Simulation of coffee fruit drying using computational fluid dynamics

Rudney Amaral¹, Ednilton Tavares de Andrade², Francisco Carlos Gomes³, Flávio Meira Borém⁴, Isabela Avila Lemos⁵, Camila de Almeida Dias⁶

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ABSTRACT: Drying is a fundamental step in post-harvest handling of coffee because moisture content at the end of drying affects several important aspects, such as sensory quality, storability, and color of the fruit coffee. Within this context, the aim of this study is to determine water distribution within the natural coffee fruit during and at the end of the drying process. For that purpose, simulations were made through finite elements using computational fluid dynamics. Experimental data on moisture content of coffee fruit in the “cherry” stage were collected during drying, which was carried out at a temperature of 40°C and relative humidity of 25% to 0.18 decimal (dry basis – d.b.) to compare the results of the experiment with the results of the simulations. Ten mathematical models of the drying process were developed for the collected data. The two-term exponential model best fit the data. The results of the simulations in computational fluid dynamics were compared to the results from experimental drying, and a satisfactory fit was obtained. The effective diffusivity coefficient ($D_{eff}$) was developed for the model proposed, obtaining the value of $2.87 \times 10^{-11}$ m² s⁻¹. At the end of drying, the model exhibited 57.1% of the projection area of the coffee fruit with moisture content below 0.18 decimal (d.b.). Thus, the model can be used for other applications.

Index terms: Moisture content, distribution, natural coffee, finite elements, diffusion.

1 INTRODUCTION

Coffee has a prominent position in Brazilian grain production, with 349.9 million dollars in exports, according to the Informe Estatístico do Café (2018).

The drying stage is fundamental in coffee to prevent the growth of microorganisms and fermentations that can compromise the quality of newly-harvested coffee, which has high moisture content and uneven maturity of the coffee fruit (berries) (RESENDE et al., 2009). The temperature of the coffee fruit must be strictly controlled because an excessive increase in temperature greatly affects its quality. Coffee should be dried at a temperature of 40°C for this operation not to affect beverage aroma and flavor (BORÉM, 2008).

Air flow during coffee drying has an effect only at the beginning of drying (Burmester; Eggers, 2010). In drying coffee fruit at low relative humidity, an increase in temperature brings about an increase in the effective diffusivity coefficient ($D_{eff}$), which ranges from 1.908 to $3.721 \times 10^{-11}$ m² s⁻¹, as well as in drying rate (Alves, et al. 2013).

Nilnont et al., (2012) modeled drying in parchment coffee through finite elements. Through this modeling, they obtained a model sufficient for predicting moisture content during the drying process. According to the authors, the two-dimensional model provides better understanding of transport processes in different components of parchment coffee. The mean values of the coefficient of liquid diffusion of the coffee bean

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¹²³⁴⁵⁶ Universidade Federal de Lavras/UFLA - Departamento de Engenharia/DEG - Cx. P. 3037 - 37.200-000 - Lavras - MG rudneyamec@yahoo.com.br, ednilton@deg.ufla.br, fgomes@deg.ufla.br, flavioborem@gmail.com, isa_lemosti@hotmail.com, camila.almeidadias@gmail.com

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and of the coefficient of liquid diffusion of the parchment found by the authors are $7.173 \times 10^{-10}$ and $6.737 \times 10^{-13}$ m$^2$ s$^{-1}$, respectively.

During the process of drying agricultural products, conditions are considered isothermal, and water transfer is restricted to the surface of the product (Bergman, et al. 2011). Thus, the aim of this study was to determine the distribution of moisture content within natural coffee fruit during and at the end of the drying process. A computational fluid dynamic model was used to describe the process of heat and matter transfer within the fruit. This model allows analysis of the liquid diffusion rate in the coffee fruit during drying, as well as the distribution of moisture content at the end of drying.

2 MATERIALS AND METHODS

Mature or “cherry” coffee fruit (Coffea arabica L. cv. Catuai Vermelho) was used. The fruit was harvested manually. Fruit with lower specific weight (shriveled, floaters, etc.) were removed through separation in water. The fruit had average moisture content of 2.11 decimal (dry basis – d.b.) at the beginning of drying. The moisture content of the coffee fruit was determined by the standard method of ISO 6673 (INTERNATIONAL ORGANIZATION for STANDARDIZATION - ISO, 2003).

