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Heat transfer simulation in corn kernel during nixtamalization process

Simulación de la transferencia de calor en el grano de maíz durante el proceso de nixtamalización

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Abstract

Maize nixtamalization is an alkaline cooking process that yields several food products. One of the critical parameters which are traditionally monitored in the process is temperature; however, to date the measurement of this variable has not been carried out inside the corn kernel itself. In this study, heat transfer inside a corn kernel during the nixtamalization process was simulated by means of finite element analysis (FEA) in a tridimensional (3D) model. In addition, thermophysical properties of corn kernel [thermal conductivity (k), specific heat capacity (C_p) and bulk density (ρ_b)] were determined as a function of temperature (25, 50 and 75 °C). The magnitudes of the thermophysical properties increased with temperature and the convective heat transfer coefficient (h) was computed as 2143 ± 407 W/m^2·K (N_{Bi} =0.0094). Also, the simulation model was good ($R^2_{adj} > 0.99$) and predictions showed that the corn kernel's surface was rapidly heated and the alkaline solution's temperature (85 °C) at corn kernel's center was achieved at 80 s of heating. Furthermore, some predictions in the anatomical parts of the corn kernel were performed. This study contributes to the understanding and improvement of the optimal conditions of the nixtamalization process which allows saving energy, having economic rewards and obtaining high quality nixtamalized products.

Keywords: nixtamalization, corn kernel, thermophysical properties, heat transfer simulation, finite element analysis.

Resumen

La nixtamalización del maíz consiste en la cocción alcalina del grano para la elaboración de diversos alimentos. El control de este proceso se ha basado sólo en la medición de la temperatura del medio de calentamiento. En este trabajo, se analizó la transferencia de calor dentro del grano de maíz sometido a nixtamalización mediante simulación por elementos finitos (FEA) en un modelo tridimensional (3D). Además, se midieron experimentalmente las propiedades termofísicas del grano de maíz [conductividad térmica (k), capacidad calorífica específica (C_p) y densidad aparente (ρ_b)] en función de la temperatura (25, 50 y 75 °C). Las propiedades termofísicas incrementaron con la temperatura y el coeficiente convectivo de transferencia de calor (h) fue 2143 ± 407 W/m^2·K (N_{Bi} =0.0094). Además, el modelo de simulación fue adecuado ($R^2_{adj} > 0.99$) y las predicciones realizadas mostraron que la superficie del grano de maíz se calentaba rápidamente y que la temperatura del centro alcanzó la temperatura del medio alcalino (85 °C) en 80 s de calentamiento. También, se realizaron predicciones en las partes anatómicas del grano de maíz. Este estudio contribuye al entendimiento y a la optimización del proceso de nixtamalización, derivando en ahorro de energía, ganancias económicas y productos nixtamalizados de mejor calidad.

Palabras clave: nixtamalización, maíz, propiedades termofísicas, simulación de la transferencia de calor, elementos finitos.

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1 Introduction

Nixtamalization is an ancient process developed by *Aztec* civilization which has been used to transform corn (*Zea mays* L) in flour, masa, tortilla and several food products (Rosales *et al*., 2016). This process mainly consists of the alkaline cooking of corn [aqueous solution at 1% $Ca(OH)_2$ concentration] using temperatures around 94 °C for 50 - 90 min followed by a steeping time of 14 h (Gutiérrez-Dorado *et al*., 2008). It has been reported that nixtamalization provides several benefits as it increases calcium uptake in tortillas (Valderrama-Bravo *et al*., 2010), increases bioavailability of niacin (Moretti *et al*., 2014) and improves protein digestibility (Gutiérrez-Dorado *et al*., 2008). Therefore, the monitoring and optimization of this process represent an important issue for food industry.

Traditionally, nixtamalization monitoring includes corn genotype, storing conditions, corn quality, $Ca(OH)_2$ concentration (Gomez *et al*., 1992), moisture, time and temperature cooking (Estrada-Girón *et al*., 2014; Moreno-Castro *et al*., 2015). The temperature measurement has been commonly carried out on the alkaline solution and its control is important due to its effect on quality parameters such as moisture and texture of masa, moisture and texture of tortilla, percentage and diffusion of calcium and solids loss (Sahai *et al*., 2001).

