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Numerical and experimental characterization of coffee roasting in a rotary drum type roaster by forced internal convection

Rafael De La Cruz Casaño[a,b*], Alberto Jesús Torres Hinostroza[c], Felipe Nestor Gutarra Meza[b] and Alejandro Alonzo García[c]

[a]*Universidad Internacional Iberoamericana, México*
[b]*Universidad Continental, Perú*
[c]*CONAHCYT/Tecnológico Nacional de México/Instituto Tecnológico de Nuevo León, Av. Eloy Cavazos No. 2001, Colonia Tolteca, C.P. 67160, Guadalupe, N.L., Mexico*

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A B S T R A C T

The effect of air injection into a coffee roasting chamber of a 2 kg rotary drum roaster is investigated on the temperature profiles and organoleptic properties of a Catuai coffee variety. In the experimental study, 1 kg of coffee beans were used and the air injection velocities were varied for the cases of 0 (standard roasting design), 1, 2 and 3 m/s; testing in triplicate and the two most representative were taken. In the coffee roaster, the temperature was monitored simultaneously in the air inlet duct, roasting chamber and gas outlet duct. The organoleptic properties were examined by a group of professionals from Negociaciones Agroindustrial Arévalo S.A. NARSA in the province of Chanchamayo - Peru, which has a G4 laboratory certified by the Specialty Coffee Association (SCA). In the organoleptic ratings, a maximum score of 83.21/100 was found for the 2 m/s test and a minimum of 80.63/100 for the 1 m/s test. For the numerical characterization, the principle of fluid mechanics such as turbulent regime flow and energy transport were used by the finite volume (FV) method using SolidWorks 2021 Flow Simulation software. The numerical results showed that for the 2 m/s test, the temperature of the bean reaches 195 °C at 500 s, indicating that the whole coffee bean reaches the cooking temperature required for the development time prior to eviction; while for the 1 m/s test, it did not exceed 190 °C. It is shown here that the effect of air injection in the roasting chamber, caused organoleptic changes with respect to the conventional design without air injection, due to a sustained cooking at different times and an adequate development time. However, there is a speed threshold where when exceeded, temperatures inside the chamber remain low, development time is extended (machine energy consumption is extended), and organoleptic properties do not improve.

1. Introduction

In recent decades the demand for coffee has risen, and it is vital to be competitive by identifying the drivers of consumer acceptance of coffee (Bhumiratana et al., 2019). According to Figueroa et al. (2015) coffee, after water, is the most consumed beverage worldwide and demand is increasing, for producing countries it is one of the main sources of income. According to Marek et al. (2020), coffee in most countries is present on the table as part of their culinary culture. The production of excellent coffee is growing as a result of trying to modulate roasting profiles, so that the consumer experiences new and varied sensory experiences (Alstrup et al., 2020); because during this process, favorably controlled, volatile compounds with potential aroma and flavor attributes are released. (Laukalja et al., 2022). This allows us to understand that there is an influence of the roasting profile on the aroma and flavor perceptions of coffee in the cup (De La Cruz, 2018).

Batali et al. (2022) declare that coffee professionals appreciate how the preparation can highlight the pleasant flavors and minimize the unpleasant ones. Although coffee possesses innate properties in flavors and aromas, characterized by the diverse varieties, it should be taken into account that, during the roasting process, changes are produced in its sensory properties; the

* Corresponding author.
E-mail addresses: rafael.delacruz@doctorado.unini.edu.mx (R. De la Cruz)

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distribution of temperature, time and volume of coffee in the roaster are important parameters associated with a good quality cup of coffee. (Figueroa et al., 2015). For Porras-Zúñiga et al. (2019) the variation of temperature in the roasting house is a little studied parameter and effects in an important way in the quality of coffee in cup. According to Castillo et al., (2016) coffee beans suffer great qualitative and quantitative changes, such as when they lose 15-20% of weight, increase from 100 to 130% of the volume according to the roasting time, sugars caramelize, more than 700 compounds responsible for giving aroma and taste are formed, the acidity decreases gradually to the roasting time. Rusinek et al. (2022) also found that the time in the roasting house influences the organoleptic ratings of coffee in the cup.

