www.foodandfeed.fins.uns.ac.rs
FOOD AND FEED RESEARCH
Journal of the Institute of Food Technology – FINS
University of Novi Sad
ISSN
2217-5369
(print version ceased in 2023)
2217-5660 (online)

UDK 663.74+581.48]:536.2:631.563.2
https://doi.org/10.5937/ffr0-62719

Original research paper

MODELING OF THE HEAT AND MASS TRANSFER IN DRYING OF FERMENTED CACAO (*THEOBROMA CACAO L.*) BEANS

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Abstract: A three-dimensional finite element model consisting of 108 cacao beans was developed to simulate heat and mass transfer during forced convection drying. The model evaluated temperature distribution within the drying chamber and individual beans as influenced by airflow, while physical and thermodynamic properties were computed and applied within the simulation. Model performance was validated experimentally, showing good agreement between simulated and observed moisture and temperature profiles. Moisture content data yielded RMSE values of 2.538 and 2.221 g water/g dry matter, while temperature RMSE ranged from 2.19–3.30 °C at 50 °C and 2.78–3.62 °C at 60 °C, indicating acceptable deviation. Results showed that beans positioned at the tray edges and upper layers exhibited higher internal temperatures than those in the bottom layer. These findings suggest that rearranging beans 60–90 minutes into the drying process may enhance drying uniformity and product quality. The presented 3D multi-bean model constitutes a significant advancement over traditional single-seed modeling approaches and provides a useful tool for optimizing cacao drying processes, with potential applicability at industrial scale.

Key words: *cacao bean processing, convective drying, Finite Element Modeling, heat and mass transfer, numerical simulation*

INTRODUCTION

The cocoa-chocolate global value chain (GVC) links producers of cocoa, also known as cacao, beans with chocolate manufacturers and consumers, forming a multimillion-dollar industry. According to both the International Institute for Sustainable Development and the International Cocoa Organization, the production of cocoa is predominantly located in developing countries, while the manufacturing and distribution of the final products occur in developed nations (IISD, 2022; ICCO, 2023). Over the last ten years, there has been a significant increase in chocolate demand, leading several countries already involved in the cacao industry to enhance their production, and prompting other nations to join the value chain. The Philippines, with its potential to produce cocoa beans, should leverage the rising global demand and the need for more contributors in the value chain. According to the report from MarkNtel Advisors, the Philippines chocolate market size was valued at around US$ 419.11 million in 2024 and is projected to reach

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USD 707.52 million by 2030 (Markntel Advisors, 2025) . The cocoa-chocolate global value chain (GVC), with cocoa beans as a vital product, is also growing swiftly. Over the past ten years, total trade in the cocoa-chocolate GVC has doubled, reaching nearly US$44 billion in 2015. In terms of value, chocolate exports account for 56% of the total exports in the industry, with cocoa beans at 20%, cocoa butter at 12%, cocoa liquor/paste at 7%, and cocoa powder at 5% (Fernandez-Stark, Hamrick & Daly, 2017).

Cacao *(Theobroma cacao)* also called the cacao tree, is a well-known tropical plant extensively cultivated for its beans. Its seeds, also known as cacao beans, are used to make tableau, cacao powder, nibs, butter, and paste/liquor, which are the primary raw materials for chocolate production. These goods are popular not just in the chocolate industry, but also in the cosmetics and medicinal sectors. Cacao production is labor-intensive and is mostly done by hand, making it a valuable source of income. The cacao-chocolate industry is a million-dollar sector that connects cacao bean producers with chocolate manufacturers and consumers. Based on the latest report of the Philippine Statistics Authority (PSA), cacao yielded a total of 8,024.02 volume of production in 2023 for the whole Davao Region and 8,031.97 in 2022 (Philippine Statistics Authority, 2023). When compared to other global and regional players, the Philippines' current output is limited, generating slightly more than US$18.6 million in exports in 2024 (OEC, 2024). Throughout the country, cacao is extensively cultivated on the island of Mindanao, specifically in the provinces of Davao, Zamboanga Peninsula and Northern Mindanao (Magallon, Patalinghug & Tangalin, 2022; Philippine Statistics Authority, 2023; Gonzales & Janaban, 2024; Penora & Magallon, 2024).

The growing demand for cacao and chocolate products both in the international and local markets presents its promising contribution to the country's economic development. Despite the promising demand for cacao, producing high quality beans remains challenging. Factors affecting the quality of cacao beans include, but are not limited to, low production of cacao as a primary raw material, poor-quality cacao beans as a result of varied standards of the fermentation process, mold growth and infestation of pests, varied fermentation periods, poor post-harvest handling and processing, specifically drying procedures, and storage of dried beans (Kongor et al., 2016; Santander et al., 2025).

The finished product quality of chocolate is often affected by the post-harvest treatments that the cacao beans undergo (Adeyeye, Akinyeye, Ogunlade, Olaofe & Boluwade, 2010; Subroto, Djali, Indiarto, Lembong & Baiti, 2023). The post-harvest treatment of cacao beans includes sorting, ripening the fruit, breaking/splitting the fruit, fermenting, drying, and storage. These treatments help initiate the formation of chocolate flavor precursors and affect the brown coloration of finished chocolate products (Subroto et al., 2023).

Although drying and fermentation have complementary effects on bean quality, poorly done drying can produce very low-quality beans from well-fermented cocoa beans because heat treatments have different effects on bean quality parameters (Mbonomo, Medap, Brecht & Eyame, 2016).

