Journal of Engineering and Applied Sciences 12 (Special Issue 3): 6600-6605, 2017
ISSN: 1816-949X

Mathematical Modeling of Food Graining Roasting Process by High Temperature Heat Agent

A.N. Ostrikov, E.Z. Mateyev, A.A. Shevtsov and L.I. Lytkina
Voronezh State University of Engineering Technologies, 1 University Square,
394006 Voronezh, Russia

Abtract: A mathematical model of food raw materials roasting (evidence from grains of coffee "Arabica") using a superheated steam as a high temperature heat agent in a form of a system of differential equations, describing heat conductivity, mass conductivity and decomposition products building-up is developed. The resulting model describes the change in the temperature and moisture fields in terms of roasted product bed height.

Key words: Mathematical model, roasting, kinetics, coffee beans, superheated steam, temperature

INTRODUCTION

Food plant materials (grain crops, barley, safflower, coffee beans, chicory, acorns, chestnuts, etc.) roasting process technological parameters behavior defines the quality parameters of finished product which are the result of biochemical, physical and colloid-chemical changes during heat treatment of grain crops (Bottazzi *et al*., 2012).

The lack of reliable kinetic dependences describing grain roasting process, affects the quality of the finished product, creates additional technological difficulties in adherence to roasting modes and complicates achieving the required quality of the finished product.

Analyzing the grain temperature behavior and its influence on the roasting intensity (Stepanov and Tatarchenko, 2009) observed that heating rate of coffee beans is far ahead of change rate of moisture content, limited by moisture internal diffusion in beans. In this regard in order to stabilize the temperature fields of moisture content and physicochemical changes in coffee beans Stepanov and Tatarchenko (Burmester and Eggers, 2010) proposed to carry out a two-fold hydration: in the middle and at the end of roasting which allow to receive the coffee with final moisture content of 4-7% and achieve greater plasticity of its beans.

In the researches by Hashim and Chaveron (1995) as well as (Zimmerman *et al*., 1996) it is proposed to determine the end of the process by the content of certain chemical substances.

Porto *et al*. (1991) and Schenker (2000) considered two modes of roasting. The first at heat agent (hot gas) temperature of 220°C and duration of 9-12 min; the second at 260°C and duration of 2.6-3 min. In the first case, the roasting temperature and other parameters are a function of the process duration: the temperature continuously grows from 20-190°C for 2 min which is 90% of the total temperature increase. In the second case, the main weight loss occurs during the first minute (75%); beans were heated to 180°C.

Feng and Michaelides (2000) proposed a dimensionless equation using the Nusselt, Reynolds and Peclet criteria of to describe the heat transfer between the spherical body and the air flow, achieving high reproducibility.

The resulting equation was applied by Dhole *et al*. (2006) and a comparative analysis with other dependencies was conducted. Burmester and Eggers (2010) and Shevtsov and Ostrikova (2011) their research demonstrated that the approach, close to one developed by Feng and Michaelides (2000) can be applied to coffee beans.

Schwartzberg (20002) presented a model that describes the heat transfer between hot air and coffee beans as well as between metal parts of the device and hot air flow. The model also describes moisture evaporation through the semi-empirical equations.

The mathematical model proposed by Bottazzi (2012) is based on the approach using distributed and lumped parameters. It describes the behavior of space-distributed physical systems as a grid of discrete objects that approximate the distributed system behavior.

Hernandez *et al*. (2007) found that the area of contact between the product particles is low due to its geometrical shape. Thermal energy, transferred from the hot air flow to coffee beans is described by Eq. 1:

Corresponding Author: E.Z. Mateyev, Voronezh State University of Engineering Technologies, 1 University Square, 394006 Voronezh, Russia

$$\dot{Q}_b = \lambda F\left(T_{air}-T_b\right) \quad (1)$$

The temperature of the coffee beans is determined from the heat balance:

$$\frac{dT_b}{dt} = \frac{\dot{Q}_b+\left(\dot{Q}_d+m_{roa}\,v\left(dW_b/dt\right)\right)}{m_{roa}\left(1+W_b\right)c_b} \quad (2)$$