An important precedent was the modeling carried out by Heyd et al. (2007), who measured the temperature of the coffee on the periphery and inside, as well as the variation of the temperature in the entrance and expulsion of gases from the roaster, with the variation of the percentage of humidity of the coffee during the roasting process; with the purpose of determining the quality of the product in line, as a proposal for the control of the process.

According to Alstrup et al. (2020) , the effect of the development time from the first crack to the removal of the roasted beans, influences the sensory characteristics of coffee. The samples were processed in a Probat Probatino 1 kg drum roaster, modifying the power of the heat source, they were able to vary the time from a fast development profile of 90 s to a baked profile of 390 s. The times for a medium and slow roast development profile were 143 and 266 sec. The 4 roasting profiles were the same until the first crack, which occurred at approximately 570 sec. They found that a short time brings out the fruity, sweet and sour flavor, while a longer time generates a bitter nutty taste.

In the work of Chiang et al. (2017), they modeled the transient-state heat transfer for a FUJI Royal R-101 1 kg type coffee roaster using computational fluid dynamics (CFD). With the 3000 W and 4000 W heat source, the air velocity in the exhaust duct varies from 8 to 10 m/s. During the roasting process, they observed that in the first 60 s, the temperature distribution in the coffee bean was very unequal; the temperature in the coffee bean became more and more uniform between 100 and 720 s as it approached 200°C.

According to the above, there is a relationship between the speed of the injected air, energy, cooking time and temperature in different roasting machines. However, there is not much precise information on the variety of organoleptic characteristics that can be achieved. Likewise, there is not much experimental information on roasting profiles, related to development times and air injection rates into the roasting chamber. In this work, an experimental and numerical characterization by CFD of the influence of injected air velocities on the temperature and organoleptic profiles of coffee for a 2 kg rotary drum roasting machine was carried out. Four cases were studied, corresponding to speeds of 0 m/s (without air injection), 1, 2 and 3 m/s, obtaining three simultaneous temperature profiles measured at the inlet, inside and exhaust of the roasting chamber. In order to obtain significant statistics, experiments were performed in triplicate. In addition, the research was complemented with a CFD analysis, for which local contours of temperature velocity as a function of time are presented, allowing to understand and analyze the evolution of baking. For the roasts obtained, an organoleptic qualification was carried out by Negociaciones Agroindustrial Arévalo S.A. NARSA, using the guidelines of the analysis protocol of the Specialty Coffee Association of America, SCAA (Pereira et al., 2017).

2. Materials and methods

2.1 Experimental characterization

A study to improve the coffee roasting process is the collection of data through sensors, which corresponds to the experimental method for heat flow analysis (Çengel & Afshin, 2011). According to Heyd et al. (2007) , when green coffee is subjected to high temperatures, over 190 °C, a series of chemical and physical processes are initiated that give rise to the development of highly appreciated organoleptic characteristics. For Marek et al. (2020) the aroma develops in the process of roasting the compounds characteristic of green coffee. Alstrup et al. (2020) manifest that the "development time" covers from the sound of the bursting of the vapor pressure release of the beans, known as "first crack", to the point of completion of the roasting, being a fundamental phase to obtain an excellent coffee product in cup in aroma and flavor. For (Porras-Zúñiga et al., 2019) determined the influence of temperature on the roasting process, through an experimental analysis, using a thermocouple to record the internal temperature of the roaster, and analyzed its relationship with the internal temperature of the coffee beans.

In relation to the experimental background, a model was used which is a coffee roasting machine of the rotary drum type of 2 kg capacity, patented by De la Cruz & De la Cruz (2018) and shown in **Fig. 1**, With a 3000 W resistor heat source, a variable speed fan was adapted in the air intake duct to regulate the three injection speeds for the roasting tests with three samples per group. Temperature variation data were collected in the inlet duct, roasting chamber and exhaust duct for the construction of the temperature profiles. For each sample we used one kilogram of Catuai variety coffee, which has a good cup quality as shown in the following **Fig. 2**.

