

Mathematical simulation of roasting of grain

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Abstract

Grain roasting and popping are important unit operations for manufacturing ready to eat products of longer shelf life. Change in moisture content and volume of grain during roasting leads to development of internal pressure for popping. A mathematical model, considering thermodynamic changes and heat and mass balances during roasting, was thus developed. The predicted internal pressure, moisture content and change in volume at 2.8 min roasting time and at 213 °C grain temperature, while roasting pan temperature was 335 °C, were found to be about 45 MPa, 14% (dry basis) and 130 mm³, respectively. The accuracy of the model's results was examined by comparing the predicted and measured values of changes in volume and moisture of the grain during roasting. Prediction performance of the developed model was found to be satisfactory.

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1. Introduction

The grains that are roasted for getting their kernel popped are paddy, corn, millets and some nuts such as peanut, gorgon nut, etc. The popping process consists of conditioning, high-temperature roasting, and popping. Conditioning creates a small gap between the kernel and the shell, equilibrates the moisture, and gelatinizes the kernel's starch. High-temperature roasting generates superheated steam and builds pressure within the grain. Majority of grains get popped during roasting, while a few whose shell wall is hard do not pop easily. The hot roasted one is hit externally to develop crack for sudden release of internal pressure for popping. A regular shape and uniform size are the desirable features of a popped kernel but it gets distorted, if shell wall breaks and popping takes place during roasting due to development of high pressure. The internal pressure

mainly is a function of roasting time, moisture content and temperature of the grain. Knowledge of the magnitude and trend of pressure development, change in moisture and volume may help in controlling the process for better quality of popped product.

A relationship amongst thermal expansion, tensile strength and cracking of corn kernels during drying (Ekstrom, Liljedahl, & Peart, 1966) gives knowledge of expansion of grain due to thermal stress. Models of simultaneous heat and mass transfer help to compute temperature and moisture of a single porous solid (Young, 1969) and agitating particulate canned foods (Stoforos & Merson, 1995). Models for drying of grains are also available but are not applicable as such in case of roasting. A very few models describing roasting operation are reported in literature (Das & Srivastav, 1993; Robbies & Fryer, 2003), but none of them provide information either for computing or measurement of internal pressure built up and change in volume of grain during roasting. So, it would be a worthy exercise to predict it mathematically, based on thermodynamic

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considerations, heat and mass balances. The objectives of this paper were thus to develop a mathematical model for prediction of internal pressure built up in grain during roasting and to examine the accuracy of prediction comparing predicted and measured values of changes in moisture and volume of the grain during roasting.

2. Mathematical modeling

A generalized model of conditioned spherical grain (Fig. 1) was considered. It is comprised of an outer shell, the starchy kernel and a small gap filled with air–water vapor mixture between the kernel and the shell. If the grain is roasted to high temperature, it is expected that the internal pressure developed due to air–water vapor mixture within the grain will induce hoop stress in the shell wall (Fig. 2). Analysis of thermal treatment of the grain mainly involves three problems, inter-linked due to the volume constraint. They are

- (i) thermo-elasticity of the spherical shell,
- (ii) expansion and shrinkage of the kernel, and
- (iii) compression of air–water vapor mixture in the gap between the kernel and the shell.

If V_s , V_k , and V_a are respectively the volume enclosed by the shell, and the volumes of the kernel and the gap between the kernel and the shell

$$V_s = V_k + V_a \quad (1)$$

For small change in the volume

$$\Delta V_s = \Delta V_k + \Delta V_a \quad (2)$$

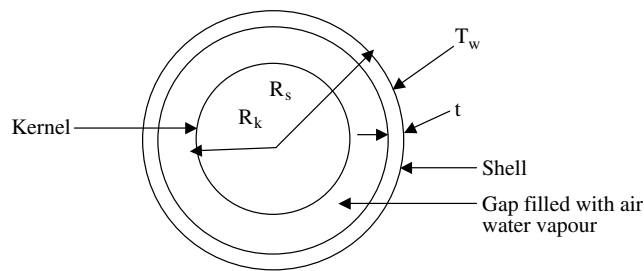


Fig. 1. A generalized spherical model of conditioned grain.