Some reports have focused on mass transport phenomena in hydration of the corn kernel (Martínez-Garza *et al*., (2018)), and nixtamalization process, during cooking and steeping (Ruiz-Gutiérrez *et al*., 2010; Gutiérrez-Cortez *et al*., 2016); however, there are no studies about the behavior of temperature and heat transfer inside the corn kernel subjected to the nixtamalization process. In this operation, two unsteady state heat transfer mechanisms are involved: conduction inside the corn kernel and convection by the alkaline solution at the surface. Time and high temperatures of nixtamalization are key parameters for analyzing heat transfer, thus, simulation methods can be an adequate tool to study heat transport phenomena inside the corn kernel. One of the simulation methods is finite element analysis (FEA) which has been applied for the assessment of several food processes as hydrocooling and blanching of broccoli florets (Iribe-Salazar *et al*., 2015); determining of watermelon quality (Abbaszadeh *et al*., 2014); and barley grains hydration (Montanuci *et al*., 2014). FEA consists in a numeric approach to solve differential equations as Fourier's second law, giving results that allow the inclusion of issues such as temperature dependence of thermal properties, food irregular geometries and nonlinear conditions. Also, data obtained by means of FEA can easily be validated by comparison with experimental results (Caro-Corrales *et al*., 2002). Therefore, simulation by means of FEA can predict the heat transport phenomenon in the nixtamalization process to ensure the achievement of the required quality of the food products derived from it. The aim of this work was to simulate heat transfer and to predict temperature histories inside a corn kernel during nixtamalization process by means of FEA.

2 Materials and methods

2.1 Material

Corn kernels (*Zea mays* L) [Pioneer genotype X6C (457W)] which were grown in Culiacan Valley, Mexico, were used for this work. After harvest, the grains were manually separated from the cob, cleaned and stored at 5 °C until used. The moisture content of corn kernels was 9.1% (d.b.).

2.2 Thermophysical properties

The thermophysical properties [thermal conductivity (k), specific heat capacity (C_p) and bulk density (ρ_b)] were measured at three different temperatures (25, 50 and 75 °C) in order to obtain values within an interval from standard conditions (25 °C) to a temperature near to starch gelatinization (75 °C). The dependence of these parameters with temperature is well known due to the temperature induces structural changes which can affect the heat transfer simulation process.

2.2.1 Thermal conductivity (k)

Thermal conductivity (k) was measured using the line heat source method (van der Held and van Drunen, 1949; Gratzek and Toledo, 1993). This method is rapid and consists in the use of a heat source as a solid with infinite length and diameter infinitely small (probe), assuming only radial conduction in a non-steady state. The temperature of the heat source was calculated from the Fourier Field equation assuming a constant thermal diffusivity. The analytical solution was given by the following equation (Espinoza-Guevara *et al*., 2010):

$$T - T_1 = \frac{Q_L}{4\pi k} \ln\left(\frac{t}{t_1}\right) \tag{1}$$

Where T is the source temperature (°C), Q_L is the heat input per unit length of the line source (W/m), t is time (s), T_1 and $\ln t_1$ correspond to coordinates in which the curve (T vs $\ln t$) started to be linear.

The procedure consisted in skewering the corn kernels into the probe by their center. The probe was constructed according to Murakami *et al.*'s work (1996) in which it was specified the use of a probe with the following dimensions: diameter = 0.12 cm, length: 14.5 cm and length/diameter ratio = 121. Probe and samples were isolated with plastic films to avoid moisture permeation and were equilibrated at 25, 50 and 75 °C. The experiment conditions were established as follows: current intensity = 140 mA, length = 14.7 cm, resistance of the probe = 69.62 Ω, and supplied heat per length unit (Q_L) = 9.3 ± 0.3 W/m. The probe's temperature as a function of time was recorded each 3 s for 3 min, using a scanning thermometer (Digi-Sense Thermocouple Scanning Thermometer, Cole-Parmer, USA). A regression analysis was performed between T and $\ln t$ to obtain the best fit.