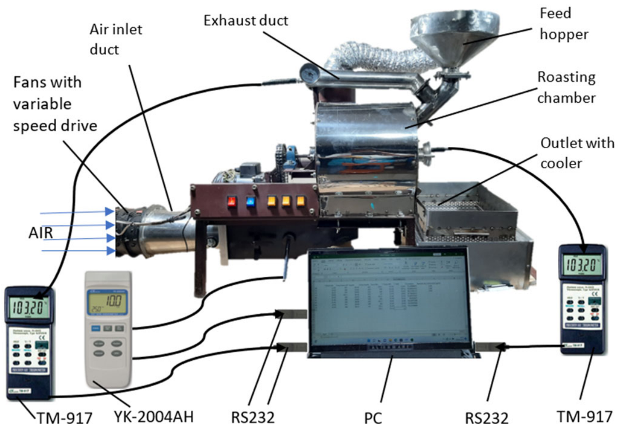

Fig. 1. Installation of the Coffee Roaster with sensors and a PC for data logging and data storage.

Fig. 2. Roasted coffee sample.

The roaster is configured for the roasting cylinder to rotate at 30 RPM. The air inlet duct to the roasting chamber has a square section of L=10 cm per side, and for the test velocities of 1, 2 and 3 m/s; we calculate a Reynolds number (Re=ρU_xD/μ) of 6764, 13528 and 20292 respectively for an air temperature at 20 ºC (Çengel & Cimbala, 2006). Here, U_x is the average flow velocity at the inlet and μ is the dynamic viscosity of the air (1.7984×10^{-5} Pa·s). In porous media flow, these Reynolds are related to the fully developed turbulent flow regime (Wood et al., 2020). **Fig. 1** shows the connections for data acquisition using the YK-2004AH hot-wire anemometer (Lutron, 2021a), which measures the average air velocity and temperature in the inlet duct. Two precision thermometers were installed TM-917 (Lutron, 2021b), one in the roasting chamber and the other in the exhaust duct. The data recording was obtained using the following protocol RS-232 (Lutron, 2016), from the instruments to the USB ports of the PC for data logging using the software SW-U801-WIN (Lutron, 2020). The sampled temperature data were obtained every 10 seconds for total roasting times ranging from 670 s to 1020 s.

2.2 Numerical characterization

For the numerical characterizations, SolidWorks Flow Simulation 2021 software was used, which numerically approximates solutions to the mass, momentum and energy transport equations using the finite volume method (VF) (Dassaul_Systemes, 2021). In this technique, the properties of a three-dimensional domain represented by a mesh are defined at the centroid of the control volumes, approximating the derivatives by means of difference schemes, in such a way that solvable matrices are obtained, which represent a numerical solution in the form of an integral of the governing differential equations, in which the balance of mass, momentum and energy is conserved.

In the applied solver, it relates the principle of conservation of matter, angular momentum and the principle of energy, which uses Cartesian coordinates for a rotation at an angular velocity "Ω", rotating around an axis located at the origin of coordinates. It is represented by the equations (1-4).

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = S_M^P \quad (1)$$

$$\frac{\partial \rho u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) + \frac{\partial \rho}{\partial x_i} = \frac{\partial}{\partial x_j}(\tau_{ij} + \tau_{ij}^R) + s_i + S_{Ii}^P \quad i = 1,2,3 \quad j = 1,2,3 \quad (2)$$

$$\frac{\partial \rho H}{\partial t} + \frac{\partial \rho u_i H}{\partial x_i} = \frac{\partial}{\partial x_i}(u_j(\tau_{ij} + \tau_{ij}{}^R) + q_i) + \frac{\partial \rho}{\partial t} - \tau_{ij}^R \frac{\partial u_i}{\partial x_j} + \rho\varepsilon + S_i u_i + S_H^P + Q_H \quad (3)$$

$$H = h + \frac{u^2}{2} + \frac{5}{3}k - \frac{\Omega^2 r^2}{2} - \sum_m h_m^0 \, y_m \quad (4)$$