In an attempt to optimize the drying process and obtain optimal cacao bean quality with minimal cost, several modifications in drying parameters have been carried out. Several studies have been done on the various drying methods, such as oven, freeze, heat pump, and microwave drying, to improve the quality of cacao beans; however, their high cost limits large-scale application (Hii, Law & Law, 2013; Banboye, Ngwabie, Eneighe & Nde, 2020; Dzelagha, Ngwa & Nde Bup, 2020a). These drying technologies vary in their performance affecting the quality of the cocoa beans. Ndukwu (2009) have studied the effect of drying temperature and air velocity under different drying conditions of cocoa bean.

Pod storage in combination with drying temperature was also studied (Streule, Freimüller Leischtfeld, Chatelain & Miescher Schwenninger, 2024). Energy parameters, vibrational spectroscopy, and changes in bioactive compounds of cocoa beans were also investigated during thin-layer hot air drying from 50 °C - 70 °C (Jiménez-Rodríguez et al., 2024). In addition to the studies focused on the effect of temperature on cacao beans, several mathematical approaches were likewise explored (Djedjro, Assidjo, Patrice & Yao, 2009; Okonkwo & Okorie, 2019; Sahadeo, Sukha, Chadee, Umaharan & Clarke, 2024).

There are many reported drying processes used to reduce the moisture content in cacao beans

(Dzelagha, Ngwa & Nde Bup, 2020b; Zulkarnain, Shahriman & Yudin, 2020; Ackah & Dompey, 2021). However, reviews of the literature show limited studies examining the effect of temperature and airflow on the quality of cacao beans (Faborode, Favier & Ajayi, 1995; Jiménez-Rodríguez et al., 2024).

There are several methods used in the assessment of the quality of dried products. One of the approaches used in the engineering principles uses finite element modeling to understand the distribution and velocity into the drying chamber; there are several reports that use FEM in the study of cereals (Carvalho et al., 2021; Jha & Tripathy, 2021; Li, Yang, Wang & Du, 2023; Yang et al., 2023; Zhou et al., 2024). There are very few articles that use FEM to study the drying of cacao beans. A research study was conducted that used a single geometry of cacao bean (Komolafe, Waheed, Chidozie & Hii, 2021; Castillo-Orozco, Garavitto, Saavedra & Man-tilla, 2023). Similarly, in a study of Adrover and Brasiello (2020), they used quarter model of a cacao bean. There were no finite element analysis studies that used multi beans to understand the temperature distribution in the drying chamber during the drying of cacao beans. This study aims to: (1) investigate and understand the drying characteristics of cacao beans in multiple layers; (2) characterize the temperature distribution during drying within single and double layers; and (3) develop a 3D finite element model to predict temperature distribution, drying duration, effective moisture diffusivity, and moisture distribution. These parameters are critical in controlling the product quality of dried cacao beans. The current work extended the previous study by Adrover and Brasiello (2020), Castillo-Orozco et al. (2023) and Komolafe et al. (2021) to obtain a better drying model.

MATERIALS AND METHODS

The method used in this present study used a combination of steps from drying experiments for the cacao beans and as well as performing a finite element modeling. To illustrate the methods used, Fig. 1 is shown below.

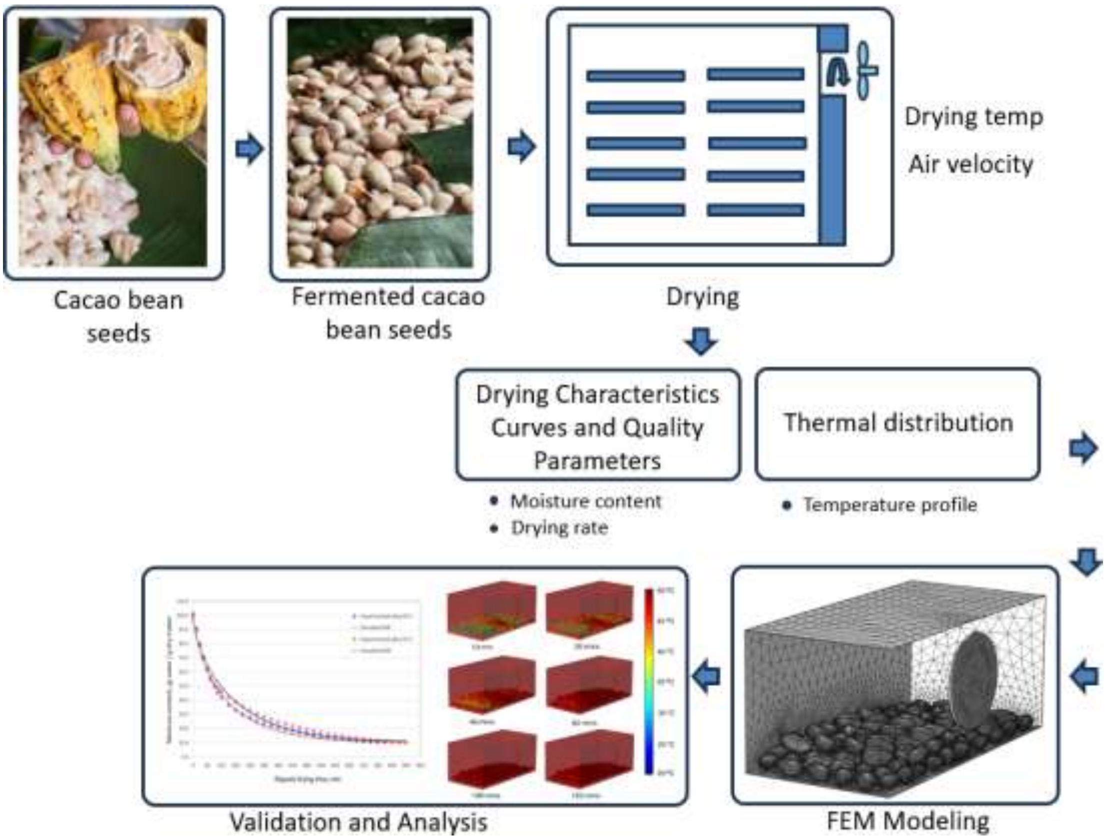


Figure 1. Schematic presentation of the methods applied in the experiment.