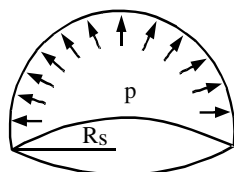


Fig. 2. Force diagram for a spherical shell of grain during roasting.

2.1. Change in volume enclosed by the shell, ΔV_s

In deriving the expression for change in volume enclosed by the shell, ΔV_s , the following assumptions were used:

- (i) The shell is spherical.
- (ii) The shell material is elastically isotropic.
- (iii) The thermal anisotropy of the shell material is restricted to the radial direction only.
- (iv) The shell's thickness is small compared to its radius, and there is no abrupt change in curvature so that bending stress can be neglected.
- (v) The roasting pan temperature is very high and the moisture content of thin shell of the grain is so low that it attains an equilibrium in moisture content and temperature almost immediately, and
- (vi) the temperature of the shell wall remains uniform with respect to thickness, so there is no thermal stress within the shell.

The net radial expansion of a thin spherical shell subjected to an internal pressure p , uniform shell wall temperature field T_w and radial contraction due to moisture loss can be obtained by using the membrane theory of shells of revolutions as follows:

Based on the above assumptions, the simpler 'membrane theory' for shell may be written (Gibson, 1965) as

$$\sigma_\theta = \sigma_\phi = \frac{pR_s}{2t} \quad (3)$$

where σ_θ , σ_ϕ , p , R_s , and t are circumferential stress, Pa; meridional stress, Pa; internal pressure, Pa; radius and thickness of shell, m; of the grain, respectively.

The circumferential membrane strain in the shell is given by

$$\varepsilon_\theta - \varepsilon_{th} + \varepsilon_m = \left(\frac{\sigma_\theta - \nu\sigma_\theta}{E} \right) \quad (4)$$

where ε_θ , ε_{th} , ε_m , ν and E are elastic circumferential strain, thermal strain, circumferential moisture strain, Poisson's ratio and modulus of elasticity, Pa; of shell material, respectively.

The circumferential thermal strain in the shell is given by

$$\varepsilon_{th} = \alpha\Delta T_s \quad (5)$$

where α and ΔT_s are coefficient of linear thermal expansion, $^{\circ}\text{C}^{-1}$; and change in temperature, $^{\circ}\text{C}$; with respect to initial temperature of shell, respectively.

Elastic circumferential strain is given by

$$\varepsilon_\theta = \frac{\Delta R_s}{R_s} \quad (6)$$

where R_s and ΔR_s are radius of shell, m and change in the same, respectively.

Circumferential moisture strain is expressed as

$$\varepsilon_m = \beta \Delta M_s \quad (7)$$

where β and ΔM_s are the coefficient of linear moisture contraction (dimensionless) and change in moisture content of shell, fraction, dry basis, respectively.

From Eq. (4)

$$\varepsilon_\theta = \left(\frac{\sigma_\theta - \nu \sigma_\theta}{E} \right) + \varepsilon_{th} - \varepsilon_m \quad (8)$$

Substituting the Eqs. (3), (5), (6), and (7) into Eq. (8) yields:

$$\Delta R_s = R_s \left[\frac{pR_s}{2tE} (1 - \nu) + \alpha \Delta T_s - \beta \Delta M_s \right] \quad (9)$$

The change in volume enclosed by the shell becomes as

$$\Delta V_s = \frac{4\pi \left[(R_s + \Delta R_s)^3 - R_s^3 \right]}{3}$$

Neglecting terms containing the higher orders of ΔR_s , the equation can be written as

$$\Delta V_s \cong 4\pi R_s^2 \Delta R_s \quad (10)$$

Substituting ΔR_s from Eq. (9) in Eq. (10), the expression for change in volume enclosed by the shell becomes

$$\Delta V_s = 3V_s \left[\frac{pR_s}{2tE} (1 - \nu) + \alpha \Delta T_s - \beta \Delta M_s \right] \quad (11)$$

2.2. Change in volume of the kernel, ΔV_k

The change in volume of the kernel can be obtained by heat and mass transfer analysis. To deduce expressions for moisture transfer from the kernel and heat transfer to the kernel from the shell following assumptions were made:

- (i) The kernel is incompressible and spherical.
- (ii) Heat transfer to the kernel from the shell is mainly through conduction via contact area of kernel and the shell wall during roasting. Heat transfer through convection and radiation, if any, are ignored, and
- (iii) specific heat and latent heat of vaporization of kernel are constant at a particular roasting temperature.