where u_i represents the velocity of the fluid, ρ its density, S_i its external force of a unit mass times the resistance of the porous medium (S_i^{porous}), floatability ($S_i^{gravity} = -\rho g_i$, where g_i is the gravity), and the rotation of the system ($S_i^{rotation}$), is given by, $S_i = S_i^{porous} + S_i^{gravity} + S_i^{rotation}$, h represents the thermal enthalpy, S_M^P, S_{Ii}^P, S_H^P are additional interfacial exchange terms caused by the Euler-Lagrange particle interaction; Q_H represents heat by volume as a source, τ_{ik} is the fluid shear stress due to viscosity, q_i is heat transfer by diffusion Ω represents the speed of rotation, r represents the distance between a point and the axis where the rotation occurs, k is the kinetic energy of turbulence, h_m^0 is the thermal enthalpy of an m-th mixed component, y_m is a concentration of the m-th component of the mixture. SolidWorks Flow Simulation, analyzes the conjugate heat transfer (between solids and fluids), as well as the thermal conductivity in solid bodies is anisotropic, characterized by:

$$\frac{\partial \rho e}{\partial t} = \frac{\partial}{\partial x_j}\left(\lambda_i \frac{\partial T}{\partial x_j}\right) + Q_H \tag{5}$$

where e is the specific internal energy, $e = c \cdot T$, c is the specific heat, Q_H is the source of the specific heat per unit volume on release or absorption, and λ_i is the thermal conductivity tensor considered diagonally and in isotropic medium $\lambda_1 = \lambda_2 = \lambda_3 = \lambda$. For the simulation of heat transfer in a transient state, developed by means of a parasolid in the form of a matrix array of 6×3×3 coffee beans. Each grain has the form of the flat half of an ellipsoid of dimension a=5 mm, b=3.5 mm and c=3.5 mm representing a unit volume of 128.2817 mm^3, the grains are distributed inside a rectangular prism of dimensions 16.5 mm × 31.5 mm × 90 mm; the ratio of the volume of the coffee and the rectangular prism represents a porosity of 15 % as we can see in **Fig. 3**. The porosity of 15 % corresponds experimentally to the ratio of the volume of 1 kg of coffee which is 6250 beans × 128.2817 mm^3/bean to half the volume of the roasting cylinder of 245 mm diameter by 230 mm length. Numerical modeling of the coffee roaster with a 3000 W heat source was performed for different average air velocities in the inlet duct of 1, 2 and 3 m/s; This found convective heat fluxes principally in the roasting chamber, giving mean air velocities of 1.2, 2.3 and 3.3 m/s respectively, which are the data for the inlet boundary condition at LID1; for the output boundary condition in LID2 we worked with the local atmospheric pressure of 92640 Pa. The side walls of the rectangular prism were considered as adiabatic.

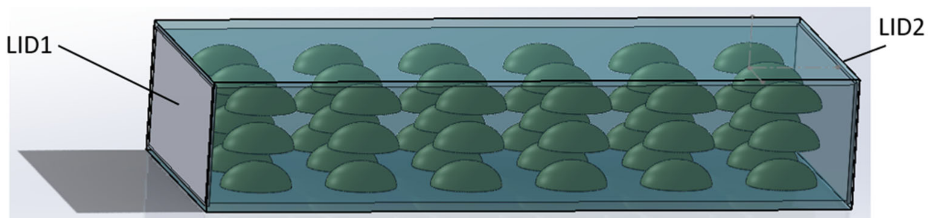

Fig. 3. Parasolid of the distribution of coffee beans within a rectangular prism, characterizing coffee roasting inside the roasting chamber.

The coffee bean material was modeled as a linear isotropic type with a mass density equal to 1247 kg/m^3, the thermal conductivity of 0.105 W/(m·K) and the specific heat of 2400 J/(kg·K). The configuration of the general parameters was the atmospheric pressure of 92640 Pa corresponding to the city of Chanchamayo-Peru, the temperature of the fluid in the rectangular prism is 205 ºC, the initial temperature of the coffee beans with 20 ºC. The times for the simulation were 730 s, 870 s y 1020 s respectively with a data logging interval of 1 s for a transient scanner on a periodical way. In **Fig. 4** visualize the meshing of the parasolid, where the global mesh is of the automatic type of level 4. The localized mesh is level 4 for refined fluid cells, level 4 for the refined solid cells and also level 4 for the refinement of fluid cells at the solid/fluid boundary.

