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Modeling and simulation of coffee bean heating during roasting: effect of heat generation

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The temperature of the coffee bean during roasting determines the sensory and nutritional quality of the beverage. Thus, evaluation of the effect of heat generated by evaporation and oxidation reactions during roasting is mandatory to elucidate this process. This work aimed to model and simulate heating. It was considered a lumped analysis on developing a physical model for estimating the temperature of the coffee bean. The model was fitted to experimental data. When evaporation is negligible, the model overestimates the temperature during the exothermic reaction period, beginning at 150°C, and up to the consumption stage of the reagents. By contrast, when exothermic reactions are ignored, the model underestimates the temperature of the bean due to cooling caused by evaporation. The temperatures estimated by the model showed R2 values between 0.973 and 0.994 at different roasting temperatures. The model can be used as an optimization and controlling tool in the roasting process.

KEYWORDS

volumetric expansion, exothermic reactions, moisture content, *Coffea arabica* L., mathematical modeling

1 Introduction

The roasting of coffee can be divided into three consecutive stages: drying, roasting or pyrolysis and cooling. During drying, water vapor is released initiating the expansion of the inner matrix, a phenomenon that continues in the second stage with the release of CO_2 and volatile compounds. The volume expansion leads to an increase in surface area and a decrease in the specific weight of grain (Hernandez et al., 2008; Jokanovic et al., 2012). The degree of roasting can be monitored through changes of these properties.

The temperature of the coffee bean, as the result of accumulation of heat transferred, is the most important parameter in the roasting process, and can be determined from the roasting time (Bonnlander et al., 2005). The evolution of this temperature during the roasting, determines the sensory and nutritional quality of the beverage as it affects the rate and intensity of reactions that generate compounds responsible for the color and aroma of coffee, as well as the antioxidant capacity of the beverage, mainly due to chlorogenic acids (Wieland et al., 2012; Ku Madihah et al., 2012; Zhou et al., 2013; Wang and Lim, 2013; Hertz-Schunemann et al., 2013; Gloess et al., 2014; Wang and Lim, 2014; Vignoli et al., 2014; Sunarharum et al., 2014; Shan et al., 2014).

Several studies have been developed to model and simulate the heat and mass transfer in coffee beans during the roasting process (Schwartzberg, 2002; Bonnlander et al., 2005;

Hernandez et al., 2008; Basile and Kikic, 2009; Fabbri et al., 2011; Bottazzi et al., 2012; Alonso-Torres et al., 2013), but sometimes its simplifications (constant physical properties, negligible heat generated) moving away from the true process conditions.

The complex phenomena that occur in the coffee roasting process still need to be studied and understood in depth, considering all the variables that can influence the process. Thorough knowledge of these phenomena will help in producing a coffee with high added value (high quality nutritional and sensory) as well as the optimization and equipment planning, in addition to reducing operating and experimental costs. The objective of this study is to add to the knowledge in better understanding of the coffee roasting process, developing a mathematical model to estimate coffee grain temperature during roasting under isothermal conditions considering the variations of physical properties. Exothermic and endothermic heat generation terms' effects on a roasting curve are intended to be evaluated using the suggested model.

2 Materials and methods

Processed coffee beans (dry process), *Coffea arabica* L., Catuaí Vermelho cultivar, with size above sieve 18 were used. A direct gas-burning roaster (Rod Bel, 4 burners) with a rotating cylinder at 45 rpm was used for the roasting operation.

For model implementation, the main heat transfer mechanisms acting on the grain were convection and radiation, in which the grain was supported by the thermocouple in the center of the roaster exposing the surface to the hot air and radiation emitted by the heated walls of the cylinder. It considered the heat flux proportional to the overall coefficient of heat transfer involving both mechanisms. For the development and mathematical formulation of the model, a lumped analysis of the following conditions was made.

i. The initial temperature and moisture content inside the grain are uniform.
ii. The mass transfer in vapor form occurs from the bean's surface to the air, by convection.
iii. The main energy transfer mechanisms are convection and radiation and are represented by the overall coefficient of heat transfer (h).
iv. Constant thermal conductivity of the bean.
v. Volume, surface area, density and grain heat capacity vary depending on the moisture content.