Exothermic heat release during the roasting process is determined by the expression proposed by Schwartzberg (2002):

$$\dot{Q}_d = m_{roa}\,A_{exp}\left[-\frac{E_\alpha}{R\,T_b}\right]\left(\frac{i_{tot}-i}{i_{tot}}\right) \quad (3)$$

He also suggested an equation describing the evaporation of water from coffee beans during the roasting process and which accounts for the moisture in the physicochemical reaction:

$$\frac{dW_b}{dt} = -\frac{4.32\times10^9\times W_b^2}{d_b^2}\times\exp\left(\frac{-9889}{T_b}\right) \quad (4)$$

MATERIALS AND METHODS

Subjects and methods of the study: In the course of development of mathematical model of food raw material roasting process coffee beans “Arabica” were selected as the subject of study and superheated steam was chosen as a high temperature heat agent. In the process of roasting coffee beans “Arabica” undergo significant physical and chemical changes that result to peculiar coffee taste and flavor. Due to the moisture evaporation from beans and decomposition of sugars, fiber and other organic compounds because of the high temperature their mass decreases and the amount of fumes (mixture of evaporated moisture and non-condensable gases) reaches 20%. Fumes result from biochemical, physical and colloid-chemical changes during heat treatment of raw coffee beans.

To predict the output of finished products it is necessary to know the amount of the resulting gaseous products of thermal decomposition. Therefore, as the characteristics of coffee beans components it is suggested to assign their bulk concentrations.

Let us, set the volume concentrations of components: C_1 the concentration of moisture (wet phase of the substance); C_2 the concentration of solids thermal decomposition products in coffee beans; C_3 the concentration of solids (dry matter phase). As the components $C_{1\text{-}3}$, represent the mass of 1 m^3 then the beans density in the beginning of the roasting process can be represented as Eq. 5:

$$\rho_0 = C'_{1H}+C'_{2H}+C'_{3H} \quad (5)$$

Then at any given time for the coffee beans density, (kg/m^3), the equality:

$$\rho(t) = \rho_0-\Delta C'_1(t)-\Delta C'_2(t) \quad (6)$$

The formation of non-condensable gases as a result of chemical reactions is accompanied by changes in the substances concentration in the dry part of coffee beans.

To model the coffee beans solids thermal decomposition process during the roasting quadratic logistic function was used (Burmester and Eggers, 2010).

$$\frac{\partial C_2}{\partial\tau} = \frac{\partial}{\partial T}\left(\frac{K_s}{\left(1+A_s\times e^{-B_S(T-T_0)}\right)^2}\right)\frac{\partial T}{\partial t} = \frac{K_sA_sB_s\times e^{-B_S(T-T_0)}}{1+A_s\times e^{-B_S(T-T_0)3}}\times\frac{\partial T}{\partial t} \quad (7)$$

Thus, the change in concentration of non-condensables in coffee beans can be specified by Eq. 5 and depends on the variation of the material dry substance density which occurs as a result of chemical reactions (thermal decomposition) under the temperature influence.

We split the transient process in zones. Within each zone we set as a constant heat and substance transfer coefficients and then the equations describing the roasting process can be represented in a spherical coordinate system as follows, heat equation:

$$c\rho_0\frac{\partial T}{\partial\tau} = \lambda\left[\frac{\partial_2 T}{\partial r^2}+\frac{2\partial T}{r\partial r}\right]+q_c+q_p,\; 0<r<R(\tau),\tau>0,\; R(0)=R_0 \quad (8)$$

Moisture transfer equation in the volume of coffee beans:

$$\frac{\partial C_1}{\partial\tau} = a'_m\left[\frac{\partial^2 C_1}{\partial r^2}+\frac{2\partial C_1}{r\partial r}\right] \quad (9)$$

Equation describing the rate of heat consumption during coffee beans solids thermal decomposition:

$$\frac{\partial C_2}{\partial \tau} = f(T)\frac{\partial T}{\partial \tau} \tag{10}$$

where, $f(T) = \frac{K_s A_s B_s \cdot e^{-B_s(T-T_0)}}{(1+A_s \cdot e^{-B_s(T-T_0)})^3}$ is a derivative of the quadratic logistic $F(T) = \frac{K_s}{(1+A_s \cdot e^{-B_s(T-T_0)})^2}$ function.