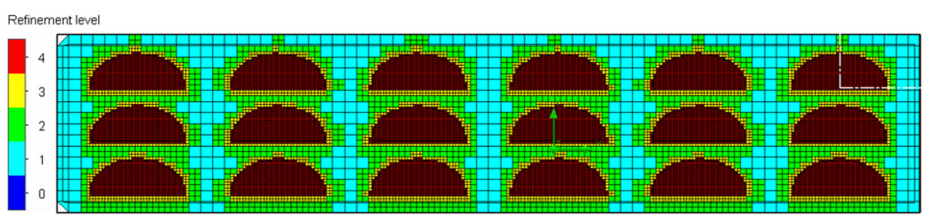

Fig. 4. Level of refinement of global meshing and localized meshing of the parasolid.

3. Results

3.1 Experimental characterization

The average roasting profiles for the 4 tests at speeds of 0, 1, 2 and 3 m/s are shown in **Fig. 5**. We start with data logging when coffee is added at the preheat temperatures of 205 °C, 201 °C, 201 °C y 200 °C. Subsequently, the grains absorb the thermal energy and the temperatures decrease to the lowest values of 128 °C, 134 °C, 146 °C y 147 °C respectively for each test, that the higher the forced convection, the higher the value of the minimum temperature of the profile. From this minimum temperature value, there is a linear increase, where the slope of the straight lines decreases and the firing time increases (the straight lines lengthen) in direct relation to the air injection velocities for forced convection. For a medium roast, the coffee was discharged at temperatures of 202 °C, 204 °C, 205 °C and 205 °C, with total times of 11.2 min, 12.2 min, 14.5 min and 17.0 min, respectively. The development times of the roasting samples, visualized in **Fig. 6**, range from the first crack at 195 °C, marked by the dotted black line H, to the end of roasting. It can be seen that the development times increase as the slopes of the curves decrease due to the higher injection speed. We corroborate the results of Alstrup et al., (2020), who indicate that this time influences the sensory characteristics of the coffee, where the tests at speeds of 2 m and 3 m/s have the ideal time for the development of roasting, which is 120 to 140 seconds.

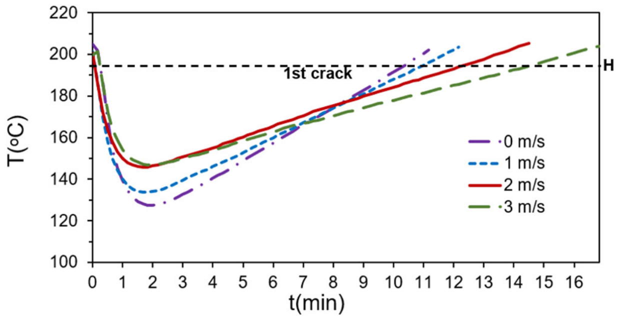

Fig. 5. Average roasting temperature profiles at different roasting tests.

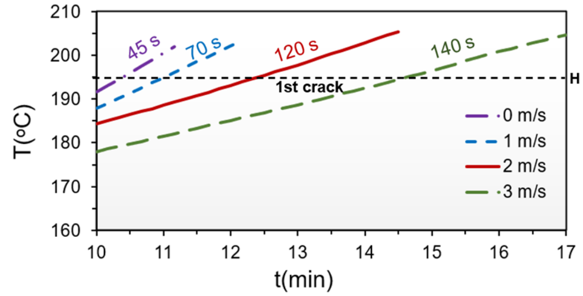

Fig. 6. Profiles of the development times of roasting trials.

On the other hand, in the tests at speeds of 0 m/s and 1 m/s, the development times are very short, between 45 s and 70 s, and the volatile chemical elements are trapped inside the coffee, thus affecting its organoleptic properties. PERFECT DAILY GRIND (2019) states that "The rate of development time and final temperature you are aiming for, will together give you a narrow margin where to finish your roasts, which will help you achieve a consistently balanced coffee profile". **Fig. 7** shows the temperature profiles recorded for the fluid in the inlet duct and the fluid in the outlet duct. For the inlet, the slopes of the temperature curves decrease for the higher speed tests, because of the injection of a greater mass of fresh air. We also observed that at the exit the temperature curves increase for the higher speed tests, i.e., part of the energy is not absorbed by the grains, it is expelled, slowing cooking. This phenomenon is strongly linked to the organoleptic properties generated by the roasting time and development time.