2.3. Moisture transfer

The moisture content of the kernel during roasting is dependent on initial and equilibrium moisture content of whole grain, roasting time and temperature. The relationship between the moisture content of kernel and the grain with roasting temperature and time can be defined by the following functions:

$$M_k = f(M_g) \quad (12)$$

$$M_g = f_1(D_g, \theta) \quad (13)$$

$$D_g = f_2(M_{go}, T, M_{ge}) \quad (14)$$

where M_k , M_g , D_g , θ , M_{go} , T , and M_{ge} , respectively, are moisture content of kernel, decimal, dry basis (d.b.), moisture content of grain, decimal, d.b.; moisture diffusivity of grain, $m^2 \text{ min}^{-1}$; roasting time, min; initial moisture content of grain, fraction, db; roasting pan temperature, °C; and equilibrium moisture content of grain, decimal, db.

Substituting Eqs. (13) and (14) in Eq. (12), the final functions for M_k can be written as

$$M_k = f[f_1\{f_2(M_{go}, T, M_{ge})\}, \theta] \quad (15)$$

Expressions for D_g , M_g and M_k assuming equilibrium moisture content of the grain at high-temperature conduction roasting, as zero (Jha, 1993; Jha & Prasad, 1993a) can be written as

$$D_g = D_o + D_1 M_{go} + D_2 T + D_3 M_{go}^2 + D_4 M_{go} T \quad (16)$$

$$M_g = M_{go} C_1 \exp(-C_2 \theta) \quad (17)$$

$$M_k = C_3 M_g - C_4 \quad (18)$$

in which $C_2 = \frac{D_g \pi^2}{R^2}$, where D_o , D_1 , D_2 , D_3 , D_4 , C_1 , C_2 , C_3 , C_4 , are constants given in Table 1, and R is the radius of the grain, m.

Putting the expression for M_g from Eq. (17) into Eq. (18)

$$M_k = C_1 C_3 M_{go} \exp(-C_2 \theta) - C_4 \quad (19)$$

The rate of moisture transfer from the kernel could be written as

$$\frac{dM_k}{d\theta} = -C_1 C_2 C_3 M_{go} \exp(-C_2 \theta) \quad (20)$$

2.4. Heat transfer

Heat input to the kernel from the shell by conduction, neglecting the convection and radiation loss and heat transfer through the point contact, can be written as

$$q_{in} = 4\pi k_v R_g R_k \left(\frac{T_w - T_k}{R_g - R_k} \right) \quad (21)$$

where q_{in} , k_v , R_g , R_k , T_w , and T_k , respectively are heat input to the kernel, kJ min^{-1} ; thermal conductivity of air–water vapor mixture, $\text{kJ min}^{-1} \text{ m}^{-1} \text{ }^\circ\text{C}^{-1}$; radius of kernel plus gap between the kernel and shell, if any, m; radius of kernel, m; shell wall and kernel temperature, °C at any time θ , min.

The heat accumulated in the kernel

$$q_{ac} = C_{pk} W_{kd} (1 + M_k) \frac{dT_k}{d\theta} \quad (22)$$

Table 1
Roasting conditions and properties of gorgon nut used in validation of model

Radius of grain, R_g	4.5 mm
Shell thickness, t	1 mm
Gap between shell and kernel, g	0.2 mm
Poisson's ratio, ν	0.3
Modulus of elasticity, E	703×10^6 Pa
Coefficient of linear thermal expansion, α	$3.88 \times 10^{-4} \text{ } ^\circ\text{C}^{-1}$
Coefficient of linear moisture contraction, β	0.0152
Coefficient of volume thermal expansion, γ	$10.15 \times 10^{-4} \text{ } ^\circ\text{C}^{-1}$
Coefficient of volume moisture contraction, γ_c	0.0603
Initial moisture content of grain (gorgon nut), M_{go}	25.9% dry basis
Initial surface temperature of grain, T_{wo}	30 $^\circ\text{C}$
Final surface temperature of grain, T_w	213 $^\circ\text{C}$
Initial mass of a single grain, W_{go}	4.585×10^{-4} kg
Initial moisture content of kernel, M_{ko}	33.4% (db)
Initial moisture content of shell, M_{so}	5% (db)
Final moisture content of shell, M_s	2% (db)
Latent heat of vaporization of moisture from kernel, L_k	2175.7 kJ kg $^{-1}$
Specific heat of kernel, C_{pk}	2.015 kJ/kg $^\circ\text{C}^{-1}$
Thermal conductivity of vapor, k_v	$1.41 \text{ J m}^{-1} \text{ min}^{-1} \text{ } ^\circ\text{C}^{-1}$
Ratio δ	0.513
Normal atmospheric pressure, P_o	101.3 kPa
Normal temperature, T_o	303.15 K
C_1	0.979
C_3	1.357
C_4	0.75