2.2.2 Specific heat capacity (C_p)

A Differential Scanning Calorimeter (DSC, TA Instruments 2920, USA) was used to determine specific heat capacity (C_p) of corn kernel. The calibration was carried out with standard sapphire (Al_2O_3). The procedure conditions were a sample size of 20 mg of manually broken corn kernels (approximately 8 fragments per grain) and a temperature scanning rate of 20 °C/min. The absorbed energy during the scanning was recorded as a thermogram. A baseline was obtained with an empty cell as a reference. Energy absorption rate was (dQ/dt) at any temperature (25, 50 and 75 °C), and was proportional to the difference between the enthalpy of the baseline and the corresponding test material curve (ΔH). C_p was computed as follows (Caro-Corrales *et al.*, 2002):

$$C_p = \frac{E}{dT/dt}\frac{\Delta H}{m} \tag{2}$$

where E is the calibration constant, m is the sample mass (kg).

2.2.3 Bulk density (ρ_b)

The bulk density (ρ_b) was calculated relating the corn kernel mass to its volume, which was obtained by the liquid (water) displacement method of 20 grains at different temperatures (25, 50 and 75 °C) (Espinoza-Guevara *et al.*, 2010).

2.3 Nixtamalization process

Nixtamalization was carried out as reported by Gutiérrez-Dorado *et al.*, (2008). The experiment consisted in cooking 5 different corn kernels in an alkaline solution [$Ca(OH)_2$ at 5.4 g/L concentration] at a temperature of 85 °C with regular stirring at 20 rpm (EuroStar Ika Labortechnik, Germany) for 30 min. Two T type thermocouples were inserted into the corn kernels, one at a depth of 6 mm and other near the surface at a depth of 2 mm. Temperature history was recorded in a Temperature Controller Software (PicoLog Recorder, USA). The experiment was carried out by triplicate.

2.4 Convective heat transfer coefficient (h)

For the nixtamalization process, the convective heat transfer coefficient (h) was computed by using the lumped parameter approach (Caro-Corrales *et al.*, 2002). An aluminum corn kernel-model (length = 14 mm, width = 9 mm, thickness = 5 mm) was manufactured for the method. Temperature histories of the aluminum grain at nixtamalization conditions (See Section 2.5) were recorded by inserting a T type thermocouple at the center of the aluminum grain (6 mm depth). The heat transfer coefficient (h) was calculated from the slope through a linear regression of the equation:

$$\frac{T - T_\infty}{T_0 - T_\infty} = \exp\left(-\frac{hA}{\rho C_p V}t\right) \tag{3}$$

where T_0 is the initial temperature of the aluminum grain (20 °C), T_∞ is bulk alkaline solution's temperature (85 °C), A and V are surface area and volume of the aluminum grain, ρ is bulk density for aluminum (2707 kg/m^3), and C_p is specific heat capacity for aluminum (896 J/ kg °C). The experiment was performed by triplicate.

2.5 Heat transfer simulation

Heat transfer modeling and predictions were performed by means of the ANSYS v. 5.3 software

(ANSYS/ED, USA). The procedure consisted in creating a 3D model of half a corn kernel to accomplish FEA. A tetrahedron (size = 1.8 mm) formed by 10 nodes was used as the finite element and composed a network, which had 462 elements and 916 nodes. The heat transfer simulation was carried out at 1 s intervals and at two locations with the following coordinates: ($x = 0.00313$, $y = 0.00623$, $z = 0.00091$) and ($x = 0.0035$, $y = 0.0015$, $z = 0.00075$) which corresponding to the center location (6 mm depth) and a point near the surface (2 mm depth), respectively.

The validation of simulation was performed by using data from: nixtamalization experiments (85 °C for 30 min), thermophysical properties as a function of temperature (25, 50 and 75 °C) and thermophysical properties at 25 °C. A comparison between the experimental and simulated unaccomplished temperature ratio $(T - T_\infty)/(T_0 - T_\infty)$ was carried out and linearized. Finally, a regression analysis was applied to evaluate the simulation goodness.

After validation, a prediction of temperature histories was carried out for analyzing the heat transfer in the anatomical parts of the corn kernel: pedicel ($x = 0.0035$, $y = 0.0813$, $z = 0.00075$), germ ($x = 0.00313$, $y = 0.00603$, $z = 0.00091$), floury endosperm ($x = 0.0035$, $y = 0.0033$, $z = 0.00075$), and vitreous endosperm ($x = 0.00513$, $y = 0.00613$, $z = 0.00091$). These boundary conditions were obtained by separating manually the pedicel, germ, floury endosperm and vitreous endosperm from 30 corn kernels, and determining the distances with a caliper. The corn kernel 3D model showing the anatomical parts for predictions is presented in Figure 1. This prediction involved only the zone's location inside the corn kernel 3D model.