Before the beginning, during, and at the end of mechanical drying, the main dimensions of 10 samples of the coffee fruit were measured. These measurements were made with a digital caliper rule with 0.01 mm readability, resulting in the mean dimensions shown in Table 1.

The volume of the coffee berry (V) was calculated by equation 01. The coffee berries were considered as oblate spheroids. The equivalent radius of the coffee berries was also calculated, defined as the radius of a sphere with volume equivalent to the volume of the berry.

$$V = \frac{4}{3} \pi (abc)$$

In which V is the volume at each level of moisture content (m$^3$), a is the length (m), b is the width (m), and c is the thickness (m).

The samples were weighed on a precision digital balance with 0.01 g readability. The true specific weight before drying the fruit was calculated by the simple ratio between weight and volume, as well as the true specific weight at the end of drying. The true mean specific weight of the fruit during the drying process was also calculated.

The system for drying the samples was composed of an air conditioning unit coupled to a fixed bed dryer (Figure 1).

The laboratory air conditioning system (LACS) was used to control the characteristics of the drying air according to the model proposed by Fortes et al. (2006). This equipment allows control of the flow, temperature, and relative humidity of the drying air and is composed of a cooling system with three air conditioning units. The dryer included four removable square trays perforated at the bottom, with sides of 0.3 m and depth of 0.1 m, located over a plenum to make the air flow uniform. The temperature of the drying air was measured in the plenum, under the perforated trays, by thermocouples connected to universal controllers (Novus N1100). A digital hygrometer inserted in the plenum measured the relative humidity of the drying air. A frequency inverter (Weg CFW-10) controlled the rotation of the centrifugal fan that blows the heated air into the plenum; it thus regulated the air flow.

The procedure began by completely filling the perforated-bottomtrays. For each hour of drying, the trays were removed from the dryer and weighed on an analytical balance with 0.01 g readability. This procedure was repeated until the fruit was dried to 0.18 decimal (d.b.); the standard laboratory oven method (BRASIL, 2009) was used to determine the moisture content of the fruit. Total drying time was 109 hours. The tray position was revolved 90° every hour to minimize possible differences of temperature and air flow among the perforated-bottomtrays.

### TABLE 1 - Dimensions of natural coffee fruit

| Axis     | Dimension (m) | Dimension used (m) |
|----------|---------------|--------------------|
| Length (a) | $1.4 \times 10^{-3}$ | $7 \times 10^{-3}$ |
| Width (b)  | $1.1 \times 10^{-3}$ | $5.5 \times 10^{-3}$ |
| Thickness (c) | $0.9 \times 10^{-3}$ | $5.5 \times 10^{-3}$ |
The air flow variables of the drying air were kept constant throughout the procedure – the temperature was 40°C, relative humidity was 25% and air speed was 0.33 m s\(^{-1}\), for a flow of 20 m\(^3\) min\(^{-1}\) m\(^{-2}\).

For the drying conditions of this study, the equilibrium moisture content of the fruit was calculated using the model proposed by Afonso Júnior (2001) and cited by Borém (2008) for “cherry” fruit (Equation 2).

\[
EMC = (2.0222 + (0.02887) - (18.7397 RH\(^{0.0101}\))) \times 10^{-3} \quad (2)
\]

In which is the equilibrium moisture content (d.b.), \(T\) is the drying air temperature (°C), and \(RH\) is the relative humidity of the drying air (decimal).