The overall energy balance in the grain, applying the first law of thermodynamics can be written according to Equation 1:

$$\dot{E}_e + \dot{E}_g = \dot{E}_{ac} \tag{1}$$

Where $\dot{E}_e$–heat rate transferred to the grain, W; $\dot{E}_g$–rate of heat generation, W; $\dot{E}_{ac}$ - heat accumulated rate in the grain, W.

The heat transferred to the grain will then be proportional to the overall coefficient of heat transfer, the surface area and the temperature difference between the grain and the air inside the roaster (Equation 2):

TABLE 1 Model parameters used for simulations.

Property	Value or reference
Volume	Proposed by Bustos-Vanegas (2015)
Initial volume	1.436×10^{-7} m^3 (Bustos-Vanegas, 2015)
Superficial area	Proposed by Bustos-Vanegas (2015)
Initial superficial área	1.63022×10^{-4} m^2 (Bustos-Vanegas, 2015)
Initial characteristic longitude	8.8056×10^{-4} m (Bustos-Vanegas, 2015)
Specific mass	Proposed by Bustos-Vanegas (2015)
Thermal conductivity	0.11 W m^{-1} °C^{-1} (Fabbri et al., 2011)
Heat capacity	Proposed by Schwartzberg (2002)
Initial moisture	0.1296 dec. d.b* (Bustos-Vanegas, 2015)
Moisture	Proposed by Schwartzberg (2002)
Air thermophysical properties	Incropera et al. (2011)
Air speed	0.02 m s^{-1} (Fabbri et al., 2011)
Roasting temperature	200, 220, 240, 260, 280°C
Roasting time	10 min
Arrhenius pre-factor **	116,200 kW kg_{dm}^{-1} (Schwartzberg, 2002)
Activation energy/Gas constant (H_a/R_g)	5500 K (Schwartzberg, 2002)
Total reaction heat produced (H_{et})	232 kJ kg_{dm}^{-1} (Schwartzberg, 2002)

* dec. d.b.: decimal dry basis. ** kg_{dm}: kg of dry matter.

$$\dot{E}_e = -hA(T_b - T_a) \tag{2}$$

Where h–overall coefficient of heat transfer, W m^{-2} °C^{-1}; A–heat transfer area, m^2; T_b–bean temperature, °C; T_a–roasting temperature, °C.

The heat generation rate is composed of an endothermic heat rate proportional to moisture variation, and a rate of exothermic heat due to the oxidation reactions produced inside the grain when it reaches temperatures above 150°C (Schwartzberg, 2002) (Equation 3):

$$\dot{E}_g = -\rho V \lambda(-dX/dt) + \rho V Q_r \tag{3}$$

Where ρ - bean specific weight, kg m^{-3}; V–bean volume, m^3; λ - water latent heat of vaporization, J kg^{-1}; Q_r - heat generated by the exothermic reactions, W kg^{-1}; dX/dt–loss humidity rate, kg_a kg_{ms}^{-1} s^{-1}.

Schwartzberg (2002) developed a model to estimate the evaporation rate considering the phenomenon governed by diffusion and a dependency on the Arrhenius type. Also taken into consideration were the driving force and the diffusion coefficient proportional to the moisture of the bean (Equation 4). Equation 4 estimates the exponential decrease in the bean moisture content with the increase in temperature. This equation considers a higher moisture removal rate at the beginning of the process (when the bean moisture content is high) and a dependence on bean size (higher rate in smaller grains). Schwartzberg (2002) modeled the generation of exothermic heat by considering the following simplifications: the rate of generation is proportional to the energy-producing reactions rate, and the rate of these reactions is proportional to the concentration of the reactants and the Arrhenius coefficient (Equation 5):

$$-\frac{dX}{dt} = \frac{4.32 \times 10^9 X^2}{d_p^2} exp\left(\frac{-9889}{T_b + 273.2}\right) \tag{4}$$

$$Q_r = Aexp\left[\frac{H_a}{R_g(T_b + 273.2)}\right]\left(\frac{H_{et} - H_e}{H_{et}}\right) \tag{5}$$