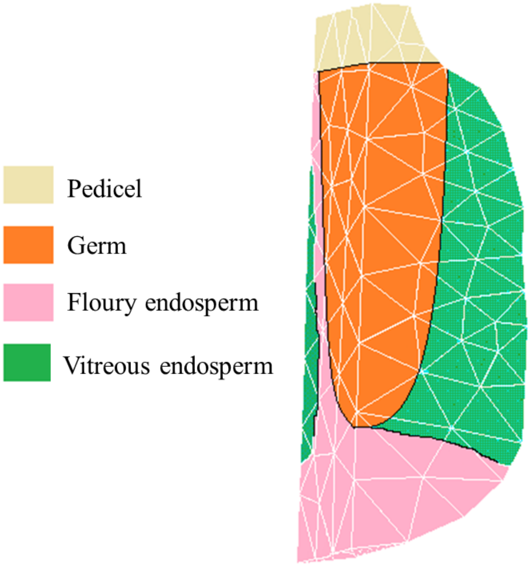

Fig. 1. Anatomical parts of corn kernel in a 3D model used for predictions by FEA.

2.6 *Statistical analysis*

The effect of the temperature (levels 25, 50, and 75 °C) on the thermophysical properties (response variables) of the corn kernel was evaluated employing a unifactorial completely randomized design. One-way ANOVA and Tukey test ($p \leq 0.05$) were performed using the Minitab 16 software.

3 Results and discussion

3.1 *Thermophysical properties of corn kernel*

Table 1 shows the thermal conductivity (k), specific heat capacity (C_p), and bulk density (ρ_b) of a single corn kernel. Thermal conductivity significantly increased ($p \leq 0.05$) at 50 °C in comparison to 25 °C. However, this property did not undergo significant ($p > 0.05$) changes when temperature increased from 50 °C to 75 °C. In literature, there are no recent works about measuring k for food grains. Kustermann *et al.* (1981) found that k in kernels of shelled corn with different moisture contents ranged from 0.1 to 0.34 W/m·K at 20 °C. These results were similar to those reported in this study and indicated the dependence of k with temperature and moisture content in food materials. In addition, k can be affected by several properties such as porosity, shape and homogeneity of the material (Mohsenin, 1980).

On the other hand, specific heat capacity of corn kernel significantly ($p \leq 0.05$) increased with temperature, which means that this property was affected as a consequence of structural changes inside the kernel associated to starch gelatinization which takes place around 70 °C. According to several reports, C_p values obtained in this study were similar to Cp of maize type "ear" (Khabba *et al.*, 1999) and wet maize (moisture content = 58%, d.b.) for drying process (Simate, 2001). It was remarkable the dependence of C_p with moisture content; therefore, the experimental value at 25 °C (1.963 kJ/kg °C) was compared with a theoretical value calculated as

Table 1. Thermophysical properties of corn kernel at different temperatures.

Property	Temperature (°C)		
	25	50	75
k (W/m K)	$0.176^b \pm 0.006$	$0.245^a \pm 0.015$	$0.262^a \pm 0.018$
C_p (kJ/kg °C)	$1.963^c \pm 0.113$	$2.177^b \pm 0.069$	$2.584^a \pm 0.040$
ρ_b (kg/m^3)	$1259.8^a \pm 44.1$	$1282.6^a \pm 45.5$	$1304.7^a \pm 45.4$

*Average and corresponding standard deviation of 5 replicates

**Means within a same row with different letters are significantly different based on Tukey test ($p \leq 0.05$)

a function of moisture content (9.1% d.b.) at 25 °C (Hahn and Rosentreter, 1991), and resulting a value of 1.789 kJ/kg °C, which was similar to the C_p reported in this study.

Moreover, ρ_b for corn kernel did not show significant differences (p > 0.05) among the analyzed temperatures. A significant variation of kernel volume was not observed in measuring ρ_b, probably due to empty cells of corn which were structurally arranged during heating. It has been reported that moisture content was the most important factor which can produce a significant change in ρ_b. In this regard, Barnwal *et al.* (2012) determined ρ_b of maize, reporting 1321.7 kg/m^3 and 1231.5 kg/m^3 for moisture contents of 12.8% and 29%, respectively.