where q_{ac} , C_{pk} , W_{kd} are heat accumulated in kernel, kJ min $^{-1}$; specific heat of kernel, kJ kg $^{-1}$ $^\circ\text{C}^{-1}$; and bone dried mass of kernel, kg, respectively.

The heat utilized for vaporization of moisture

$$q_{out} = -L_k W_{kd} \frac{dM_k}{d\theta} \quad (23)$$

where q_{out} and L_k , are heat utilized in vaporization of moisture of kernel; kJ min $^{-1}$ and latent heat of vaporization of moisture of the same, kJ kg $^{-1}$, respectively.

Now,

$$q_{ac} = q_{in} - q_{out} \quad (24)$$

On substituting the Eqs. (21)–(23) into Eq. (24) and rearranging the terms

$$\frac{dT_k}{d\theta} = \frac{4\pi k_v R_g R_k (T_w - T_k)}{C_{pk} W_k (R_g - R_k)} + \left(\frac{L_k}{C_{pk} (1 + M_k)} \right) \frac{dM_k}{d\theta}$$

Let $\frac{W_{sd}}{W_{gd}} = \delta_1$ then

$$W_k = W_{gd} [1 + M_g - \delta_1 (1 + M_s)]$$

where W_{sd} , W_{gd} , W_k , and M_s are bone dried mass of shell, kg; bone dried mass of whole grain, kg; mass of kernel, kg; and moisture content of shell, fraction, db; respectively.

Expressing the mass of the kernel in terms of the mass of grain and rearranging the terms in the above equa-

tion, the simplified form of heat transfer equation can be written as

$$\frac{dT_k}{d\theta} = A(T_w - T_k) + B \frac{dM_k}{d\theta} \quad (25)$$

where

$$A = \frac{4\pi k_v R_g R_k (1 + M_{go})}{C_{pk} W_{gd} \{ (1 + M_g) - \delta_1 (1 + M_s) \} (R_g - R_k)}$$

$$B = \frac{L_k}{C_{pk} (1 + M_k)}$$

If $T_w - T_k = T$, $\frac{dT}{d\theta} = -\frac{dT_k}{d\theta}$ and using the expression for $\frac{dM_k}{d\theta}$ from Eq. (20), Eq. (25) can be written as

$$\frac{dT}{d\theta} + AT = C \quad (26)$$

where

$$C = B_1 \exp(-C_2 \theta)$$

$$B_1 = BC_1 C_2 C_3 M_{go} \exp(-C_2 \theta)$$

Eq. (26) is first-order differential equation with boundary (initial) conditions $\theta = 0$, $T = T_{ko}$ the solution is (Agnew, 1960)

$$T_k = T_w - \frac{B_1 [\exp(-C_2 \theta) - \exp(-A\theta)]}{A - C_2} - (T_w - T_{ko}) \exp(-A\theta) \quad (27)$$

From Eqs. (19) and (27) the moisture content and temperature of the kernel respectively could be obtained at different time interval during roasting.

Now change in volume of the kernel due to change in moisture and temperature can be written as

$$\Delta V_k = V_k [\gamma (T_k - T_{ko}) - \gamma_c (M_{ko} - M_k)] \quad (28)$$

where γ and γ_c are coefficients of volume expansion and contraction due to change in temperature and moisture of the kernel, respectively.

2.5. Change in volume of air–water vapor mixture, ΔV_a

Let P_o , V_o , T_o and m respectively be the initial pressure, Pa; volume, m 3 ; absolute temperature, K; and mass of the air–water vapor mixture, kg; in the gap under ambient conditions. Assuming the shell of grain impermeable to the air–water vapor mixture for the short period of roasting, the changes in pressure, volume, temperature and mass during roasting period of θ be p , ΔV , ΔT , and Δm , respectively.