Where d_p - effective bean diameter, mm; X–bean moisture, $kg_a\ kg_{ms}^{-1}$; A–Arrhenius pre-factor, J kg_{ms}^{-1} s^{-1}; H_a–activation energy, J mol^{-1}; R_g–gas constant; H_{et} - total reaction heat produced, J kg_{ms}^{-1}; H_e–reaction heat produced at time t, J kg_{ms}^{-1}.

Thus, the governing equation (Equation 6) and its initial temperature and moisture content conditions were established.

$$\rho V C p_b \frac{dT_b}{dt} = -hA(T_b - T_a) - \rho V \lambda \frac{dX}{dt} + \rho V Q_r \tag{6}$$

$$T_{b(0)} = T_i = 28°C$$

$$X_{(0)} = X_i = 0.1296\, kg_a\, kg_{ms}^{-1}$$

Where Cp_b–bean specific heat, J kg_{ms}^{-1} °C^{-1}.

The convection heat transfer coefficient (h_c) was calculated by Ranz-Marshall correlation (Equation 7). Parameters used for the solution of the Equations 8–10 are listed in Table 1.

$$Nu = h_c\frac{d_p}{k_a} = 2 + 0.6Re^{0.5}\, Pr^{0.33} \ \ (1 < Re < 10^5;\ 0,6 < Pr < 380) \tag{7}$$

$$Re = \frac{vel \times L_c}{\nu} \tag{8}$$

$$d_p = \left(\frac{6\forall}{\pi}\right)^{1/3} \tag{9}$$

$$Pr = \frac{\mu C_{pa}}{k_a} = \frac{\nu}{\alpha} \tag{10}$$

Where L_c - length characteristic, m; Nu–Nusselt number, dimensionless; Re–Reynolds number, dimensionless; Pr–Prandtl number, dimensionless; vel–air velocity, m s^{-1}; ν–air kinematic viscosity, m^2 s^{-1}; μ–air dynamic viscosity, kg m^{-1} s^{-1}; Cp_a–air specific heat, kJ kg^{-1} °C^{-1}; k_a–air thermal conductivity, W m^{-1} °C^{-1}; α–air thermal diffusivity, m^2 s^{-1}.

The numerical solution was performed by the finite difference method, calculating the bean's temperature and moisture for each instant of time later. The step size for the discretization in time (Δt) was determined by Equation 11 (Incropera et al., 2011):

$$Fo = \frac{\alpha \Delta t}{L_c^2} \le \frac{1}{4} \tag{11}$$

Where Fo–Fourier number, dimensionless time.

It is considered that Fo = 0.2, and average and constant values of k, Cp and ρ (only for calculation of Δt, but in the model, these properties are variable):

$$0.2 = \frac{0.11\Delta t}{1500 \times 800 \times (8.8056 \times 10^{-4})^2}$$

Thereby determining: Δt ≤ 1.69 s. To facilitate this, the numerical calculations are established Δt = 1 s.

Derivatives temperature and humidity over time were discretized explicitly by calculating the value for each time step later using Microsoft Excel spreadsheet, stated by Equations 12–15:

$$\frac{dT}{dt} = \frac{T^{j+1} - T^j}{\Delta t} \tag{12}$$

$$\frac{dX}{dt} = \frac{X^{j+1} - X^j}{\Delta t} \tag{13}$$

$$X^{j+1} = X^j - \Delta t\left(\frac{4.32 \times 10^9 X^{j^2}}{d_p^2}\right) exp\left(\frac{-9889}{T^j + 273.2}\right) \tag{14}$$

Substituting Equation 6:

$$T^{j+1} = T^j - \Delta t\left(\frac{hA_s}{C_p \rho \forall}\right)(T^j - T_a) + \left(\frac{\lambda}{C_p}\right)(X^{j+1} - X^j) + \Delta t\left(\frac{Q_{reac}}{C_p}\right) \tag{15}$$

The overall heat transfer coefficient was calculated using Microsoft Excel Solver tool by minimizing the square error between the experimental and estimated temperatures by the model. The convergence criterion was defined at 1E-4.