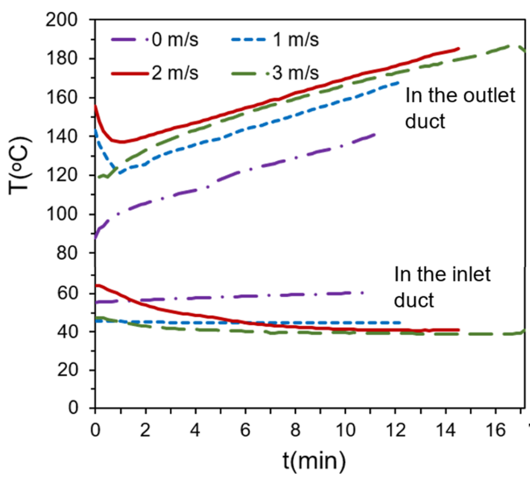

Fig. 7. Temperature profiles recorded in the fluids of the inlet duct and outlet duct for the different tests.

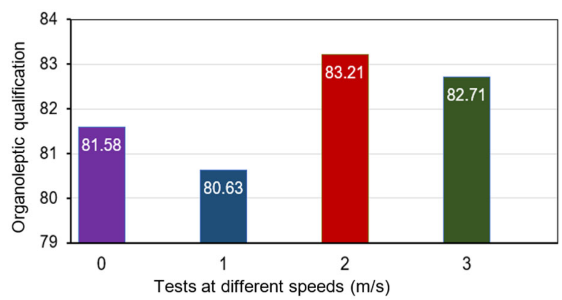

Fig. 8. Bar chart of the average of the organoleptic ratings of the 3 tasters for each roasting test.

Fig. 8 shows the average organoleptic scores of the 3 tasters for the two most representative tests, where we observed that the organoleptic qualification increased for the 2 m/s test and decreased for the 1 m/s test, with development times of 70 s and 120 s shown in **Fig. 6.**

Table 1
Organoleptic characteristics found by tasters for the different tests.

Descriptors	0 m/s	1 m/s	2 m/s	3 m/s
Fragrance/ Aroma	Dry, barley grains (cereals), sweet lemon, honey and peanuts	Peanuts, cinnamon, floral, panela, chocolate, almond milk, tangerine or orange	Honey, cinnamon, floral, tangerine, orange, chewing gum and herbal	Peanuts, chocolate, blancmange, cranberry, butter and milk
Taste	Chocolate, sweet peanuts, caramel, fruit, citrus and nuts	Chocolate, sweet peanuts, fruits, citrus, nuts, dry, cereals.	Chocolate, sweet peanuts, ripe banana, panela, tangerine, orange and pineapple.	Caramel, dried nuts, cereals, bread, vegetables and dried fruits and nuts.
Residual flavor	Baked, green acid, dried fruits, rough, corn, and panela	Baked, dried fruit, coarse, raw to banana, cooked pineapple, beans and cereal	Green acid, dried fruits, sweet lemon peel, hot spicy and vegetables.	Dried fruit, sweet lemon zest, passion fruit, hints of peach, juicy grapefruit.
Acidity	Dried citrus, orange and mandarin orange,	Dry citrus, soft, sharp, sharp and short bitterness.	Dry citrus, orange, tangerine and mild.	Dry citrus, soft, sharp, sharp grapefruit.
Appreciation	Baked dry finish, clean, smooth, soft, sweet, light red berries.	Baked dry finish, clean, smooth, sweet red fruit, with notes of tobacco, dried fruit, orange peel,	Clean, smooth, sweet, light red berry, sweet acid, exotic flavor, and mild cinnamon finish.	Clean, smooth, sweet, floral and dark chocolate finish.