3.2 *Heat transfer modeling*

The convective heat transfer coefficient (h), at the nixtamalization conditions, was 2143 ± 407 W/m^2·K (N_{Bi} = 0.0094). The magnitude of h was attributed to the high temperature (85 °C) and the high stirring velocity (20 rpm) of the experiment, which increased the turbulence of the alkaline solution, producing a lower thickness of the thermal boundary layer between the liquid and the corn kernel. In another work (Iribe-Salazar *et al.*, 2015), it was reported lower h values for blanching (h = 1011 W/m^2·K) and hydrocooling (h = 468 W/m^2·K) of broccoli florets, which were the result of a higher thickness of the thermal boundary layer, produced by the absence of stirring. The lumped parameter approach seemed to be a good experimental method to compute h, due to the obtained coefficient was similar to h calculated by theoretical equations reported in a study for agitated tanks (López *et al.*, 2018).

Figure 2 shows the 3D model of corn kernel which was used for heat transfer simulation during nixtamalization (Figure 2A). The element shape was a tetrahedron with 10 nodes each (Figure 2B), creating a fine network of elements which were adequate for the curvy shape of corn kernel. The amount, the size and the volume shape of the elements provided good approximations to the behavior of heat transfer inside the corn kernel during nixtamalization process. Experimental and simulated temperature histories of corn kernel by FEA using the thermophysical properties as a function of temperature (Table 1) are shown in Figure 3. The results indicated that the geometric center of the corn kernel (6 mm depth) reached the alkaline solution's temperature (85 °C) at 80 s after immersion (1.3 min) while at the location of 2 mm near the surface, alkaline solution's temperature was reached at 20 s after immersion. Also, N_{Bi} was 12.14, showing that the conductivity inside the corn kernel (internal resistance) mainly affected the heat transfer flux of the nixtamalization process. Therefore, alkaline solution's temperature was reached at a short time due to the small geometry of the corn kernel. Thus, the measurement and control of temperature of the alkaline solution for the nixtamalization process as has traditionally been carried out is adequate (Yglesias *et al.*, 2005), because the temperature of the alkaline solution was reached rapidly by the corn kernel and remained constant after reached it. The variation of nixtamalization's temperature has been also analyzed, finding an increase in gelatinization temperature which was associated to calcium interaction with amylose chains in starch (Ruiz-Gutiérrez *et al.*, 2010). Furthermore, a good fit between experimental and simulated data along the heat transfer process was observed, obtaining high determination coefficients: R^2_{adj} = 0.9962 and R^2_{adj} = 0.9991 ($p \leq 0.05$); for 6 mm and 2 mm depth, respectively. Also, the use of thermophysical parameters as a function of temperature (25, 50 and 75 °C) caused better simulation results in comparison to a simulation performed with thermophysical properties at 25 °C (R^2_{adj} = 0.9634 for the location of 2 mm depth).

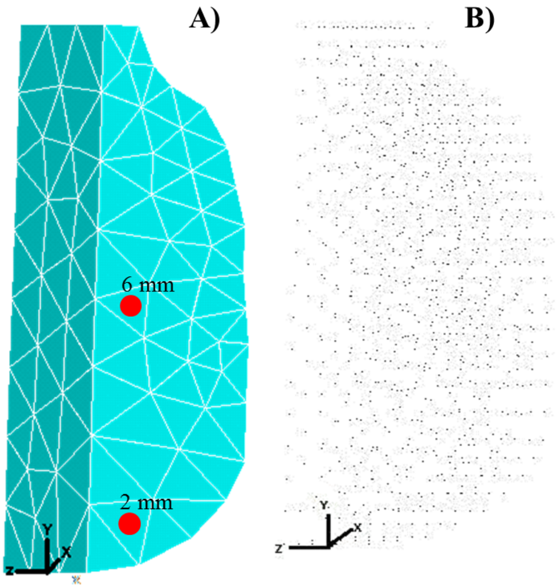

Fig. 2. A) Corn kernel 3D model for FEA. Red circles are the thermocouple locations for 6 mm and 2 mm depth. B) Nodes.