The moisture ratio was calculated from fitting equation (3) to the data observed using the STATISTICA® 5.0 (Statsoft, Tulsa, USA) software. The moisture ratio (MR) is essential for describing different drying models in a thin layer. Equation (3) is the analytical solution for Fick’s second law, considering the geometric form as spherical and considering the surface contour condition as known (Brooker et al., 1992).

\[
MR = \frac{M - EMC}{M_i - EMC} = 6 \sum_{n=1}^{\infty} \frac{1}{n^2} \exp \left[ -\frac{n^2 \pi^2 D t}{9} \right] \left( \frac{3}{R} \right)^2 \quad (3)
\]

in which MR is the moisture ratio of the product, adimensional; \(M\) is the moisture content of the product, decimal (d.b.); EMC is the equilibrium moisture content of the product, decimal (d.b.); \(M_i\) is the initial moisture content of the product, decimal (d.b.); \(D\) is the effective diffusivity coefficient (m\(^2\) s\(^{-1}\)), and \(R\) is the equivalent radius of the coffee fruit (m).

The mathematical models disposed in Table 2 by Equations (4) to (14) were fitted to the experimental data of coffee drying.

For the purpose of understanding heat and mass transfer in coffee fruit during drying, the distribution of moisture content can be identified within the coffee berry by mathematical modeling. Under computational fluid dynamics, hypotheses can be analyzed more easily since computational fluid dynamics is a technique that has been used for evaluation of various physical phenomena using the finite element method. This technique is a set of computational tools based on numerical algorithms to solve and interpret problems in the flow of fluids (Schneider; Maliska, 2000).

For fluid flows, the mathematical model is based on equations of conservation of the amount of movement, conservation of mass, and conservation of energy. Analytical solution of these equations is only possible for very simple flows.
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TABLE 2 - Mathematical models used to predict drying.

| Model                  | Equation                                                                 |
|------------------------|---------------------------------------------------------------------------|
| Diffusion Approximation| $MR = a \cdot \exp(-k \cdot t) + (1 - a) \cdot \exp(-k \cdot b \cdot t)$ (04) |
| Two Term               | $MR = a \cdot \exp(-k_0 \cdot t) + b \cdot \exp(-k_1 \cdot t)$ (05)     |
| Two-Term Exponential   | $MR = a \cdot \exp(-k \cdot t) + (1 - a) \cdot \exp(-k \cdot a \cdot t)$ (06) |
| Logarithm              | $MR = a \cdot \exp(-k \cdot t) + b$ (07)                                  |
| Midilli                | $MR = a \cdot \exp(-k \cdot t) + b \cdot t$ (08)                        |
| Newton                 | $MR = \exp(-k \cdot t)$ (09)                                            |
| Page                   | $MR = \exp(-k \cdot t^n)$ (10)                                          |
| Modified Page          | $MR = \exp(-k \cdot t^n)$ (11)                                          |
| Thompson               | $MR = \exp((-a \cdot (a^2 + 4 \cdot b \cdot t)^{0.5}) / 2 \cdot b)$ (12) |
| Verna                  | $MR = a \cdot \exp(-k \cdot t) + (1 - a) \cdot \exp(-k_1 \cdot t)$ (13) |
| Wang and Singh         | $MR = 1 + at + bt^2$ (14)                                                |

MR is the moisture ratio (dimensionless); $k, k_0, k_1$ are drying constants (s\(^{-1}\)); $t$ is the drying time (h); $a, b, n$ are constants that depend on the nature of the product (dimensionless). (BROOKER et al., 1992; Corrêa et al., 2001; Alves et al., 2013; Filho et al., 2015).

To analyze real problems in which strong temporal variations and turbulence are found, numerical methods are used that are able to analyze flows in a general manner through discretization of the equations cited. Computational fluid dynamics is divided into three basic steps: the first is pre-processing, in which the geometry and the numerical mesh is generated and the contour conditions are defined; the second step is processing, which is solution of the mathematical equations using discretization; and the third step is post-processing in which the information, graphs, and analyses generated in the solution are visualized (SILVA et al., 2012).

According to Crank (1975), there is an analogy between thermal conduction and liquid diffusion. The mathematical theory of diffusion in isotropic bodies is based on the hypothesis that the transfer rate of a substance diffused through the unit area of a section is proportional to the gradient of concentration measured normally at the section. In an analogous manner, the transfer rate of heat through the unit area of a section is proportional to the temperature gradient measured normally at the section. Table 3 shows the analogy between the two processes:

The analogy between liquid diffusion and thermal conduction was used to develop the computational simulation of coffee drying using modeling by the commercial software ANSYS® ED® (version 9.0) through programming in APDL (Ansys Parametric Design Language) language.