Initial conditions:

$$T(r,\tau)\big|_{\tau=0} = T_i \tag{11}$$

$$C_1(r,\tau)\big|_{\tau=0} = C_{1i} \tag{12}$$

$$C_2(r,\tau)\big|_{\tau=0} = C_{2i} \tag{13}$$

The boundary condition of the third kind for the heat equation:

$$-\lambda \frac{\partial T}{\partial r}\bigg|_{r=R(\tau)} = \alpha\left(T_n - T_c\right) \tag{14}$$

The boundary condition of the third kind for the equation of moisture transfer:

$$-a_m \frac{\partial C_1}{\partial r}\bigg|_{r=R(\tau)} = \beta\left(C_n\text{-}C_p\right) \tag{15}$$

Symmetry conditions:

$$\frac{\partial C(0,\tau)}{\partial r} = \frac{\partial T(0,\tau)}{\partial r} = 0 \tag{16}$$

where, R (τ) is a function characterizing the variation of coffee beans volume (volumetric shrinkage) during roasting q_c is a specific heat release rate of the moisture phase transition:

$$q_c = \varepsilon r_u W_c \tag{17}$$

Where:

$W_c = \partial C_1/\partial \tau$ = A moisture removal rate

q_c = A specific heat release rate of the coffee beans solids thermal decomposition

$$q_d = Q_d W_d \tag{18}$$

The dimensionless form of system of Eq. 8 and 16 will be as follows heat equation:

$$\frac{\partial \theta}{\partial Fo} = \frac{\partial^2 \theta}{\partial z^2} + \frac{2\partial \theta}{z \partial z} + k_1 \frac{\partial \overline{C}_1}{\partial Fo} + k_2 \frac{\partial \overline{C}_2}{\partial Fo} \tag{19}$$

Moisture transfer equation in the volume of coffee beans:

$$\frac{1}{Lu}\frac{\partial \overline{C}_1}{\partial Fo} = \frac{\partial^2 \overline{C}_1}{\partial z^2} + \frac{2\partial \overline{C}_1}{z \partial z} \tag{20}$$

The equation of formation of non-condensable substances in the solids thermochemical decomposition:

$$\frac{\partial \overline{C}_2}{\partial Fo} = k_3 \times f(\overline{T} \times T_i)\frac{\partial \overline{T}}{\partial Fo} \tag{21}$$

Initial conditions:

$$\theta\big|_{Fo=0} = 1;\ \overline{C}_1\big|_{Fo=0} = 1;\ \overline{C}_2\big|_{Fo=0} = 0 \tag{22}$$

Border conditions:

$$-\frac{\partial \theta}{\partial z}\bigg|_{z=1} = Bi \times \left(\theta_s - \theta_f\right);\quad -\frac{\partial \overline{C}_1}{\partial z}\bigg|_{z=1} = Bi_m \times \left(\overline{C}_s - \overline{C}_f\right) \tag{23}$$

Symmetry conditions:

$$\frac{\partial \theta}{\partial z}\bigg|_{z=0} = \frac{\partial \overline{C}_1}{\partial z}\bigg|_{z=0} = 0$$

Thus, the system of Eq. 19-24 provides a fields distribution of temperature, distributed moisture concentration and formation of non-condensable substances concentration during the thermal decomposition of solids at a certain interval of time. $\Delta_m = \tau_{m+1}\text{-}\tau_m$. Splitting the entire period of the roasting process in the intervals $\Delta_m, m = \overline{i, k-1}$ (τ_1 = 0 is the beginning of the roasting process; τ_k is the end of roasting process; k is the number of grid points here the variable k coincides with the variable τ_k index) and performing calculations by the model Eq. 7-24 allows to get a full understanding of the process on the interval from 0 to τ_k.

To simplify the calculations and make a representation of the finite-difference scheme of coffee beans roasting model implementation more compact, we introduce the following designations, $t = Fo, C_1 = C_1, \overline{C}_2 = \overline{C}_2$.