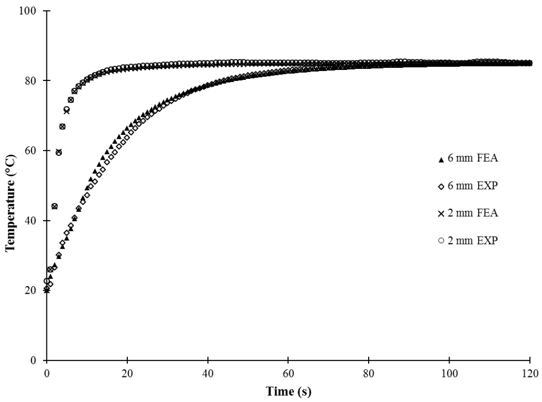

Fig. 3. Temperature histories of corn kernel during the nixtamalization process simulated by finite element analysis (FEA) and experimental (EXP), corresponding to 6 mm and 2 mm depth.

Therefore, the simulation by means of FEA of the nixtamalization process was satisfactory for those locations.

3.3 *Predictions*

The simulations by FEA showed that the zones located near the corn kernel surface had higher temperatures, whilst the nucleus at the corn kernel's center presented cooler temperatures (Figure 4).

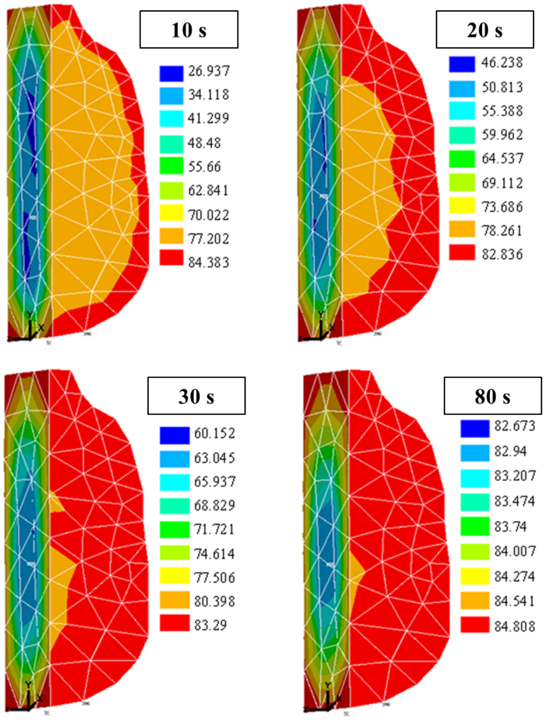

Fig. 4. Simulated temperature distribution of corn kernel during the nixtamalization process by FEA. Numbers in legends are temperature in °C.

The predictions indicated that the corn kernel's surface reached a temperature near the alkaline solution (85 °C) at 10 s of heating. After 20 s of heating, almost all the surface achieved a temperature of 85 °C; however, the corn kernel's center remained at low temperature (46 °C). Also, at 30 s of nixtamalization process, most of corn kernel structure had a temperature higher than 60 °C. Finally, after 80 s of heating, temperature of the corn kernel center was 83 °C, approximately. There are reports about the intrinsic relationship of cooking temperature with quality parameters in food process, as an example, the temperature of meat during water-bath cooking was modeled by FEA, finding that at low temperature, moisture content was dependent on the meat type (Oillic *et al*., 2011).

Furthermore, Figure 5 shows heat flux distribution at different nixtamalization times inside the corn kernel. Simulations computed that heat flow was concentrated to the corn kernel central axis in radial and axial directions, which means that the kernel center achieved the alkaline solution's temperature (85 °C) at a longer time (increasing the value of the energy flux) in comparison to other corn kernel locations, due to the distance was longer towards the center.

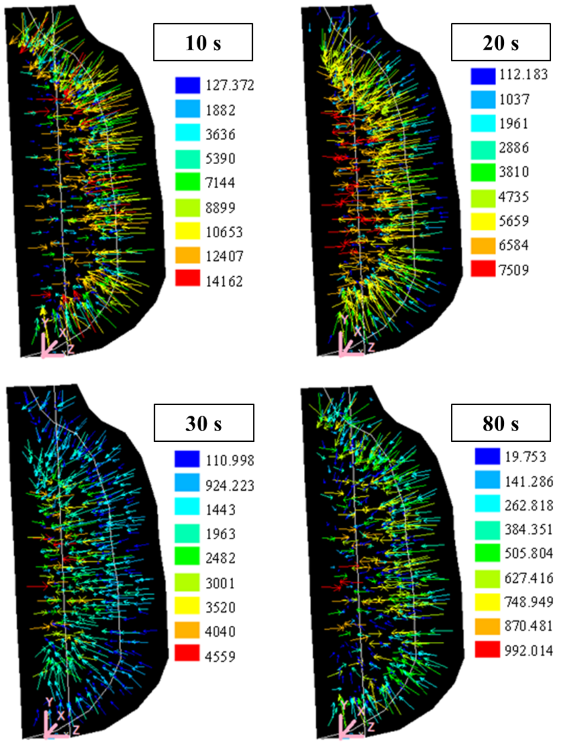

Fig. 5. Simulated heat flux distribution of corn kernel during the nixtamalization process by FEA. Numbers in legends are flux in J/s·m^2.