To carry out simulations, geometry that corresponds to one fourth of a coffee berry (axisymmetric) was chosen, as shown in Figure 2, considering axial symmetry of the coffee berry.

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The main dimensions of “cherry” coffee fruit were measured with a digital caliper rule with 0.01 m readability. The main dimensions of a coffee berry are shown in Table 1. The a and b values of 6.9132 x 10^{-3} m and 5.7347 x 10^{-3} m, respectively, were used for the geometry implemented.

A thermal element called PLANE77 (Figure 3) was chosen, which is a two-dimensional quadrangular element with eight nodes applicable to two-dimensional thermal analyses according to Ansys (2011) to make up the computational mesh. The mesh was regular with its three sides divided into the same number of elements. This procedure divided the geometry presented into 507 elements and 1600 nodes (Figure 4).

The initial conditions and the contour conditions were also defined in pre-processing.

The effective diffusivity coefficient (\(D_{\text{eff}}\)) used in the simulation was fitted to the real data to represent the experimental data.

The total fruit drying time in the computational model was 109 hours, which was the same time obtained experimentally with the fruit in order to dry to mean moisture content of 0.18 decimal (d.b.).

The initial condition used for solution of the problem was to apply the same concentration of moisture content to all the nodal points of the mesh. For that purpose, the initial concentration of moisture content was calculated at 861.55 kg(H\(_2\)O).m\(^{-3}\). This value was obtained from the product of the fruit moisture content in dry basis and the specific weight of the fruit. This initial condition corresponds to moisture content of 2.11 decimal (d.b.). For the value of specific weight, its mean variation in time was considered, obtaining the value of 1305 kg m\(^{-3}\). The dry matter part of this specific weight was considered for use of the model (408.3 kg m\(^{-3}\)).

**TABLE 3** - Analogy between liquid diffusion and thermal conduction.

| LIQUID DIFFUSION                          | THERMAL CONDUCTION                  |
|-------------------------------------------|-------------------------------------|
| Occurs through random movements           | Occurs through random movements     |
| Fick 1855                                  | Fourier 1822                        |
| D is the diffusion coefficient             | K is thermal conductivity           |
| C is concentration of the substance        | is temperature                      |

\[ F(t) = -D \frac{\partial C}{\partial x} \]

\[ F(t) = -K \frac{\partial \theta}{\partial x} \]

\(F\) is the diffusive flux and/or heat flux.

**FIGURE 2** - Representation of a coffee berry as an oblate spheroid.

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The concentration of equilibrium moisture content was applied on the outside surface of the fruit, represented by the arc in the geometry implemented in the simulations. The concentration of equilibrium moisture content is the product of the equilibrium moisture content of the coffee fruit (calculated by equation 02) and its specific weight. The value of the concentration of the equilibrium moisture content was calculated at 34.53 kg(H₂O).m⁻³.

Considering the above, the source program was developed from the menu of commands available in the library of the Ansys® software, applying the initial conditions and contour conditions calculated. Thus, the problem of the process for removing water from the coffee fruit was resolved.

Through simulation, the nodal values of concentration of moisture content were obtained in each minute of the drying process, as well as the distribution of moisture content within the fruit. The simulation came to an end exhibiting 720 iterations in all.

To evaluate the efficiency of the model developed computationally in APDL language for liquid diffusion of the coffee fruit, the results of the model were compared to the results obtained experimentally. The moisture ratio curve for the two cases was compared.

The mean relative error (P) was calculated by equation 16 from the drying curves obtained by the computational model in order to carry out statistical parameterization.
3 RESULTS AND DISCUSSION

The mean calculated volume of the coffee berry before drying was $9.922 \times 10^{-5}$ m$^3$. The mean measured weight of the coffee berry was 1.52g and the true specific weight of the fruit before drying was 1540.69 kg m$^{-3}$. At the end of drying, when the fruit had a moisture content of 0.18 decimal (d.b.), the true specific weight was 918.84 kg m$^{-3}$, and the true mean specific weight during drying was 1305 kg m$^{-3}$.