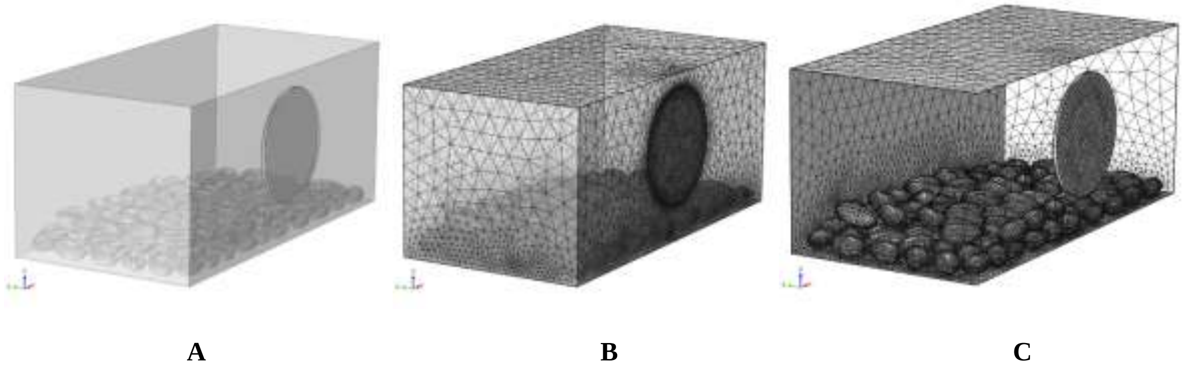


Figure 2. 3D Finite Element Model showing both A) unmeshed; B) transparent meshed geometry; C) meshed geometry with 2 faces of the rectangular geometry hidden

3D Finite Element Model Formulation

The 3D model was created using a 20 cm x 10 cm x 8 cm rectangular cuboid with 108 embedded ellipsoids (Fig. 2). The mathematical model represents cacao beans ellipsoids. The ellipsoids have average dimensions of the semi major (a), semi minor (b) and semi intermediate axes (c), 1.087 cm, 0.574 cm, 0.442 cm respectively. A thin cylindrical domain (r = 3 cm; h = 0.2 cm) was placed at the center of the cuboid to represent the fan blade region. The cylindrical domain is used to represent the fan blade installed in the drying chamber.

The cylindrical domain houses the axial fan where the heated air is blown throughout the entire drying chamber. The physical parameters used in the simulation are presented in Table 1. The 3D finite element model was solved using COMSOL Multiphysics solver v4.3a.

The model was solved using the Conjugate Heat Transfer and Transport of Diluted Species modules with a time-dependent solver. The mesh consisted of 891,053 tetrahedral elements, 109,280 triangular surface elements, and 12,216 edge elements.

The rectangular block and thin cylinder representing the air domain were set to a finer mesh, while the ellipsoids were assigned a normal mesh size. A fully coupled linear iterative solver with a BDF time-stepping scheme was applied. Similar solver settings were adopted in previous study of Perez, Tanaka, Tanaka, Hamanaka and Uchino (2015). The finite element analysis was computed using an Acer Nitro 5 laptop computer with 12th Gen Intel(R) Core(TM) i5-12500H (3.10 GHz) processor and 16 GB RAM.

Parameters used in the simulation

Table 1 summarizes the parameters used in the simulation. Some values were obtained through trial and error from the results of the simulation while the rest are taken from published literature (Bart-Plange & Baryeh, 2003; Giretti, Lemma, Larghetti & Ansuini, 2012; Perez et al., 2015; Koua, Koffi & Gbaha, 2017)

The physical properties of the air were modeled using both piecewise and analytic functions in COMSOL Multiphysics. Piece-wise function is defined as a single function that uses different formulas for different intervals of its domain. On the other hand, the analytic function is equal to a power series that converges to it within some radius of convergence around each point in its domain. These functions were also used in the past by Giretti et al. (2012) and Perez et al. (2015) using the same software. Below are the functions of the properties of air.

Governing equations

In numerous engineering and food processing applications, mathematical models are employed to represent both experimentally observed and theoretically derived phenomena (Djekic et al., 2019; Kumar, Vatsa, Madhumita & Prabhakar, 2021; Erdogdu, 2023; Lončar & Pezo, 2024).

These models provide a systematic framework for analyzing complex systems, predicting performance, and optimizing design and operation conditions.