For the numerical implementation of the coffee beans roasting process, model we use a grid method. Area: $G = (0 \le z \le 1, 0 \le t \le t^*)$ where a solution by grid is to be found is a discrete set of points in a plane (t, θ):

$$(t^n, z_m),\ t^n = t_0 + n\Delta t,\ z_m = z_0 + m\Delta z \tag{25}$$

where, Δ_t, Δ_z are positive values, called step grid by t, z respectively m, n are integers t^e is a number corresponding to the end of the system (Eq. 19-24) integration process, t^e = Fo (t*), t* coffee beans roasting time. According to the grid method we replace the functions $\theta(t,z), \bar{C}_1(t,z), \bar{C}_2(t,z)$ in the G area by grid functions:

$$\theta_m^n = \theta(t_m^n, z_m^n),\ C1_m^n = C1(t_m^n, z_m^n),\ C2_m^n = C2(t_m^n, z_m^n) \quad (26)$$

Defined in the grid nodes (Eq. 25) using the diagram. The set of nodes corresponding to the fixed value n, defines the bed where the grid functions are determined. Along with the designations Δ_t, Δ_z we use designations $\tau\Delta_t$, $h = \Delta_z$.

For Eq. 19-24, we draw the approximation implicit scheme having a second order of accuracy in relation to (τ, z), i.e., O (τ^2)+O (h^2) for the second derivatives with respect to space variable: for the heat equation:

$$\theta_j^{n+1} - \theta_j^n = \tau\left(0.5\cdot\frac{\theta_{j+1}^{n+1} - 2\theta_j^{n+1} + \theta_{j-1}^{n+1}}{h^2} + 0.5\times\frac{\theta_{j+1}^n - 2\theta_j^n + \theta_{j-1}^n}{h^2}\right) + \frac{2\tau}{z_j}\left(\frac{\theta_{j+1}^n - \theta_{j-1}^n}{2h}\right) + k_1(C1_j^{n+1} - C1_j^n) + k_1(C2_j^{n+1} - C2_j^n); \quad (27)$$

For the equation of moisture transfer in the volume of coffee beans:

$$C1_j^{n+1} - C1_j^n = \tau Lu\left(0.5\times\frac{C1_{j+1}^{n+1} - 2C1_j^{n+1} + C1_{j-1}^{n+1}}{h^2} + 0.5\times\frac{C1_{j+1}^n - 2C1_j^n + C1_{j-1}^n}{h^2}\right) + \frac{2\tau Lu}{z_j}\left(\frac{C1_{j+1}^n - C1_{j-1}^n}{2h}\right) \quad (28)$$

For the carry-over equation of non-condensable substances formed by the solids thermal decomposition:

$$C2_j^{n+1} - C2_j^n = k_3\times f(\theta\times T_i)(\theta_j^{n+1} - \theta_j^n) \quad (29)$$

For the boundary conditions (Eq. 28):

$$-\frac{\theta_T^{n+1} - \theta_{m-2}^{n+1}}{2h} = Bi\left(\theta_m^n - \theta_c\right) \quad (30)$$

$$-\frac{C1_m^{n+1} - C1_{m-2}^{n+1}}{2h} = Bi_m\times\left(C1_m^n - C1_p\right) \quad (31)$$

For the symmetry conditions (Eq. 28):

$$\frac{\theta_3^{n+1} - \theta_1^{n+1}}{2h} = 0 \text{ or } \theta_3^{n+1} = \theta_1^{n+1} \quad (32)$$

For a solution of the system (Eq. 27-33), the following initial conditions are adopted: temperature and moisture content at the beginning of the process are distributed uniformly; no substances are formed in coffee beans, i.e.:

$$\frac{C1_3^{n+1} - C1_1^{n+1}}{2h} = 0 \text{ or } C1_3^{n+1} = C1_1^{n+1} \quad (33)$$

Using the grid approximations (Eq. 27-34), the algorithm of resolving linear equations system formation for determination of the grid functions values for the bed n+1 can be represented as performing the following sequence of steps. Preliminary we note that the dimension of resolving linear equations system AX = B equals to M = 3 m.

The program, implementing coffee beans roasting process in the environment of superheated steam is developed in C# in the IDE Microsoft Visual Studio 2013 and implemented on a PC with a processor intel core i5-4570 in the environment Windows 8.