If the air–water vapor mixture obeys the ideal gas law, it can be written for ambient condition as (Shvets, Tolubonsky, Kivakovsky, Neduzhy, & Sheludko, 1987):

$$P_o V_o = m G_o T_o \quad (29)$$

and after elapsed time θ

$$(P_o + p)(V_o + \Delta V) = (m + \Delta m) G_1 (T_o + \Delta T) \quad (30)$$

where G_o and G_1 are gas constants, $\text{J kg}^{-1} \text{K}^{-1}$; at initial conditions and after time θ , respectively.

Dividing Eq. (30) by Eq. (29)

$$\frac{T_o(P_o + p)(V_o + \Delta V)}{(T_o + \Delta T)P_oV_o} = \frac{G_1(m + \Delta m)}{G_o m}$$

As $\Delta V = \Delta V_a$ and $V_o = V_a$

$$\Delta V_a = V_a \left(\frac{G_1 P_o (M + \Delta m) (T_o + \Delta T)}{G_o m T_o (P_o + p)} - 1 \right) \quad (31)$$

Let the volume of the air–water vapor gap V_a be a fraction of δ of the total enclosed initial volume of the shell, V_s

$$\text{therefore } V_a = \delta V_s \quad (32)$$

and

$$V_k = (1 - \delta)V_s \quad (33)$$

Now substituting the expressions for ΔV_s , ΔV_k and ΔV_a from the Eqs. (11), (28) and (31) respectively in Eq. (2) and replacing V_a and V_k by Eqs. (32) and (33) respectively in the above equation and rearranging the terms,

$$\begin{aligned} 3pR_s \frac{(1 - v)}{2tE} - \frac{\delta G_1 P_o (m + \Delta m) (T_o + \Delta T)}{G_o m T_o (P_o + p)} \\ = (1 - \delta) [\gamma (T_k - T_{ko}) - \gamma_c (M_{ko} - M_k)] \\ - 3(\alpha \Delta T_s - \beta \Delta M_s) - \delta \end{aligned}$$

Assuming the right hand side of the above equation equal to X and rearranging the terms, simplified equation can be written as

$$\begin{aligned} 3R_s m G_o T_o (1 - v) p^2 + G_o T_o m [3R_s P_o (1 - v) - 2tEX] p \\ - 2tEP_o [\delta G_1 (m + \Delta m) (T_o + \Delta T) + G_o m T_o X] = 0 \end{aligned} \quad (34)$$

Eq. (34) is in a quadratic form of p which can be solved for any time θ .

3. Materials and methods

3.1. Solution of model

A grain, known as gorgon nut (*Euryale ferox*), representing fully assumed generalized model (Fig. 1), was taken as an example. A material surface temperature of 213°C , when the nut was roasted at a pan temperature of 335°C for the highest percentage of popping (Jha & Prasad, 1996) was taken as a point of prediction. Properties and processing conditions reported elsewhere (Jha, 1993; Jha & Prasad, 1993a,b, 1996) were used. Some other basic data required for solution of the model were determined separately (Table 1) and a computer program for knowing moisture content of whole nut and kernel, change in volume of the nut and pressure built up within the nut during roasting, was developed.

3.2. Measurement of change in volume and moisture

Ninety medium size (8–10 mm diameter) conditioned nuts of known moisture content (29.9%) and diameter were randomly selected for measurement of change in volume and moisture of the nut during roasting. Different groups of three nuts were made and numbered. All nuts of each group were roasted together for a specified time period, ranging from 0.5 to 5 min at 0.5 min interval, in a cast iron pan at 335°C surface temperature. Electric heater of 1.5 kW or gas burner was used as heat source. The pan temperature was measured by means of a mercury thermometer of range $0\text{--}500^\circ\text{C}$ with 1°C graduations. The accuracy of temperature measurement was later verified by fixing an iron–constantan (J type) thermocouple to the pan surface and measuring temperature connected to a digital temperature indicator. Conditioning of the nut was carried out following the procedure suggested in literature (Jha & Prasad, 1996). The diameter and outer wall temperature of each nut (out of three being roasted) immediately after end of pre-decided roasting time were measured using a vernier caliper having the least count of 0.001 mm and probe-type temperature indicator with least count of $\pm 1^\circ\text{C}$, respectively. The change in volume of nut with respect to initial one was computed. Moisture contents of another whole nut and kernel, obtained decorticating the third nut, were determined using air oven method (Hall, 1970). The experiment was replicated three times using different sets of sample and the average values are reported.