Table 1.
Numerical values of the parameters for cacao beans and air used in the simulation

Parameter	**Value/Function**	**Source**
	Air properties	
Inlet velocity (m/s)	2.0	This study
Initial temperature of air (^oC)	27	This study
Inlet air temperature (^oC)	50 and 60	This study
Density of air (kg/m^3)	ρ (pA[1/Pa],T[1/K])	Giretti et al., 2012; Perez et al., 2015
Dynamic viscosity of air (Pa-s)	μ_a (T[1/K])	Giretti et al., 2012; Perez et al., 2015
Heat capacity at constant pressure of air (J/(kg-K))	C_p(T[1/K])	Giretti et al., 2012; Perez et al., 2015
Thermal conductivity of air (W/(m-K))	k(T[1/K])	Giretti et al., 2012; Perez et al., 2015
Density, ρ	pA*0.02897/8.314/T	Giretti et al., 2012; Perez et al., 2015
Dynamic viscosity, μ	-8.38278 x10^{-7} + 8.35717342 x10^{-8}T - 7.69429583 x10^{-11}T^2 + 4.6437266 x10^{-}	Giretti et al., 2012; Perez et al., 2015
Heat capacity at constant pressure, C_p	1047.63657 - 0.372589265T + 9.45304214 x10^{-4} T^{2} - 6.02409443 x10^{-}	Giretti et al., 2012; Perez et al., 2015
Thermal conductivity, k	-0.00227583562 + 1.15480022 x10^{-4} T- 7.90252856 x10^{-8} T^2 + 4.11702505 x10^{-11}T^3 - 7.43864331 x10^{-15}T^4	Giretti et al., 2012; Perez et al., 2015
	Cacao bean properties	
Density of cacao beans (kg/m^3)	828	Bart-Plange & Baryeh, 2003
Heat capacity at constant pressure of cacao beans (J/(kg-^{o}C))	2623	Koua et al., 2017
Thermal conductivity of cacao beans (W/(m-^{o}C))	1.256	This study
Total mass of dry solids (108 pcs) (kg)	3.4891 x 10^{-3}	This study
Total volume of cacao beans (108 pcs) (m^3)	120.324 x10^{-6}	This study

Furthermore, the developed mathematical models were used to simulate and predict the outcome for multiple applications irrespective of the prevailing conditions. These equations are embedded in the COMSOL Multiphysics software where it is used in obtaining the solution of the model (Giretti et al., 2012; Perez et al., 2015).

The heat and mass transfer equations used in the present study are based on Fourier's law of heat conduction, which serves as the mathematical model for describing heat transfer in solids.

$$\rho C_p \frac{\partial T}{\partial t} = \nabla.(k\nabla T) + Q \qquad \text{Eqn. 1}$$

where, ρ is the density (kg/m^3) , Cp is the heat capacity (J/kg- ^{o}C), T is the temperature at any time t, Q is the conductive heat flux and k is the thermal conductivity of the product (W/m ^{o}C).

The fluid flow that helps facilitate the heat transfer caused by the moving fluid uses the Navier-Stokes momentum equation in the conservation form.

$$\rho\frac{\partial \boldsymbol{u}}{\partial t} + \rho(\boldsymbol{u}\cdot\nabla)\boldsymbol{u} = \nabla\cdot\left[-p\mathrm{I} + \mu(\nabla\boldsymbol{u} + (\nabla\boldsymbol{u})^T) - \frac{2}{3}\mu(\nabla\cdot\boldsymbol{u})\mathrm{I}\right] \qquad \text{Eqn. 2}$$

where u is the velocity (m/s), ρ the fluid density (kg/m^3), P the pressure (N/m^2), T temperature (°C), t elapsed time (s), and | is the unit tensor.

For the fluid domain, the heat and mass transfer can be assessed using the equations shown below as:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0 \qquad \text{Eqn. 3}$$

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \boldsymbol{u} \cdot \nabla T = \nabla \cdot (k \nabla T) \qquad \text{Eqn. 4}$$

Eq. 2, is the conservative form of the Navier-Stokes equation in terms of the vector and stress tensor while the conservation of mass for the drying air is presented in Eq.3. The continuity equation, also known as the law of conservation of mass, stipulates that the mass entering a fluid system must precisely balance the mass exiting the system. Stated differently, mass is transferred from one point to another rather than created or lost, as explained by equation 3. This flow is governed by the driving force of concentration gradients.

Moreover, the heat transfer equation with consideration of fluid flow is presented in equation 4.

The mass transfer in the solid domain was modeled using

$$\frac{\partial C_i}{\partial t} + \nabla \cdot (-D_i \nabla C_i) + u \cdot \nabla C_i = R_i \qquad \text{Eqn. 5}$$

Initial and boundary conditions

The boundary conditions for the cacao beans and the drying air were expressed below as:

$$t(x,y,z)\,|_{\tau=0} = t_0 \text{ and } C(x,y,z)\,|_{\tau=0} = C_0 \qquad \text{Eqn. 6}$$

The values for the initial moisture content and temperature for the cacao beans were 102 g water/g dry matter and 26.15 ºC, respectively. The initial temperature of the ambient air is around 45.15 ºC.

Assumptions for the model

The present 3D model used the following assumptions to calculate the solutions for the drying conditions under study.

1) The cacao beans are both homogeneous and isotropic allowing for the use of a single set of material properties across the entire domain;
2) The heat and mass transfer in the air occur through conduction and convection;
3) Moisture movement and heat transfer are three-dimensional;
4) The shrinkage that occurs during drying is negligible. Shrinkage of the solid medium during drying was not incorporated in the model as it will complicate further the implementation of the finite element analysis. In addition, it will also cause trouble in executing the coupled analysis;
5) Air is considered as an ideal gas and incompressible;
6) Heat generation due to friction is also negligible;
7) The kernel-kernel conduction is negligible. Conduction occurs between two contacting surfaces. However, the software has a meshing issue between two contacting and/or overlapping surfaces. Thus, in this present study, kernel-kernel conduction was neglected;
8) No chemical reaction takes place during drying.

