quantities λ_{ij} and a_{mij}, are the components of a second order tensor. When the solid presents some symmetry type, the previous expressions can be simplified by appropriate choice of the system of co-ordinated axes.

3 APPLICATION TO THE DRYING OF SWEET POTATO

Sweet potato is an anisotropic product, which has fibers in its structure. The flow of heat and mass naturally presents two preferential directions, normal and parallel to these fibers.

A cylinder of radio R and height L was chosen as domain of analysis. The samples were cut with the fibers of sweet potato parallel to the axis to the cylinder. The bases were insulated to allow only heat and mass flux in a radial direction as shown in Figure 1.

The drying experiments of sweet potato were described in detail in previous works.[8,9] Two samples of 29 mm diameter and 15 mm height were used in the test. One was used for monitoring and recording the weight change by means of an electronic balance scale. Two thermocouples were placed in the other sample (Figure 2) and the temperatures were recorded by means of a data-logging system.

For axial symmetry the resulting Luikov's equations are:

$$\rho\,c\,\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\,\lambda_{\perp}\,\frac{\partial T}{\partial r}\right) + \varepsilon\,L_V\,\rho_0\,\frac{\partial X}{\partial t} \tag{5}$$

$$\rho_0\,\frac{\partial X}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\,a_{m\perp}\,\rho_0\,\frac{\partial X}{\partial r}\right) \tag{6}$$

with the following initial and boundary conditions:

$$\lambda_{\perp} \left. \frac{\partial T}{\partial r} \right|_R = \alpha \left(T_a - T_R \right) + a_{m\perp} \, \rho_0 \left. \frac{\partial X}{\partial r} \right|_R L_V \left(1 - \varepsilon \right) \tag{7}$$

$$a_{m\perp} \, \rho_0 \left. \frac{\partial X}{\partial r} \right|_R = - \alpha_m \, \Delta p \quad \text{where} \quad \Delta P = a_w \, F(T_s) - H_{rel} F(T_a) \tag{8}$$

$$\left. \frac{\partial X}{\partial r} \right|_0 = 0 \qquad \left. \frac{\partial T}{\partial r} \right|_0 = 0 \tag{9}$$

$$T(r,0) = T_0 \qquad X(r,0) = X_0 \tag{10}$$

where α is the convective heat transfer coefficient and α_m is the convective mass transfer coefficient based on vapor partial pressures difference (ΔP) between the air adjacent to the sample surface and the environment. The second term in equation (7) represents the energy used to evaporate the water at the surface.

For the vapor pressure difference evaluation (equation (8)), it is assumed that the air layer close to the boundary is instantaneously in equilibrium with the sample surface, which is at temperature T_s.

Table 1 displays the expressions and material properties used for sweet potato in this work.[8,10,11,12].

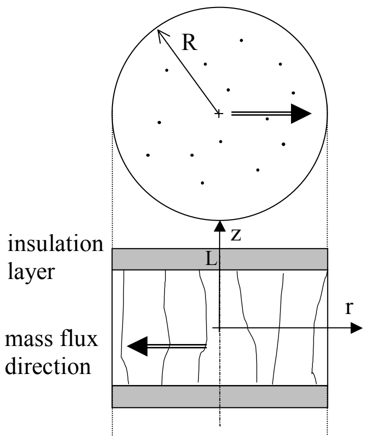

Figure 1: Orientation of sweet potato samples.

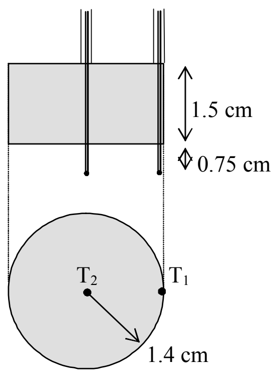

Figure 2: Thermal insulation of the samples and thermocouple location.

Table 1: Material properties and heat and mass transfer coefficients.