The effect of heat generated during the process of heating the coffee beans, was simulated for the roasting process at 240°C by adding and/or deleting the term's source, endothermic and exothermic, in Equation 6.

3 Results and discussion

The obtained results apply to the roasting process of an individual coffee bean, considering variations in physical properties and terms of exothermic and endothermic heat generation. This model can be used to strengthen predictive models for masses of coffee beans being roasted, in which the effects of collisions between particles (beans) should be included.

Table 2 presents the values of the convective (h_c) and global (h) coefficient heat transfer for each process temperature, the average relative and estimated mean error, and the determination coefficient.

As seen in Table 2, the convection heat transfer coefficient is slightly influenced by the temperature of the process, and its value is low because of the low air velocity that is generated by the rotation of the roasting drum. The overall coefficient of heat transfer, covering convection and radiation, increased exponentially with the temperature of the process, and its value indicates that radiation is the governing phenomena. In the current work, a individually bean was roasted, supported by a thermocouple, and exposed only to the convection and radiation heat transfer mechanisms. Since there was no contact with the walls or other beans, heat conduction did not act in the process. The low values of the convective coefficient (Table 2) correspond to the low air velocities inside the drum, caused solely by the drum's rotational movement. It is then deduced that the bean heating rates are due to an additional mechanism beyond convection, and in the present case, it is mainly by radiation.

Basile and Kikic (2009), through a global heat capacity approach and considering constant physical properties, calculated the external heat transfer coefficients between 12.7 and 82.7 W m^{-2} °C^{-1} for roasting temperatures between 180 °C and 240 °C in fluidized bed

TABLE 2 Convective and overall heat transfer coefficient calculated for different roasting temperatures.

Roasting temp. (°C)	Convective h_c (W m^{-2} °C^{-1})	Overall h (W m^{-2} °C^{-1})	P (%)	SE (% d.b.)	R^2
200	15.91	60.20	1.03	2.19	0.994
220	16.27	72.36	1.55	2.95	0.993
240	16.65	68.00	3.05	5.77	0.986
260	17.04	81.62	3.50	7.57	0.985
280	17.43	102.55	1.98	6.51	0.973

Relative (P) and estimated (SE) mean error; determination coefficient (R^2).