The initial equivalent ratio of the samples was $6.18 \times 10^{-3}$ m, and the equilibrium moisture content was 8.458 $\times 10^{-2}$ decimal (d.b.).

The moisture ratio according to time was calculated by equation (03). Figure 5 shows the comparison of the simulated values and the experimental values for the variation of the moisture ratio (MR) as a function of time by the two-term exponential model, which best fit the experimental data. In Table 4 are the values of the coefficient of determination ($R^2$), mean relative error ($P$), standard deviation of the estimate (SE), chi-square and the constants of the two-term exponential model. This model exhibited satisfactory values of the mean relative and estimated errors, as well as a high coefficient of determination ($R^2$). Values of mean relative error below 10% mean a good fit of data to the drying phenomenon according to Madamba et al. (1996) and confirmed by Mohapatra and Rao (2005).

The effective diffusivity coefficient ($D_{\text{eff}}$) was calculated at the value of $1.86 \times 10^{-11}$ m$^2$ s$^{-1}$. This result is corroborated by Alves et al. (2013), who found a variation of this coefficient from 1.908 to $3.721 \times 10^{-11}$ m$^2$ s$^{-1}$.

Table 4 - Coefficient of determination ($R^2$, %), mean relative error ($P$, %), standard deviation of the estimate (SE), chi-square ($\chi^2$), and the constants of the two-term exponential model.

| Temperature | Statistical parameter | Constants of the model |
|-------------|-----------------------|------------------------|
|             | $\chi^2$ P SE $R^2$ a b k |
| 40°C        | 0.0004 0.73 0.022 99.99 | 30.467 0.9789 -0.0302 |

$$MR = -30.4672 \cdot \text{exp}(-0.0302 \cdot t) + (31.4672) \cdot \text{exp}(-0.0296 \cdot t)$$

$R^2 = 99.99\%$

- Moisture ratio (Experimental)
- Moisture ratio (Simulated)

Figure 5 - Values of the experimental and simulated moisture ratio by the two-term exponential model for drying of coffee fruit as a function of time (h).
The value obtained for the effective diffusivity coefficient \( (D_{\text{eff}}) \) that best fit the experimental data was \( 2.87 \times 10^{-11} \text{ m}^2\text{s}^{-1} \). This value is in agreement with the results presented in the study of Isquierdo (2011), who studied the drying kinetics for natural coffees under different temperatures and relative humidities of the drying air and concluded that the effective diffusivity coefficient ranges from \( 1.460 \times 10^{-11} \) to \( 3.993 \times 10^{-11} \text{ m}^2\text{s}^{-1} \). This is also in agreement with the result obtained by Alves et al. (2013), who obtained the effective diffusivity coefficient \( (D_{\text{eff}}) \) of water in coffee fruit ranging from \( 1.908 \times 10^{-11} \) to \( 3.721 \times 10^{-11} \text{ m}^2\text{s}^{-1} \). The value obtained in a computational manner for the effective diffusivity coefficient \( (D_{\text{eff}}) \) is a mean value since the components of a coffee berry were not considered, such as the parchment. In fact, each component has a specific effective diffusivity coefficient \( (D_{\text{eff}}) \).

The knowledge of the distribution of water inside the fruit provides better drying, seeking mechanisms to accelerate the process without compromising its structure and quality, enabling the development of new forms and more efficient drying equipment. In addition, it is possible to obtain a better way of handling the drying in order to maintain the quality of the product with a less aggressive drying. Distribution of the moisture content within the coffee berry at the end of the drying process for the berries analyzed in this study is shown in Figure 6. Each color in the Figure indicates a range of concentration of moisture content.

The numbered areas in Figures 6 and 7 were calculated, as well as the percentage of each one in relation to the area of the entire berry.