4. Results and discussion

4.1. Validation of model

Accuracy of prediction of model was determined comparing the predicted values with the measured ones. As measurement of pressure developed within the moving nut during roasting was not possible, accuracy of its predicted values was assumed to be that of moisture content and change in volume of the nut.

Internal pressure predicted in the nut during roasting increased rapidly in the beginning, and later its rate of increase declined (Fig. 3). This may be due to higher rate of moisture migration from the kernel and temperature rise at the initial stage and accumulation of the former in the gap between the shell and the kernel. The pressure built up within the nut at 2.8 min, optimum roasting time reported in literature (Jha & Prasad, 1996), and 213°C nut temperature was found to be about 45 MPa. The high rate and magnitude of pressure built up within the nut revealed that the hard grain like this nut could burst on its own during roasting. It may cause injuries to the nearby persons and also produces inferior quality of

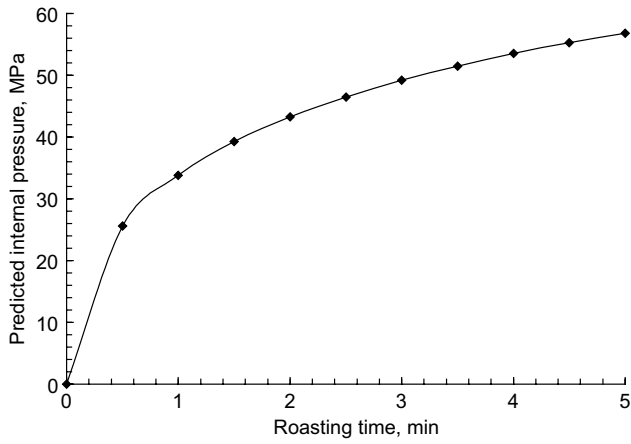


Fig. 3. Predicted internal pressure in gorgon nut during roasting.

popped kernel. The experiments conducted to measure the change in volume of the nut showed bursting of few nuts even at about 2.5 min of roasting and yielded fractured and distorted popped kernel. It suggested that the nut should be hit externally before 2.8 min to avoid the self-bursting for better quality popped kernel, which is in agreement with the reported optimum roasting conditions for this nut (Jha & Prasad, 1996).

The measurement of pressure built up within the nut during roasting was neither possible nor reported in the literature for any grain as far as direct validation is concerned. The predicted and measured values of change in volume of the gorgon nut, which is very much dependent on internal pressure, were thus compared (Fig. 4). Variation between predicted and measured values was found to be high (24–136%) till 1 min of roasting (Fig. 5). The large variation at initial stage could be due to the assumptions made that the shell of the nut is impervious and attains an equilibrium temperature almost immediately at high-temperature roasting, which may not be completely valid in the real situation. In addition, use of ordinary differential equation instead of partial differential equation in the model may be causing this initial variation. The maximum variation between the

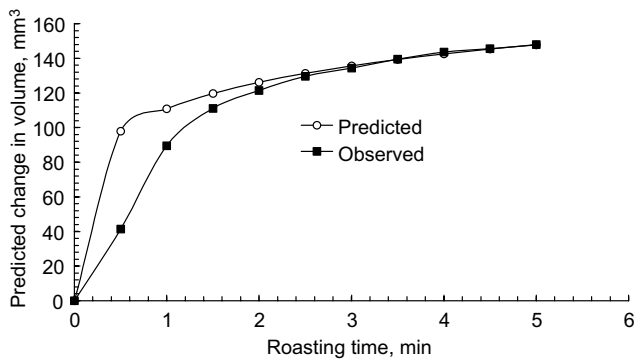


Fig. 4. Observed and predicted change in volume of whole gorgon nut during roasting.