Preparation of materials

The cacao pods used in the present study were taken from Brgy Lingating, municipality of Baungon, Province of Bukidnon, Northern Mindanao, Philippines. Ripe cacao pods were carefully selected for the study. The cacao pods were harvested during February and March.

The cacao pods were split open to remove the ripe beans. After the beans were removed from the pods, they were placed in a plastic woven basket lined with fresh banana leaves for fermentation. The fresh cacao beans were fermented for 5 days until the slimy parts were partially removed from the seeds by the fermentation process.

After completing the fermentation period, the harvested beans were then brought to the laboratory for drying.

Drying of fermented cacao beans

The drying experiment was carried out using a laboratory dryer (UF160 Plus, Memmert, Germany). The laboratory dryer was preheated at the 50 ºC and 60 ºC temperatures for 30 minutes until the drying temperature had stabilized. The freshly fermented cacao beans were brought to the laboratory for drying. The airflow inside the laboratory oven was monitored using a digital air velocity meter (Lutron ABH 4225, Taipei, Taiwan). The temperature inside the drying chamber was also monitored using a type K thermocouple wire connected to a data logger (Model UT 320A, UNI-T Beijing China). About 157 grams of the fermented cacao beans were used in the drying experiment. The beans were placed on a prefabricated aluminum wire mesh tray with dimensions of 20 cm x 10 cm x 4 cm. Then the beans were manually arranged so that there would be two layers of beans in the middle portion of the tray while a single layer on the sides of the tray. The change in the weight of the cacao beans was monitored at intervals of 15 minutes for the first 2 hours and every 30 minutes over the duration of drying. The experiment was replicated in three trials. The average of the three replicates was analyzed for the drying characteristics curves. The drying characteristics data were used in the finite element modeling. The drying process was terminated once the weight of the samples remained constant.

Temperature monitoring in select cacao beans

During drying, temperature within the beans is affected, especially if there is clustering and double layering. Clustering and the formation of double layers of beans in the drying tray commonly occur due to an oversupply of cacao beans and insufficient drying space. Moreover, the relative position and proximity of the seed to the heat source position is also a factor in the temperature rise. Thus, monitoring of temperature increase in the cacao beans was performed. To measure the internal temperature of the cacao beans, a stainless steel wire with a diameter of approximately 1 mm was first inserted into the bean to create a cavity extending to the center of the seed. A Type K thermocouple wire connected to a data logger was then carefully inserted into this cavity (Fig. 4A). Temperature monitoring was done until readings reached stability.

Drying characteristics of the cacao beans

The change in the weight of the cacao beans was used to calculate the moisture content. The moisture content of the cacao beans expressed in g water / g of dry matter were calculated using the formula:

$$MC_{d.b.} = \frac{M_i - M_{dm}}{M_{dm}} \qquad \text{Eqn. 7}$$

The drying rate of the cacao beans was also calculated:

$$\frac{dM}{dt} = \frac{MC_t - MC_{(t+\Delta t)}}{\Delta t} \qquad \text{Eqn. 8}$$

where dM/dt is the drying rate; MC(t + Δt) is the moisture content at time, t + Δt, (g water/g dry matter); t is the time (min).

The difference between observed and predicted values for the moisture content was measured using the root mean square error (RMSE), which is used to compare simulated and experimental data. A lower RMSE suggests that the simulation and experimental data fit each other better. In essence, RMSE measures the average magnitude of errors; predictions that are more accurate are indicated by a lower value.

Validation of simulated and experimental data

The simulated data and the experimental data for the moisture content were validated using the Root Mean Square Error (RMSE) and the coefficient of determination (R^2) which is the square of the Pearson correlation coefficient (R) shown in the following equations below. The RMSE is a standard metric used to measure the differences between values predicted by a model and the actual observed values. The root mean square error has been used in the studies of several researchers (Perez et al., 2015; Murayama, Ishikawa, Genkawa & Ozaki, 2018).
The RMSE is calculated using:

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_o - y_s)^2} \qquad \text{Eqn. 9}$$

$$R = \frac{\sum_{i=1}^{n}(x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum_{i=1}^{n}(x_i - \bar{x})^2}\sqrt{\sum_{i=1}^{n}(y_i - \bar{y})^2}} \qquad \text{Eqn. 10}$$

where:
n – is the total number of measurements in each run;
y_o – the i^{th} actual or observed value;
y_i – the i^{th} simulated or predicted value;
$\sum_{i=1}^{n}$ –the sum of all the terms from i=1 to n;
x and y are the experimental and predicted values at time/place i;
$\bar{x}$ are $\bar{y}$ are the sample means.

RESULTS AND DISCUSSION

Drying characteristics of cacao beans

The drying characteristics of the cacao beans expressed in moisture content over time (g water / g dry matter) are shown in Fig. 3. The drying characteristic curves for both drying temperatures are average values from three trials. As shown in Fig. 3A, the initial moisture content of the fermented cacao beans is about 99 and 101 g water /g dry matter for 60 ºC and 50 ºC, respectively.

As anticipated, the drying characteristic curve of the cacao beans exhibited a sharp decrease in moisture content within the first 120 minutes of drying, leading to a corresponding reduction in weight. The moisture content subsequently stabilized at 10 % (g water/g dry matter) after approximately 800–900 minutes of drying. This observation is similar to the observations of Faborode et al. (1995) in the drying of fermented cacao beans. During the drying process, the bean's length, thickness, and breadth decrease as the cotyledons shrink and the testa hardens and becomes brittle. The moisture content reached stable levels after steadily declining over the 13 and 14 hours of drying period. Moisture contents between 7 % and 11% g water /g dry matter are considered good for storage.