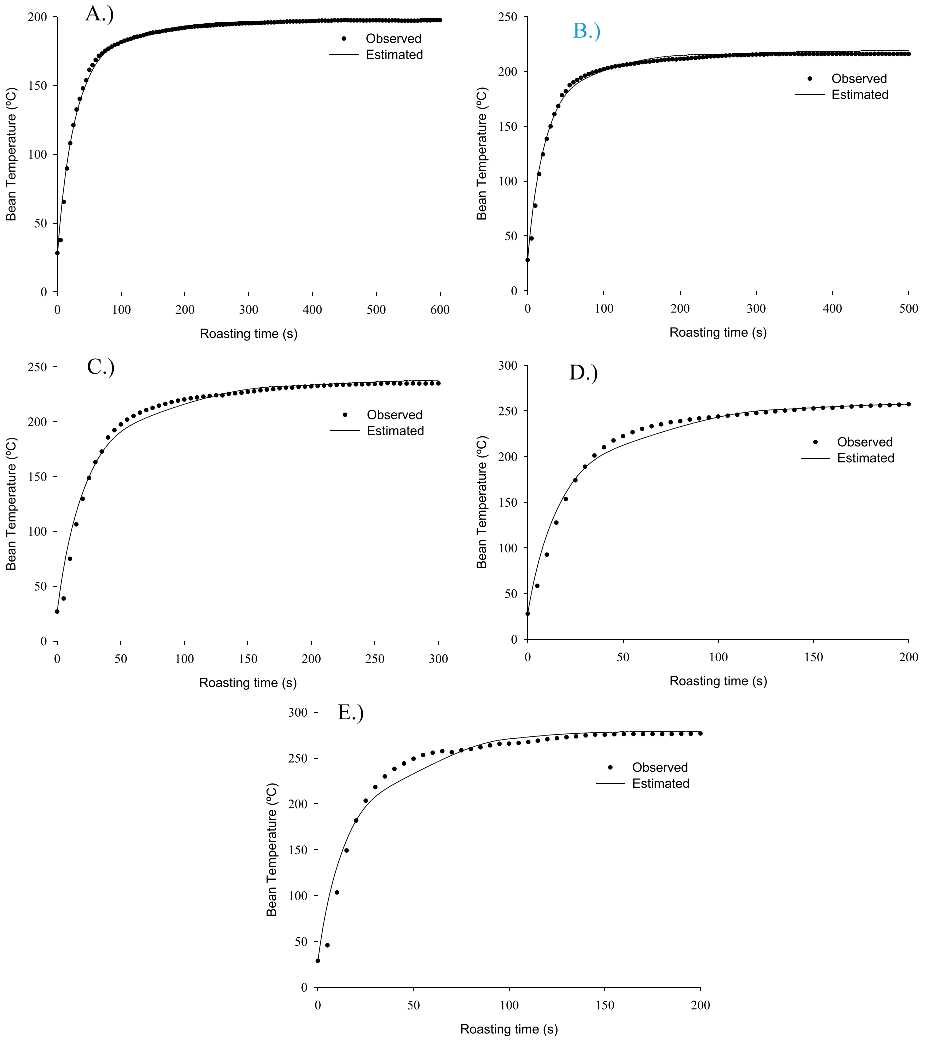

FIGURE 1
Observed (•) and estimated values (–) of the coffee bean temperature during the roasting process: **(A)** 200°C; **(B)** 220°C; **(C)** 240°C; **(D)** 260°C; **(E)** 280°C.

conditions. Putra et al. (2019) conducted a theoretical study on heat transfer in a fluidized bed coffee roaster. Assuming spherical bean geometry, the researchers determined convection heat transfer coefficient values ranging between 74.5 and 77.4 W m^{-2} °C^{-1}. The overall heat transfer coefficient in a fluidized bed coffee roaster with a spouted bed type was assessed by Yohanes et al. (2022). The values of the coefficients ranged from 26.63 to 92.02 W m^{-2} °C^{-1} at 225°C and from 44.85 to 139.98 W m^{-2} °C^{-1} at 240°C. These differences can be mainly due to the gradual increase in the transfer area considered in our study, which is as a result of bean expansion.

Values of the Biot number obtained for overall heat transfer coefficients were 0.48; 0.58; 0.54; 0.65 and 0.82 for roasting

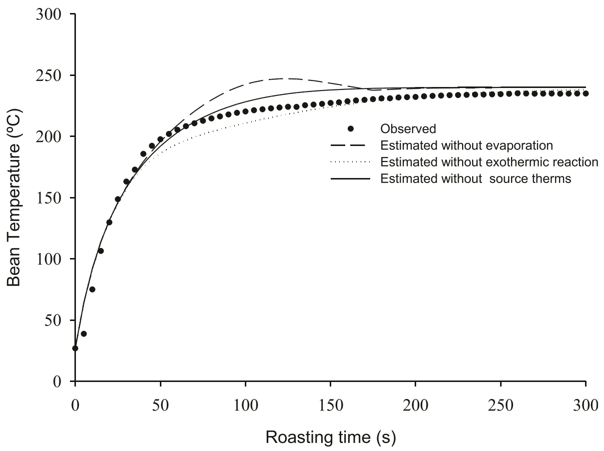

FIGURE 2
Effect of source terms (evaporation and exothermic reactions) in grain temperature estimated by the model to 240°C.

temperatures of 200, 220, 240, 260°C and 280°C, respectively. These amounts reflect the relevant role of conductive resistance within the grain in later studies. Alonso-Torres et al. (2013), using computational fluid dynamics, determined a temperature difference of 16°C between the center and the surface of the bean, still considering constant bean volume. The internal resistance to heat transfer increases with the temperature and roasting time due to formation of pores in the solid grain structure, as observed by Schenker et al. (2000) and Frisullo et al. (2012). Using X-ray microtomography, these last authors determined an increase of up to 37% in porosity of the grain during roasting at 220 °C for 5 min.