Arabica coffee beans thermal and physical characteristics c, a and λ in the drying process are being reduced (Bottazzi *et al*., 2012). The true values of the coefficients c and λ during the heat treatment vary slightly.

The equivalent thermal and physical characteristics vary significantly because they are significantly affected by the heat of the phase transition. The moisture diffusion coefficient a_m for a wide range of food products takes values $0.64\cdot10^{-8}$, … , $0.222\cdot10^{-8}$ m²/sec.

Arrhenius law sets the rate of non-condensable substances formation during thermal decomposition of coffee beans solids. Arrhenius law is described by an exponential law, according to which the formation rate of thermal decomposition products increases monotonically with increasing temperature of the product.

The pre-exponential factor characterizes the speed limit of non-condensable gases formation rate which in the limit case should be equal to zero.

To modulate the process of thermal coffee beans solids decomposition during the roasting logistic quadratic function is used which is set by Eq. 35:

$$F(T) = \frac{k}{(1 + a\times\exp(-b(T-T_0)))^2} \quad (35)$$

Approximation was performed by Software Math CAD Prime 3.0. The parameters of the logistic function: $k = 22; \alpha = 8.670557.10^9 : b = 0.071614$. To calculate the values of the heat and mass transfer coefficients of roasting proc ess criteria equations were used (Bottazzi *et al*., 2012):

$$Nu_q = 0.05 \cdot Re^{0.8}(T_c/T_s)^{-0.5} \quad (36)$$

$$Nu_m = 0.0086 \cdot Re^{0.8}(T_c/T_s)^{-0.5} \quad (37)$$

RESULTS AND DISCUSSION

As a result of modulation using the developed program the possibility of using the criteria equations to determine the of heat and mass transfer coefficients: heat transfer coefficient α and β mass transfer coefficient.

According to a comparative analysis of the calculated and experimental data approximation it was found that the deviation of the absolute value does not exceed 3.5% for the temperature and 11.0% for moisture content.

Thus, the results of modeling with sufficient for engineering calculations accuracy reflect the kinetic regularities of the coffee beans roasting s process by superheated steam as an object with distributed parameters and can be used to analyze occurring physicochemical changes, process calculation, roasters design and development of program-logical algorithms of technological parameters control.

CONCLUSION

The mathematical model of coffee beans roasting in a superheated steam environment as a system of partial differential equations that describes the processes of heat conductivity, mass conductivity and thermal decomposition products formation is developed. S-shaped logistic function was used as the equation describing thermal decomposition process. It is established, that intensity of coffee beans roasting process is determined by the superheated steam temperature.

NOMENCLATURE

F = Heat exchange surface between the flow of heat agent (superheated steam) and coffee beans (m^2)

T_{air} = Temperature of the incoming flow of heat agent (superheated steam) (K)

T_b = Temperature of the coffee beans (K)

Q_b = Thermal energy released by the reactions occurring during roasting (W)

m_{roa} = Mass of roasted coffee (kg)

v = Latent heat of vaporization and desorption of moisture from coffee (kJ/kg)

W_b = Moisture content of coffee beans fraction

t = time (sec)

C_b = Specific heat of the coffee beans (J/(kg K))

A = Pre-exponential arrhenius factor (kJ/(kg sec))

E_a = Activation energy (kJ)

i_{tot} = Total enthalpy of reactions during roasting (kJ/kg)

I = Cumulative enthalpy of reactions during roasting (kJ/kg)

d_b = Grain diameter (m)

$\Delta c_i(\tau) = -C_{ii}-C_i(\tau)$ = Concentration of the moisture being removed from coffee beans at a point of time (τ)

$\Delta C_2(\tau) = C_2(\tau)-C_{2i} = C_2(\tau)$ = Concentration of solids thermal decomposition products in coffee beans being removed

$W_d = \partial C_2/\partial_\tau$ = Formation rate of non-condensable substances

Q_d = Thermal effect characterizing non-condensables formation process during the solids thermal decomposition (kJ/kg)

$Nu_q = \alpha R_H/\lambda$ = Heat transfer Nusselt number

$Nu_q = \beta R_H/\alpha_m$ = Mass transfer Nusselt number (Re = R_2^H)