The drying process of the cacao beans showed two drying rate periods (Fig. 3B). This observation is similar to the findings of Wan Daud et al. (1996) and Waheed and Komolafe (2019). It is observed from Fig. 3B that the drying rate formed two patterns of falling rate periods in which the slope of the first falling rate period descended steeply while flattening off at the second falling rate period. The first falling rate of the cacao beans for both drying temperatures, 50 ºC and 60 ºC, have the same steepness. On the contrary, the slope of the second falling rate period at 60 ºC is a little higher than that of the 50 ºC. To validate the similarity of the steepness of the slope during the first falling rate period in both drying temperatures, regression lines were fitted in all falling rate periods. The equation of the regression lines as well as the coefficient of determination describing the first and second falling rate periods for both temperatures are shown in Fig. 3B. The coefficients of determination R^2 of all the fitted regression lines ranged from 0.9495 to 0.9883, indicating varying degrees of fit in describing the falling rate characteristics of the cacao beans. The regression analysis between the measured and CFD-predicted final moisture content of fermented cacao beans under different drying conditions (Fig. 3C–3D) demonstrates a strong correlation between the subsample measurements and model outputs. The model achieved a high coefficient of determination (R^2 = 0.9929–0.9938), indicating excellent predictive accuracy at both drying temperatures. These results confirm that the developed CFD model provides a robust and reliable tool for predicting moisture content in cacao beans during drying.

Simulated air and bean temperatures inside the drying chamber

In most drying systems, cacao beans are scattered over the drying trays either in single and multiple layers. In times where there is abundance of cacao beans with limited drying trays, over stacking of cacao beans in drying trays happen. To simulate this scenario, cacao beans stacked and dried in single and double layers are simulated for this purpose and shown in Fig. 2A-C. Cacao beans situated in the left, right, and both the top and bottom layer in the middle sections of the drying tray were monitored for temperature profiling. Results of the temperature profiling are shown in Fig. 4C-4D. The quality of dried cacao beans is often affected by the drying temperature. Because cacao beans are typically dried in batches, overlapping or layering of beans is un-avoidable, particularly when the drying tray is insufficiently large to hold the intended volume, resulting in double or triple layers of beans. In this manner, the rate of heat transfer is slowed down in those sections where there are double or triple layers of the cacao beans.

This scenario does not only happen in sun drying but also in mechanical dryers. To better understand the rate of heat transfer during drying with beans placed on top of the other beans, the temperature profile in cacao beans dried in more than one layer requires monitoring. The temperature of the cacao beans in a single layer located in the outer boundary of the drying tray gradually increased during the first 30-150 minutes of drying before reaching stable values during drying.

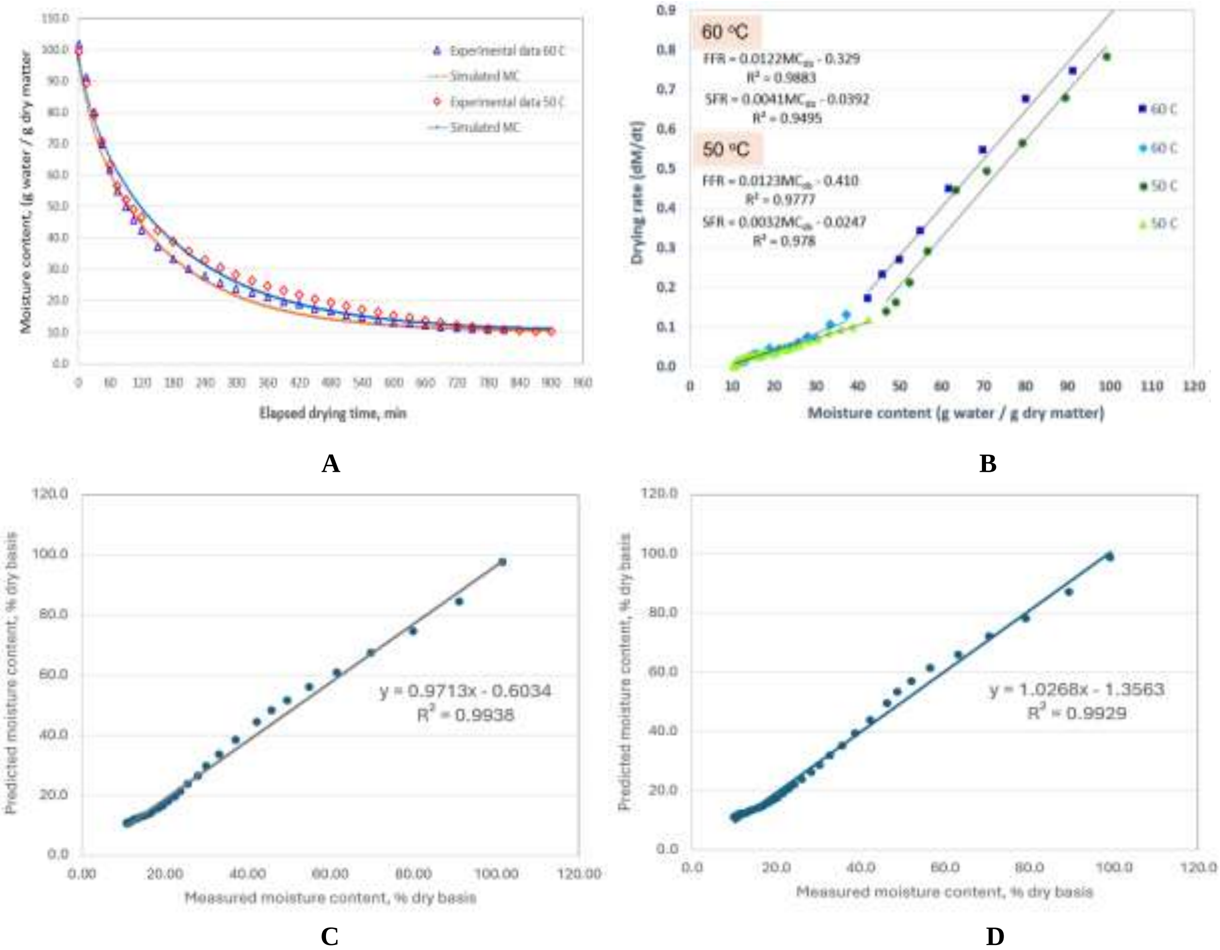
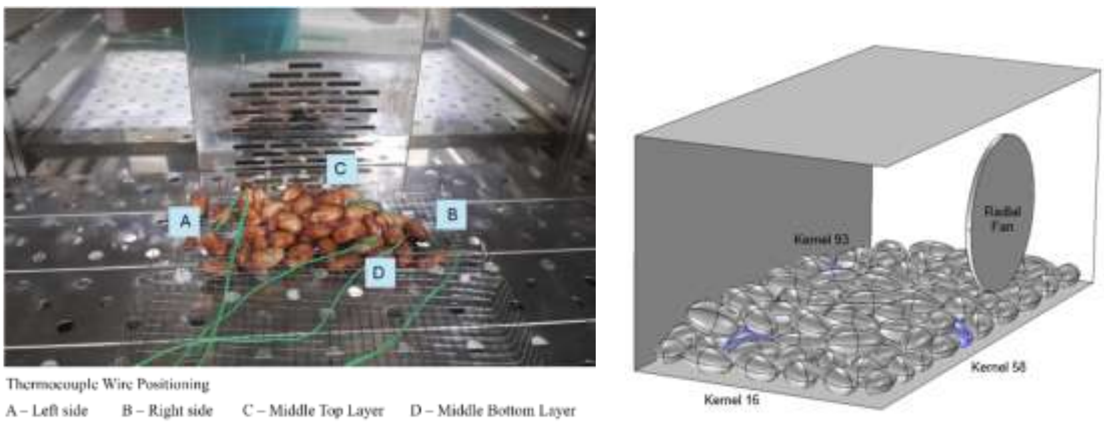