In Table 05, the approximate percentage of each area of Figure 07 is shown.
Area 1 (shown in blue) is the largest and the one that lost most water, as expected, because it is the outside surface of the berry. A band composed of the sum of areas 1, 2, 3, and 4 is equivalent to 57.1% of the total area of projection of a coffee berry. In Table 04, the values of the range of concentration of moisture content in each area are shown. In areas from 1 to 4, the highest concentration of moisture content is 74.06kg(H2O)m-3, equivalent to 0.18decimal (d.b.) of moisture content.

The evolution of the liquid diffusion process of moisture content in coffee fruit over the drying time is illustrated in Figures 08 and 09, for which each figure represents 24 hours of evolution of the liquid diffusion process.

Figures 8 and 9 show that evolution of the water diffusion process within the coffee berry is inversely proportional to drying time; that is, liquid diffusion is increasingly slower over time. This generates greater difficulty in removing water from the fruit at the end of drying, thus increasing the risks of losses in product quality. This is in agreement with several studies already described in the literature, such as the study of Saath et al. (2010).

Figure 10 shows the liquid diffusion that occurred within a coffee berry during simulation in vector format. The difficulty of removing water from the points nearest the center of the berry can be noted from the figure.

Figure 11 shows the values of concentration of moisture content (kg(H2O)m-3) for some nodal points of the computational mesh as a function of time. From Figure 11, it can be observed that in the center of the berry, moisture content is higher. The line that represents the drying curve for nodal point 08 is very different from the drying curve of nodal point 48. This occurs because nodal point 08 is at 0.12 x 10^-2 m from the center of the berry and nodal point 48 is at 0.54 x 10^-2 m from the center of the berry. In addition to the drying curves of nodal points 08 and 48, Figure 11 shows the drying curves for nodal points 18, 28, and 38 indicated in Figure 7.

The values of moisture ratio for the experimental data compared to the simulated data as a function of time are shown in Figure 12. The simulation carried out adequately represents coffee fruit drying. The experimental data and simulated data matched satisfactorily. Thus, the model can be used for other applications that require representation of this phenomenon. The mean relative error (P) was 1.8%, which is considered satisfactory.

| No. | Area (m²) | Equivalence (%) | Water concentration (kg(H₂O)m⁻³) | Moisture content decimal (d.b.) |
|-----|-----------|----------------|----------------------------------|-------------------------------|
| 1   | 2.09E-05  | 16.4           | 34.54 – 44.42                    | 0.08 – 0.11                   |
| 2   | 1.75E-05  | 13.7           | 44.42 – 54.30                    | 0.11 – 0.13                   |
| 3   | 1.67E-05  | 13.1           | 54.30 – 64.18                    | 0.13 – 0.16                   |
| 4   | 1.77E-05  | 13.9           | 64.18 – 74.06                    | 0.16 – 0.18                   |
| 5   | 1.21E-05  | 9.5            | 74.06 – 83.94                    | 0.18 – 0.21                   |
| 6   | 1.19E-05  | 9.4            | 83.94 – 93.82                    | 0.21 – 0.23                   |
| 7   | 1.12E-05  | 8.8            | 93.82 – 103.70                   | 0.23 – 0.25                   |
| 8   | 9.65E-06  | 7.6            | 103.70 – 113.58                  | 0.25 – 0.28                   |
| 9   | 9.72E-06  | 7.6            | 113.58 – 123.46                  | 0.28 – 0.30                   |
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**FIGURE 8** - Visualization of the field of moisture content for 24 and 48 hours of drying.

**FIGURE 9** - Visualization of the field of moisture content for 72 and 96 hours of drying.

**FIGURE 10** - Vector representation of liquid diffusion that occurred within the coffee berry.
According to the results obtained in this study, we conclude that:
- The model developed in a computational manner by the technique of computational fluid dynamics for drying natural coffee fruit satisfactorily fit the experimental data with a mean relative error of 1.8%.
- For drying air temperature of 40°C and relative humidity of 25% at the end of drying, 57.1% of the area of projection of natural coffee fruit has moisture content below 0.18 decimal (d.b.).
- The effective diffusivity coefficient found by the model was $2.87 \times 10^{-11}$ m$^2$ s$^{-1}$.

4 CONCLUSIONS

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