Density of dry material	$\rho_s = 1444$ kg/m^3
Density of wet material [kg/m^3]	$\rho = \dfrac{m}{V}$
Content of solids [kg/m^3]	$\rho_0 = \dfrac{m_s}{V} = \rho_s \left(1 + \beta X\right)^{-1}$
Shrinkage coefficient	$\beta = \rho_s / \rho_w$
Specific heat of dry product	$c_s = 1381$ J/kg K
Specific heat of wet product	$\rho_0\, c' = c\, \rho \qquad c' = c_s + X\, c_w$
Thermal conductivity [W/mK] normal to the fibers	$\lambda_{\perp} = 0.48$
Effective water diffusivity [m^2/s] normal to the fibers	$a_{m\perp} = 2.5 10^{-6}\, exp\left(-\dfrac{E}{RT}\right)$
Mass transfer coefficient [kg/m^{2}s P$_a$]	$\alpha_m = 2.4 10^{-8} \left(\dfrac{X_S}{X_0}\right)^{0.7}$
Heat transfer coefficient [W/m^2 C]	$\alpha = 43$

4 FINITE ELEMENT FORMULATION

By use of the weighted residual statement, the weak form of equations (1) and (2) can be obtained:

$$\iint_{\Omega} W \left[\frac{\partial X}{\partial t} - \nabla \cdot \left(a_m\, \nabla X \right) \right] d\Omega = 0 \tag{11}$$

$$\iint_{\Omega} W \left[\rho_0\, c \frac{\partial T}{\partial t} - \nabla \cdot \left(\lambda\, \nabla T \right) - \varepsilon\, \rho_0\, L_v \frac{\partial X}{\partial t} \right] d\Omega = 0 \tag{12}$$

Application of Galerkin method[13], Green's theorem and boundary conditions to the above expressions yields the following algebraic systems of equations:

$$C^X\ \dot{X} + K^X\ X = F^X \tag{13}$$

$$C^T\ \dot{T} + K^T\ T = F^T \tag{14}$$

where C is the global capacitance matrix and K the global conductance matrix, defined by the following expressions:

$$C_{kl}^{X} = \iint_{\Omega} N_k \; N_l \; d\Omega$$

$$C_{kl}^{T} = \iint_{\Omega} \rho_0 \, c \, N_k \; N_l \; d\Omega$$

$$K_{kl}^{X} = \iint_{\Omega} a_m \left(T\right) \nabla N_k \bullet \nabla N_l \; d\,\Omega$$

$$K_{kl}^{T} = \iint_{\Omega} \lambda \left(T\right) \nabla N_k \bullet \nabla N_l \; d\Omega + \int_{\partial\Omega} \alpha \; N_k \; N_l \; d\Gamma$$

$$F_k^{X} = \int_{\partial\Omega} \eta_m \; N_k \, N_l \; d\Gamma \qquad \eta_m = \alpha_m \Delta \; p$$

$$F_k^{T} = \iint_{\Omega} Q \; N_k \; d\Omega + \int_{\partial\Omega} \left(\alpha \, T_a \, N_k + \eta\right) d\Gamma$$

$$Q = \varepsilon \, \rho_0 \, L_V \, \frac{\partial X}{\partial t} \qquad \eta = \left(1-\varepsilon\right) \alpha_m \, \Delta p \; L_V$$

and N_k are the shape functions. Linear triangular elements were used to discretize the domain. To solve the differential equations (13) and (14), the Crank-Nicolson central difference scheme was employed because it is unconditionally stable and second-order accurate in time.

Assuming that the variation of density is negligible, average temperature and moisture content of a sample are calculated from nodal values according to the following expressions for axial symmetry[14]:

$$\overline{T}\left(t\right) = \frac{\sum_{e=1}^{N_e} \left(\left(2\,r_i + r_j + r_m\right)T_i^{e} + \left(r_i + 2\,r_j + r_m\right)T_j^{e} + \left(r_i + r_j + 2\;r_m\right)T_m^{e}\right)\frac{\pi\,\Delta_e}{6}}{\sum_{e=1}^{N_e} \Delta_e}$$

$$\overline{X}\left(t\right) = \frac{\sum_{e=1}^{N_e} \left(\left(2\,r_i + r_j + r_m\right)X_i^{e} + \left(r_i + 2\,r_j + r_m\right)X_j^{e} + \left(r_i + r_j + 2\;r_m\right)X_m^{e}\right)\frac{\pi\,\Delta_e}{6}}{\sum_{e=1}^{N_e} \Delta_e} \qquad (15)$$

After studying the effect of mesh density and time step size on the temperature and average moisture content, a time step of 5 sec and a mesh with 76 elements refined at the surface were chosen to perform the numerical solution.

5 ESTIMATION PROCEDURE

Based on the different periods that characterise the drying process described in section 1, the phase change criterion variation between 0 and 1 was represented by a sigmoidal relationship (SIG1) as function of the moisture ratio $W = X / X_0$:

$$\varepsilon(W) = \frac{1}{exp\{\sigma(W - W_c)\} + 1} \tag{16}$$

where σ is the slope at W_c. This point represents the critical moisture ratio at which the process changes from a constant to a falling rate drying period. The parameter W_c was determined from the experimental drying rate curves and was found to be equal to 0.94.