$\rho_n \upsilon/\mu$ = Reynolds number

(T_c/T_s) = Temperature simplex

T_c, T_s = Temperature of superheated steam at the flow center of the and product surface temperature

r = Current radius of the coffee beans particle (m)

τ = Current time of coffee beans roasting (sec)

C_1, C_{1i}, C_s, C_f = Concentration of the dispensed substance moisture in the bulk of coffee beans, initial one, at the surface and in superheated steam flow, respectively, kg/kg (with superheated steam roasting it is set ($C_f = 0$))

C_2, C_{2i} = Concentration of non-condensables during coffee beans solids thermal decomposition in the bulk of coffee beans and initial one, respectively, kg/kg ($C_{2i} = 0$)

T, T_H, T_s, T_f = Body temperature in the bulk of the coffee beans, initial one, at the surface and in a superheated steam flow

K; λ = Thermal conductivity of product (W/(m.K))

α = Heat transfer coefficient (m/sec)

$a'_m = a_m/(1-\varepsilon)$ = Equivalent coefficient of product moisture conductivity (m^2/sec)

a_m = Moisture conductivity coefficient of the product (m^2/sce)

β = Moisture transfer coefficient (m/sec)

ρ = Density of coffee beans absolutely dry substance kg of (DS/m^3)

k_0 = Pre-exponential factor characterizing the probability of interaction between the molecules of substances whose energy is sufficient to perform thermal conversion (1/sec)

r_u = Heat of phase transition (specific heat of vaporization) (kJ/kg)

K_s, A_s, B_s = Coefficients of quadratic logistic function

ε = Phase transition criterion

REFERENCES

Bottazzi, D., S. Farina, M. Milani and L. Montorsi, 2012. A numerical approach for the analysis of the coffee roasting process. J. Food Eng., 112: 243-252.

Burmester, K. and R. Eggers, 2010. Heat and mass transfer during the coffee drying process. J. Food Eng., 99: 430-436.

Dhole, S.D., R.P. Chhabra and V. Eswaran, 2006. A numerical study on the forced convection heat transfer from an isothermal and isoflux sphere in the steady symmetric flow regime. Intl. J. Heat Mass Transfer, 49: 984-994.

Feng, Z.G. and E.E. Michaelides, 2000. A numerical study on the transient heat transfer from a sphere at high Reynolds and Peclet numbers. Intl. J. Heat Mass Transfer, 43: 219-229.

Hashim, L. and H. Chaveron, 1995. Use of methylpyrazine ratios to monitor the coffee roasting. Food Res. Intl., 28: 619-623.

Hernandez, J.A., B. Heyd, C. Irles, B. Valdovinos and G. Trystram, 2007. Analysis of the heat and mass transfer during coffee batch roasting. J. Food Eng., 78: 1141-1148.

Porto, D.C., M.C. Nicoli, C. Severini, A. Sensidoni and C.R. Lerici, 1991. Study on physical and physico-chemical changes in coffee beans during roasting Note 2. Ital. J. Food Sci., 3: 197-207.

Schenker, S., 2000. Investigation on the hot air roasting of coffee beans. Ph.D Thesis, Swiss Federal Institute of Technology, ETH Zurich, Zürich, Switzerland.

Schwartzberg, H.G., 2002. Modelling Bean Heating During Batch Roasting of Coffee Beans. In: Engineering and Food for the 21st Century, Welti-Chanes, J., G. Barbosa-Canovas and J.M. Aguilera (Eds.). CRC Press, Boca Raton, Florida, USA., pp: 253-268.

Shevtsov, A.A. and E.A. Ostrikova, 2011. Rationale multistage mode of chestnuts roasting on the basis of the types of moisture binding study. Bull. Voronezh State Technol. Acad., 1: 39-41.

Stepanov, D.E. and I.I. Tatarchenko, 2009. Influence of coffee beans roasting conditions on the quality. Proc. Univ. Food Technol., 4: 121-122.

Zimmermann, R., H.J. Heger, C. Yeretzian, H. Nagel and U. Boesl, 1996. Application of laser ionization mass spectrometry for on-line monitoring of volatiles in the headspace of food products: Roasting and brewing of coffee. Rapid Commun. Mass Spectrom., 10: 1975-1979.