Figure 1 shows the dependence of the bean's heating rate on the temperature of the process.

The models developed by Basile and Kikic (2009), Fabbri et al. (2011), Bottazzi et al. (2012) and Alonso-Torres et al. (2013) describe similar behavior. It can be observed to be a better fit with lower roasting temperatures. At temperatures higher than 240°C, the model tends to underestimate data when the bean

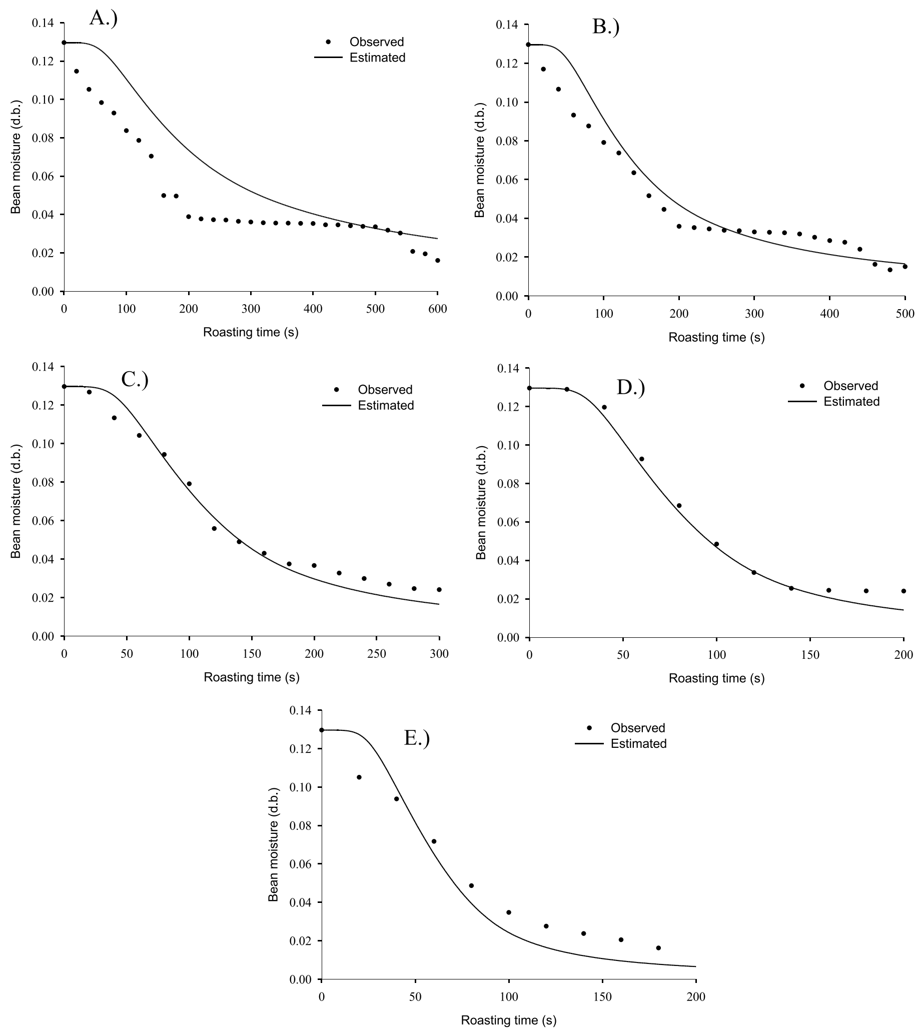

FIGURE 3
Observed (•) and simulated values (–) of the coffee bean moisture during roasting process: **(A)** 200°C; **(B)** 220°C; **(C)** 240°C; **(D)** 260°C; **(E)** 280°C.

reaches temperatures between 180°C and 230°C, approximately. This may be caused by the intensity of the exothermic reactions taking place at these temperatures. Using differential scanning calorimetry and thermogravimetric analysis, Rivera et al. (2011) observed a rapid and sharp decomposition in coffee between 208 °C and 230°C. The authors attributed this phenomenon to the rapid changes of some components in coffee, such as sucrose, cafestol and kahweol in this temperature range.