The energy flux decreased with increasing time in the center and in the surface, due to the temperature gradient between alkaline solution and corn kernel was low as well. The analysis of heat flux inside the corn kernel helps in the selection of the optimum location of thermocouples in other food grains which can be useful to standardize measure methods of temperature for several cooking process.

On the other hand, temperature predictions of the anatomical parts of corn kernel were carried out for the nixtamalization process (Figure 6). A slow increasing of temperature of floury endosperm was observed during 5 s of heating and it was increasing exponentially towards alkaline solution's temperature (85 °C at 60 s of heating). Regarding vitreous endosperm, temperature increased rapidly at first; however, the rate of temperature decreased and alkaline solution's temperature was reached at 80 s of heating. The temperature history obtained for the germ was similar to the experimental data at 6 mm, due to the location of this anatomical part is at the center of the corn kernel. An analogous result was computed for the pedicel, which location was the surface, thus causing in a similar curve to 2 mm depth.

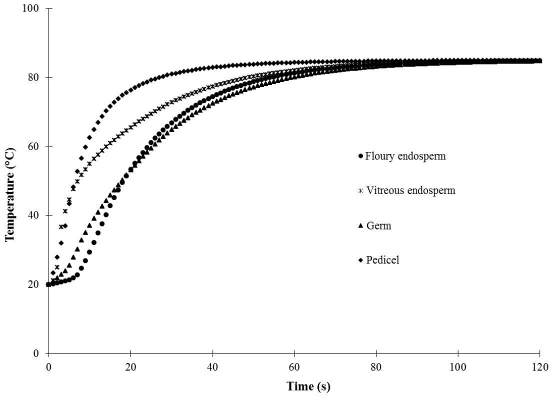

Fig. 6. Simulated temperature histories of corn kernel anatomical parts during the nixtamalization process by FEA.

It should be noted that these estimations were related to the locations of the anatomical parts and nor to the chemical composition and structure of each.

Conclusions

The heat transfer simulation of the corn kernel during nixtamalization reported in this work was satisfactory and can predict the temperature and heat flux at any location of the corn kernel. The thermophysical properties of the product were experimentally calculated together with their dependence on temperature. These properties of the corn kernel were indicators of structural changes which are produced inside the grain owing to a heating process. The temperature of the alkaline solution was achieved inside the corn kernel in a short time; thus, the traditional control of this process variable has been adequate. Also, the heat flux distribution inside the corn kernel decreased with nixtamalization's time and it was concentrated towards the center of the grain. In summary, experimentally obtained knowledge of the heat transfer coefficient and thermophysical properties combined with FEA tridimensional modeling allowed the simulation of the heat transfer inside the corn kernel during the nixtamalization process. The high coefficients of determination between estimated and experimental temperatures demonstrated the validity of the model.

Acknowledgements

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Nomenclature

3D	tridimensional
A	surface area of the aluminum grain, m^2
$Ca(OH)_2$	calcium hydroxide
C_p	specific heat capacity, kJ/kg °C
E	calibration constant
FEA	finite element analysis
h	convective heat transfer coefficient, $W/m^2 \cdot K$
k	thermal conductivity, W/m K
m	sample mass, kg
N_{Bi}	Biot number
Q_L	heat input per unit length of the line source, W/m
R^2_{adj}	adjusted coefficient of determination
T_∞	bulk alkaline solution's temperature, °C
T_0	initial temperature of the aluminum grain, °C
T_1	temperature value in which the curve (T vs $\ln t$) started to be linear, °C
t	time, s
t_1	time value in which the curve (T vs $\ln t$) started to be linear, s
V	volume of the aluminum grain, m^3
Greek symbols	
ΔH	enthalpy difference of the baseline and corresponding test material curve, kJ
ρ_b	bulk density, kg/m^3

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