Seeking for a model prediction improvement two other functions were also considered: a piecewise linear and a corrected sigmoidal function (SIG2).

Figure 3a illustrates the proposed linear function. This function was defined between 0.6 and 1 because this is the range of moisture ratio variation during the drying process as can be seen from the calculated moisture ratio at the surface and center of the sample presented in Figure 3b.[8]

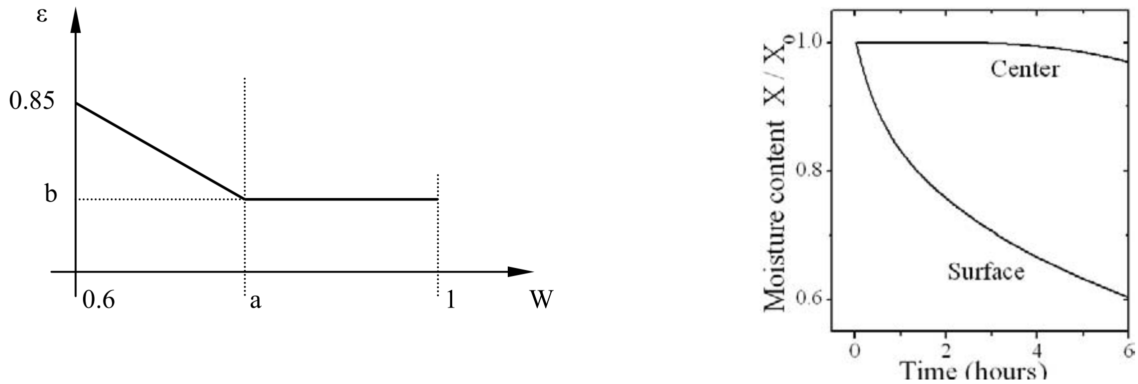

Figure 3: a. Piecewise linear phase change criterion *vs.* moisture ratio
b. Calculated evolution at the surface and center of the sample.

The corrected sigmoidal function (SIG2) was defined as:

$$\varepsilon(W) = \frac{(1-e)}{d\, exp\{cW\} + 1} + e \tag{17}$$

The parameters a, b, σ, c, d and e appearing in the above expressions were estimated by minimizing the sum of square deviations between measured and predicted values[5]:

$$S = \sum_{j=1}^{n} \left[\left(\frac{T_{exp,j} - T_j}{T_{exp,j}} \right)^2 + \left(\frac{\overline{X}_{exp,j} - \overline{X}_j}{\overline{X}_{exp,j}} \right)^2 \right] \tag{18}$$

The Modified Box Kanemasu method was applied for the estimation of parameters as recommended by Beck and Arnold[15] for non-linear systems.

In matrix form,

$$S^{(j)} = \left[\boldsymbol{Y} - \boldsymbol{\eta}^{(j)}\right]^T \boldsymbol{\Pi}\left[\boldsymbol{Y} - \boldsymbol{\eta}^{(j)}\right] \tag{19}$$

where $\boldsymbol{Y}$ is the vector of measured dependent variable, $\boldsymbol{\eta}$ is the vector of estimated dependent variable, $\boldsymbol{\Psi}$ is the matrix sensitivity coefficient and $\boldsymbol{\Pi}$ is the inverse of the matrix of variance of measurements.

The estimated parameter vector is given by:

$$\begin{gathered} \boldsymbol{b}^{(j+1)} = \boldsymbol{b}^{(j)} + z^{(j+1)}\delta^{(j)} \\ \delta^{(j)} = \boldsymbol{P}^{(j)}\left[\boldsymbol{\Psi}^{T(j)}\boldsymbol{\Pi}\left(\boldsymbol{Y} - \boldsymbol{\eta}^{(j)}\right)\right] \\ \boldsymbol{P}^{-1(j)} = \boldsymbol{\Psi}^{T(j)}\boldsymbol{\Pi}\boldsymbol{\Psi}^{(j)} \end{gathered} \tag{20}$$

where $z^{(j+1)}$ is a scalar interpolation factor that modifies the step size in the direction provided by the Gauss method $\delta^{(j)}$, which is iteration-dependent.