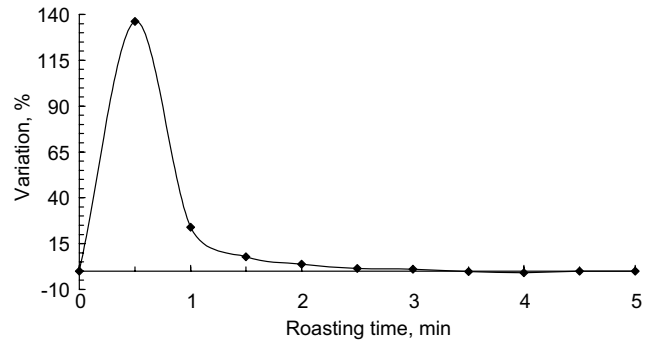


Fig. 5. Variation between predicted and observed volume of gorgon nut during roasting.

observed and predicted values after 1 min however was within 8%, and is only about 0.1% beyond 2.8 min of roasting which suggests that the model could be used well for the purpose beyond 1 min of roasting time of the gorgon nut.

Internal pressure built up within the nut during roasting is also very much dependent on moisture content of the nut during roasting. Scatter plots of measured versus predicted moisture content of whole gorgon nut and its kernel are presented in Figs. 6 and 7 for entire period of roasting. Slopes and correlation coefficients of curves are very near to 1. The small intercepts in the regression equation show little deviation from the real values, which is negligible as compared to its initial moisture content of 25.9% and 33.4% of whole nut and kernel, respectively. The moisture content of about 14% predicted by the model for the best time of popping (2.8 min of roasting) is also in agreement with the reported values for maximum expansion ratio of popcorn (Gokmen, 2004). Prediction of moisture by this model is also better than that by models available for drying (Young, 1969) and roasting (Das & Srivastav, 1993) and one thus may use it to regulate the internal pressure in the grain to avoid unregulated self-bursting during roasting to get a popped kernel of regular shape,

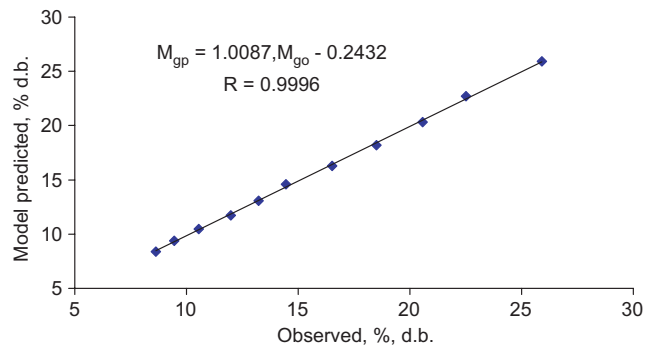


Fig. 6. Observed and predicted moisture content of whole gorgon nut during roasting: M_{gp} , predicted moisture content; M_{go} , observed moisture content; R , regression correlation coefficient.

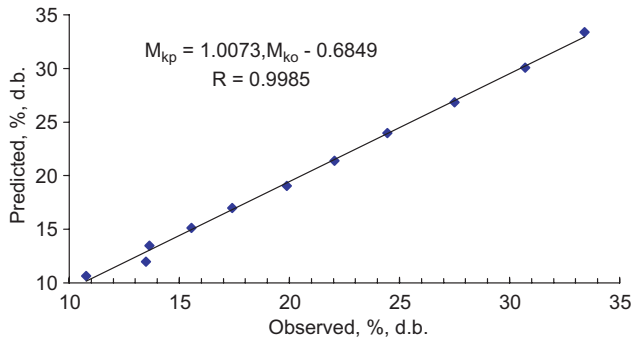


Fig. 7. Observed and predicted moisture content of kernel during roasting: M_{kp} , predicted kernel moisture; M_{ko} , observed kernel moisture; R , correlation coefficient.

uniform size and prevent injury to nearby person by minimizing jumping of grain from the roasting pan.

5. Conclusions

The internal pressure predicted within the selected grain at 335 °C pan temperature and 2.8 min of roasting time was found to be about 45 MPa and it increased rapidly in the beginning of roasting. This pressure was though not get verified directly but its associated parameters such as moisture content of whole nut and its kernel and change in volume during roasting were found to be predicted very closely to the measured values, except change in volume till 1 min of roasting. In later stage of roasting variations between the predicted and measured values of all parameters were negligible and thus the model appears to be adequate for prediction.

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