According to **Table 1**, we observe that there is an improvement in the organoleptic characteristics for the speeds of 2 m/s and 3 m/s with a smooth clean finish, sweet with tangerine sweet acidity, exotic flavor; as well as a decrease in the organoleptic characteristics for the speed of 1 m/s as a dry finish, baked with notes of tobacco, dry citric acidity and bitterness.

3.2 Numerical characterization results

The results of the numerical characterization for a transient state heat flux of the minimum temperature profile in coffee beans, with heat flux and streamlines recorded in the virtual solid at 100 s intervals, are given in **Figs. (9-10). Fig. 9** shows the results of the 1 m/s test, where the average temperature in the coffee bean center does not exceed 190 ºC during the cooking process. Also, temperature growth tends to be linear, as compared to the 2 m/s and 3 m/s tests, where a logarithmic type of behavior is observed. For these speeds of 2 m/s and 3 m/s, the minimum bean temperatures exceed 195 ºC at 500 s and 400 s. This indicates that the entire coffee bean reaches the cooking temperature required for the development time from the first crack, which is not the case for the 1 m/s test.

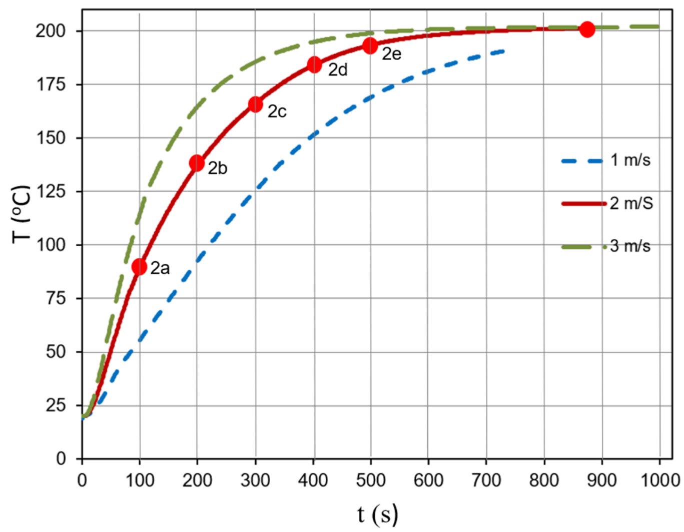

Fig. 9. Results of the numerical characterization of the profile of minimum temperatures of coffee beans for the three roasting tests.

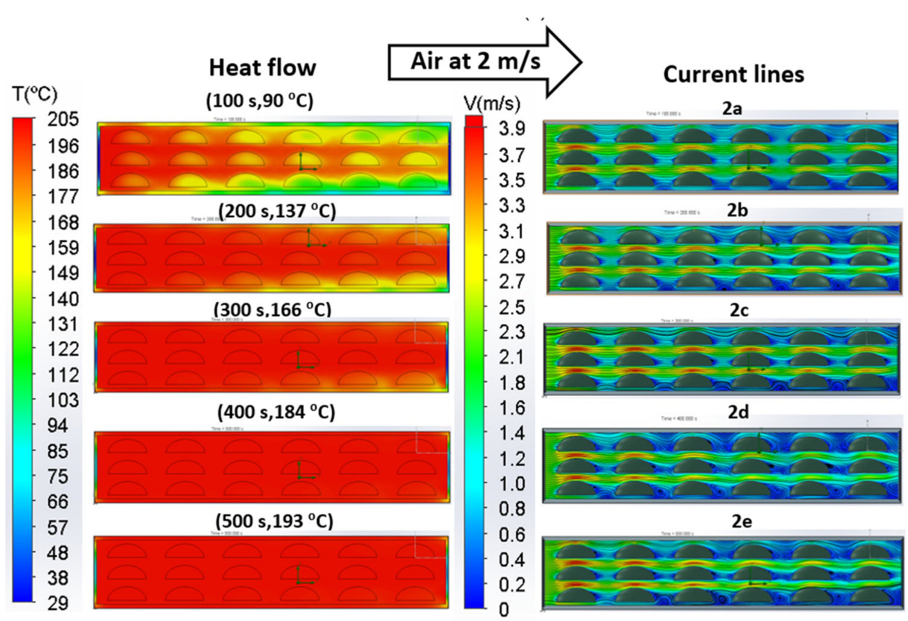

Fig. 10. Result of the numerical characterization of the development of heat flow and streamlines for the 2 m/s roasting condition of coffee beans, which has the best organoleptic qualification.