6 RESULTS

Figure 4 shows the fitted values assuming a constant phase change criterion and experimental temperature and moisture evolution of cylindrical samples of sweet potatoes. The temperature values present a rapid increase, followed by a plateau, more evident for the inner temperature. After three hours, temperatures start to rise and the drying rate decreases.

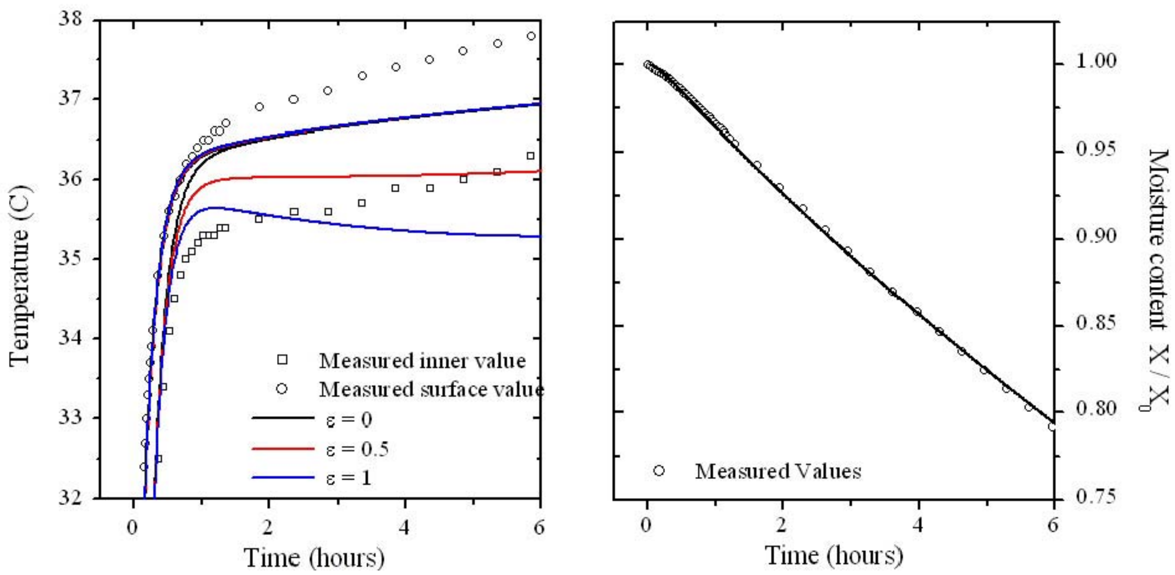

Figure 4: Calculated temperature at thermocouples locations and global moisture ratio for three different constant values of ε.

As reported in previous works[5,8], constant values of the phase change criterion have no significant effect on the global moisture content predictions and good agreement with experimental data was obtained. This is because the moisture transfer equation does not explicitly depend on temperature gradients and is coupled only through the temperature dependent effective moisture diffusivity.

On the contrary, the predicted temperature values were strongly dependent on the phase change criterion and the overall experimental temperature evolution could not be reproduced.

Figure 5 compares the temperature calculated with the proposed functions for the phase change criterion. The values of the estimated parameter and minimum sum square are given in Table 2.

Table 2: Summary of parameter estimates

Equation	Parameter	Estimates value	SSD
Linear Function	a b	0.7748 0.6971	0.028
Sigmoidal SG1 Eqn (16)	σ W_c	0.3549 0.94 (fixed)	0.03275
Sigmoidal SG1 Eqn (16)	σ W_c	0.4118 3.807	0.0314
Sigmoidal SG2 Eqn (17)	c d e	19.58 1.912×10^{-6} 0.7623	0.0293

Applying the sigmoidal function (SIG1) the temperature presented a similar prediction as the one corresponding to $\varepsilon = 0.5$ and a sum of squares of 0.03275 was obtained. In fact, this relationship produced a smooth, almost linear variation between 0.53 and 0.49 in the 0.6-1 range of moisture ratio. When both parameters were simultaneously estimated in SIG1, the fitting was improved to some extent. The variation of ε was still smooth and these new parameters shifted the curve to the constant value of 0.8. Now, W_c has no physical meaning because its values is greater than one.

With the piecewise linear function it was possible to reproduce the trends of behaviour of temperatures profiles and the minimum sum of squares (SSD) decreased to 0.02988.

Based on the previous results, the sigmoidal function was corrected so as to give a similar behaviour to that of the linear function. Thus, parameter e was set equal to 0.7 and c and d were simultaneously estimated. With the converged values of c and d a further calculation was performed to estimate just e. A minimum sum of squares (SSD) of 0.0293 was obtained.