The effect of the term's source (evaporation and exothermic reactions) on temperature is estimated by the model shown in Figure 2.

Endothermic heat due to water evaporation influences more strongly the model response. When this term is neglected, the model overestimates the temperature during the exothermic reaction period, starting at 150 °C until the reagent's consumption. Schwartzberg (2002) established that the end of the reaction is when it reaches the total heat of reaction (H_{et}). By contrast, when exothermic reactions are ignored, the model underestimates the temperature of the bean due to evaporative cooling, which starts at 100°C and gradually decreases up to the end of the process. Schenker, (2000) evaluated the effect of the bean's initial moisture on the heating rate, and he observed a rapid increase in bean temperature in grains with low initial values, which is expected to be caused by the lower energy requirement for evaporation and benefit the sensible heat.

Evolution of the bean's moisture content during the roasting process (Figure 3) shows the typical trend of a grain's drying curve.

It can be seen that the first step corresponds to the grain heating up to reach approximately 100°C, at which moisture remains approximately constant. Then, an exponential decay proportional to temperature process takes place until it achieves equilibrium moisture, where the curve becomes asymptotic. The final moisture content was between 2% and 4%, decreasing with time and roasting temperature. Alonso-Torres et al. (2013) simulated one roasting at 260 °C reaching a 2% moisture content for a 300 s process. Similar results were observed by Burmester and Eggers (2010), who found that the drying rate was mainly influenced by temperature and controlled by diffusive mass transfer inside the grain matrix. A very low (<3%) moisture content can lead to poor quality and yield losses. Monolayer moisture content indicates the moisture content that must be reached to ensure the quality and stability of the product in storage. Iaccheri et al. (2015) determined a monolayer moisture content for roasted coffee of 4.3%, which can be achieved in a more controlled way in medium and low roasting temperatures. Thus, in addition to the bean's temperature, moisture content is an important parameter in the coffee bean roasting process.

4 Conclusions

1. A physical model to estimate coffee bean temperature during the roasting process was developed. The model is based on combined heat and mass transfer phenomena and has been developed considering the variation of the grain's physical properties (heat capacity, specific mass, volume and surface area), which ensures their versatility. The major simplifications in the model were grouping the heat transfer mechanisms (convection and radiation) in an overall heat transfer coefficient and considering a constant bean thermal conductivity.
2. Although the two source terms have to be taken to get the best fit for the experimental data, evaporation has a greater effect on the temperature estimated by the model when compared with the effect of the exothermic reactions. In order to facilitate the control of the roasting process, a low initial moisture content in the beans is recommended.
3. Values of the overall heat transfer coefficient calculated by the model are between 80% and 90% higher than the convective heat transfer coefficient calculated under the experimental conditions, allowing one to find that the dominant heat transfer mechanism is radiation.
4. The model is a complementary tool for real-time control and optimization of the roasting process under conditions whereby radiation and convection are the main heat transfer mechanisms. The model could be used in future research to help model the kinetics of formation and/or degradation of compounds responsible for flavor and aroma, as these are influenced by the process temperature.

Data availability statement

The raw data supporting the conclusions of this article will be made available by the authors, without undue reservation.

Author contributions

JB-V: Data curation, Formal Analysis, Conceptualization, Writing – original draft, Investigation, Methodology. MM: Writing – review and editing, Investigation, Validation, Resources, Visualization. PC: Resources, Writing – review and editing, Funding acquisition, Visualization, Conceptualization, Project administration, Supervision. FB: Investigation, Visualization, Writing – review and editing. Gd: Visualization, Writing – review and editing.

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Conflict of interest

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