Figure 3. Drying characteristics of the cacao beans dried at the two drying temperatures. A) reduction of moisture; B) drying rate curves; C) regression line for the moisture content at 50 ^{o}C; and D) regression line for the moisture content at 60 ^{o}C



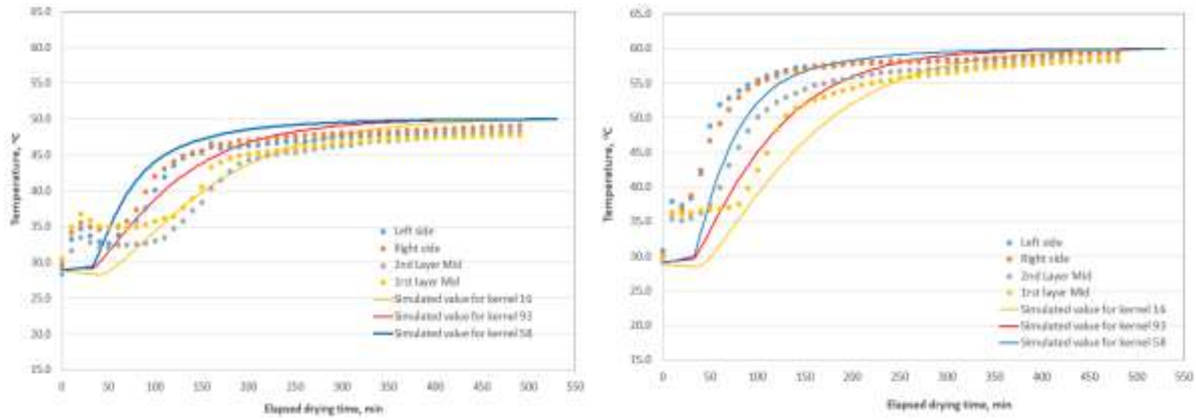
A B

For the cacao beans dried at 60 ºC, the initial temperature of the beans was only 30 ºC when the beans were loaded into the dryer and gradually increased to 58 ºC in just 150 minutes. At the same drying temperature, however, for the cacao beans located in the middle, both the bottom and top layers, there is a delay in the temperature rise. The cacao bean's temperature increases to about 35 ºC, and then after 50 minutes, it slowly increases until it reached 58 ºC after 390 minutes. Monitoring of the temperature profile within the cacao beans was carried out up to the 480th minute of drying. This is because the temperature had already reached near the temperature setting for both drying temperatures.

Simulated temperature and moisture in cacao beans

The simulated temperature profile of the drying air surrounding the cacao beans is shown in Fig. 6A and 6B. Considerably, the simulated air temperature surrounding the cacao beans remained stable and within the set range.