Figure 6 compares the phase change criterion functions calculated with the estimated parameters.

Figure 7 compares predicted and measured mean temperature. The experimental mean temperature was calculated by a volume-weighted sum of the thermocouple measurements and the numerical values applying equation (15). On average, the proposed functions give very similar predictions in contrast to the poor prediction with $\varepsilon = 0$ or $\varepsilon = 1$.

Results depicted in Figures 4 and 5 shows that the predicted temperatures at the surface are underestimated after one hour of drying and overestimated at the center of the sample for the constant or variable phase change criterion.

It is possible that thermocouple attached to the surface might loosen and thus measured the temperature of the air layer adjacent to the surface. To some extent, this may explain the deviations between measured and predicted surface temperatures.

Table 2 shows that the best fit was obtained with a linear moisture dependency. Unfortunately, the sigmoidal function SG1 in which W_c parameter was defined on physical ground did not reproduced the experimental temperature behaviour.

Taking into account that the experimental errors of the thermocouple temperature were within 5%, the predicted values showed good agreement with experimental results. The relative difference between the calculated temperatures and the experimental values were less than 1.5%.

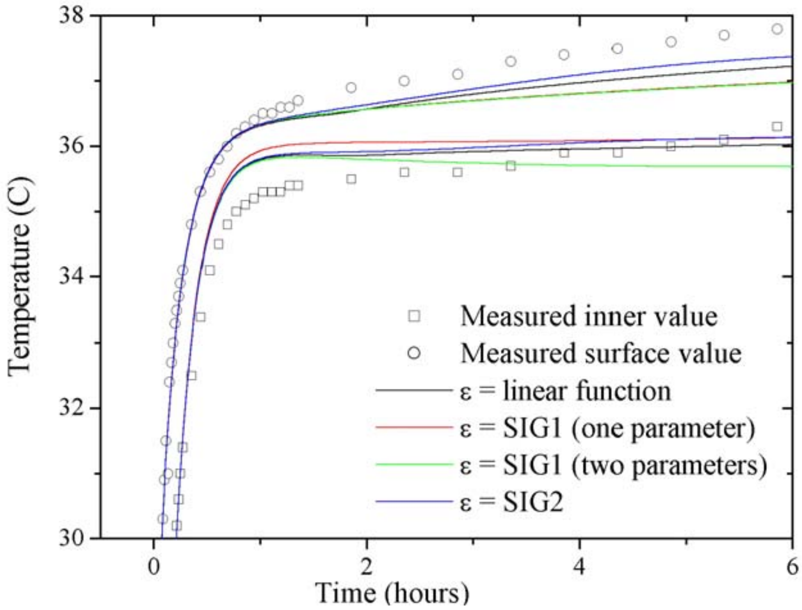

Figure 5: Temperature calculated with the proposed functions for the phase change criterion.

7 CONCLUSIONS

The Luikov heat and mass transfer model was used to study the drying of sweet potato. A finite element formulation was adopted to solve the coupled system of equations.

The finite element model was applied to predict the temperature evolution and moisture content variation of cylindrical samples of sweet potato. By including a variable phase change coefficient it was possible to reproduce the trends of behavior of temperatures profiles and good agreement with experimental results was obtained.

It can be concluded that the phase change must present a sharp variation from 0.95 to 0.7 in the 0.6–0.75 range moisture ratio. These variation was represented by two empirical function. The relationship based on physical reasoning failed probably because the critical moisture ratio is not well defined and the drying process developed in the falling rate period.

Possibly, further improvement in the predictions of inner temperatures could be obtained if a thermal conductivity dependent on temperature and moisture content is included in the model.