The time evolution of the local minimum temperature distributions and their corresponding streamlines for the 2 m/s test (best organoleptic characteristics) are shown in **Fig. 10**. For a better understanding, the temporal substages were selected according to the red dots in **Fig. 9**. It shows how the hot fluid packets penetrate sequentially from the interconnected channels of the domain linking the inlet to the outlet, and then disperse in the transverse coordinate of the domain after 200 s, where the grains increase their firing temperatures. On the other hand, the streamlines show regions where the velocity increases in the vertical spaces between grains, and others of recirculation from the back side of the grain. These velocity patterns were independent of temperature and remained nearly constant. Although not shown here for brevity, very similar velocity patterns were present for the other blowing velocities, indicating that the flow regime was sustained, in this case, subcritical. This behavior is related to the constant turbulence values in the range $1000<Re<100,000$ obtained in other porous media (Alonzo-Garcia et al., 2021).

4. Discussion

In the experimental characterization of studied the impact of the development time on the sensory characteristics of coffee, they concluded that for a short development time between 90 s and 143 s, the sweet and sour fruity flavor increases. In the same way for our experiment, we found that for the samples of 2 m/s and 3 m/s which are for a development time of 120 s and 140 s there is an improvement of the organoleptic characteristics to a smooth clean finish, sweet with sweet tangerine acidity, exotic flavor, and a sweet, exotic taste. The difference is that in the work of Alstrup et al. (2020) they modulated the heat source to find different development times, while in the present investigation the air injection into the roasting chamber was modulated at different speeds.

In the numerical characterization performed by Chiang et al. (2017) of the roasting profile of a coffee, by the finite element method (FEM) and previously described; found an unequal temperature distribution between the periphery and the interior of the coffee bean at the beginning of the process, then the average temperature of the coffee increased sequentially until the end of roasting at 720 s, when the average temperature of the coffee reached 200 °C. Similarly, in the present work for the 2 m/s test, it was found that the minimum temperature of the center of the coffee bean reaches 195 °C at 500 s, understanding that the whole bean reaches the necessary temperature for the development time (from the first crack), thus highlighting its organoleptic characteristics.

From the above we found a convenient development time to be 120 s, with a score of 83.21/100 for the 2 m/s test.

5. Conclusions

We present the experimental and numerical characterization of the effect of injecting air into the roasting chamber, on the organoleptic properties for a 2 kg rotary drum machine, using 1 kg samples of the Catuaí coffee variety. The tests were evaluated at speeds of 1 m/s, 2 m/s and 3 m/s through the air inlet duct, comparing the results with the operation of the machine without a blower element (standard design). The experiments were performed in triplicate, choosing the two most representative ones, and the analysis of the temperature profiles obtained and roasting times is presented. The injection Reynolds numbers were 6764, 13528 and 20292 respectively, corresponding to the fully developed turbulent flow regime.

According to the experimental results, for an air injection speed of 2 m/s in the combustion chamber inlet duct, the best organoleptic rating of 83.21/100 was found for the Catuaí coffee variety, with a roasting time of 14.5 min (870 s) and a development time of 120 s (870 s); tasters found improvements in their sensory descriptors to a clean, smooth, sweet finish with sweet tangerine acidity and exotic flavor. This is due to a delay in the cooking times and a better penetration of the thermal energy in the coffee, which releases volatile elements contained within the bean.

From the numerical point of view, the average temperature profiles distributions of the coffee beans showed different baking slopes, which varied from an almost linear behavior at a speed of 1 m/s, to a logarithmic trend at a speed of 3 m/s. In the latter case, the cooking times were the longest, affecting both the energy consumption of the machine and the organoleptic properties of the device. This work finds relevance given that most of the works are oriented to the type of machine used to extract flavors from a certain variety of roasted coffee beans, but very few have been oriented to the roasting process itself. This is very important, since it provides added value for the promotion of domestic consumption and the export of coffee as a processed product.

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