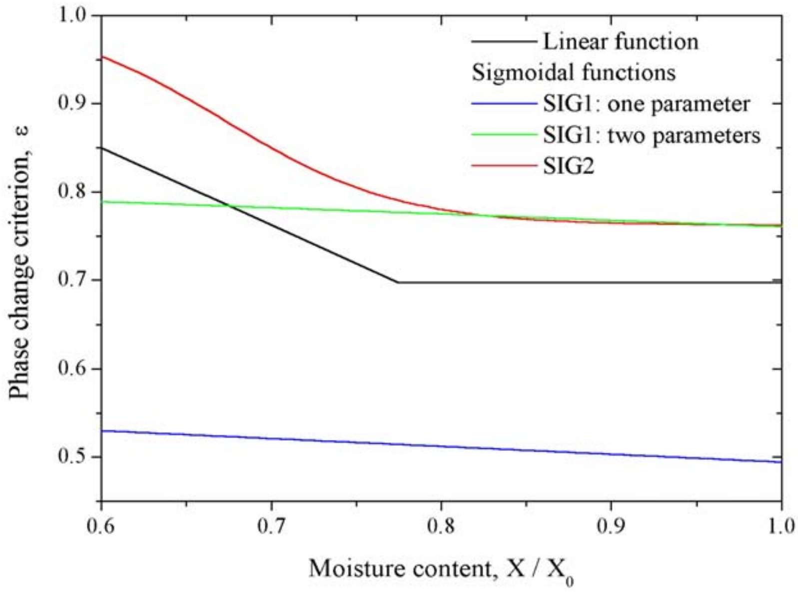

Figure 6: Phase change criterion proposed functions.

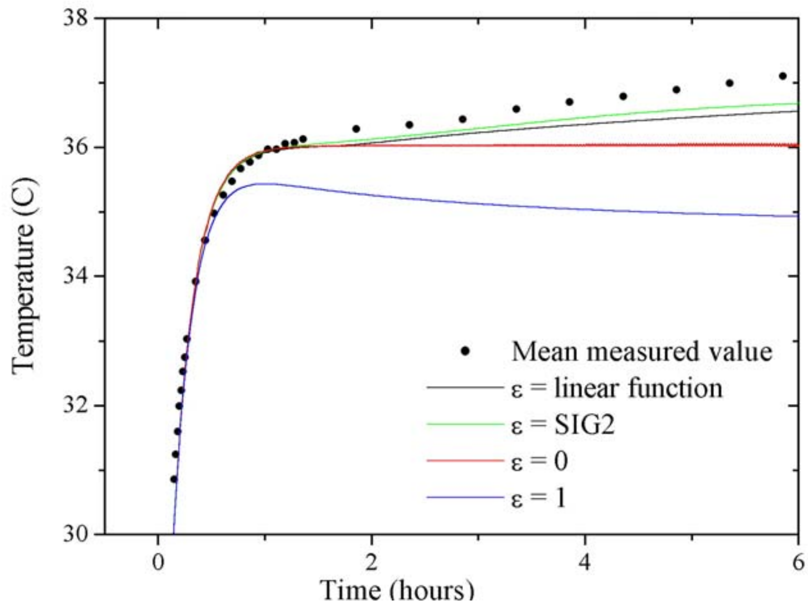

Figure 7: Predicted and measured mean temperature with constant and proposed variable phase change criterion.

NOMENCLATURE

r,θ,z	cylindrical coordinate
$a_{m\perp}$	mass diffusivity normal to the fibers (m^2/s)
a_w	water activity
$\mathbf{b}$	estimate of the vector parameters
c_s	specific heat of the dry product (J/kg K)
c_w	specific heat of the water (J/kg K)
c	specific heat for unit of total mass of the wet product (J/kg K)
c'	specific heat for unit of dry mass of the wet product (J/kg dry K)
$F(T)$	air pressure saturation at the temperature T (Pa)
$\mathbf{J_q}$	flow of heat (W/m^2)
$\mathbf{J_m}$	flow of mass (kg/m^2s)
L	cylinder long (m)
L_v	latent heat of water vaporization (J/kg)
R	cylinder radius (m)
t	time (s)
T	temperature (C)
$\overline{T}$	mean temperature (C)
T_a	ambient temperature (C)
T_0	initial temperature (C)
Ts	surface temperature (C)
V	volume (m^3)
X	moisture content (dry base, kg / kg dry)
$\mathbf{Y}$	vector of measured dependent variable
W	moisture ratio
W_c	critical moisture ratio
α	convective heat transfer coefficient (W/m^2 C)
α_m	convective mass transfer coefficient (kg/m^2sPa)
ε	phase change criterion
Δp	difference of vapor partial pressures (Pa)
$\lambda_\perp$	thermal conductivity normal to the fiber (W/mK)
$\boldsymbol{\eta}$	vector of estimated dependent variable
ρ	density (kg/m^3)
ρ_0	content of solids (kg dry/m^3)
$\boldsymbol{\Psi}$	matrix sensitivity coefficient
$\boldsymbol{\Pi}$	inverse of the matrix of variance of measurements

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