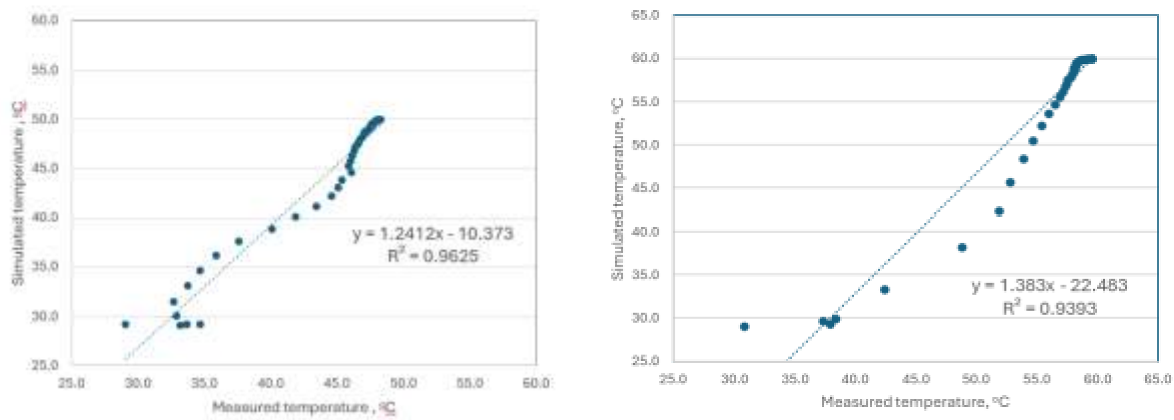
The simulated temperature values are within the temperature range as indicated in the color legend on the right side of the Fig. 6A and 6B.



C

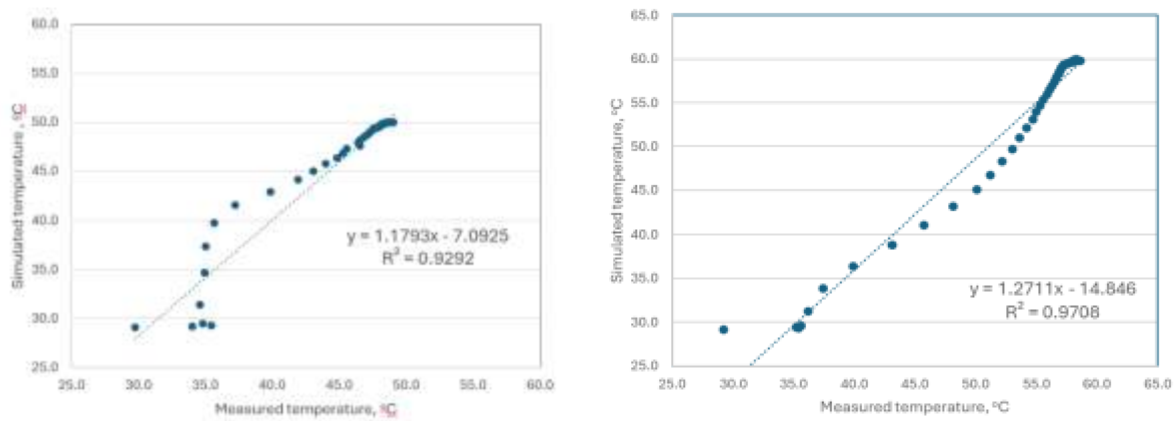
D

Figure 4. Temperature monitoring of the cacao beans inside the drying chamber in various location within the drying tray. A) thermocouple wires inserted into the cacao beans; B) position of the select beans in the 3D model C) temperature profile of the monitored cacao beans at 50 °C; D) temperature profile of the monitored cacao beans at 60 °C

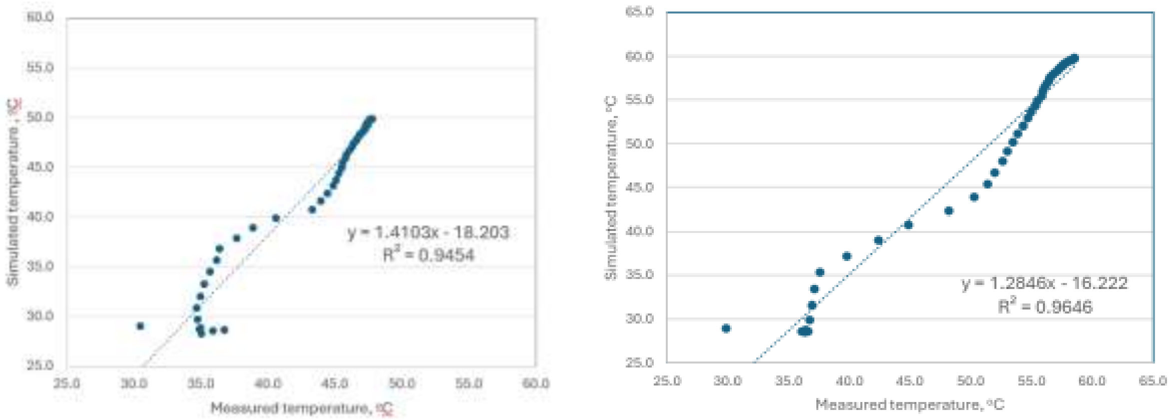


A

D



B E



C F

Figure 5. Regression curves for the simulated versus measured temperature for the cacao beans at the different locations. A) left side 50 ºC; B) right side 50ºC; C) bottom layer 50 ºC; D) left side 60 ºC; E) second layer 60 ºC; F) first layer 60 ºC

Figure 6C illustrates the distribution of moisture content inside the cacao domain for several times. Depicted in the figure are the slices of the 3D ellipsoid geometry representing cacao beans with varying colors in different drying times.

The regression correlation between the observed and simulated temperatures of fermented cacao beans under different drying conditions (Fig. 5A-F) illustrates a close correspondence between experimental subsample readings and CFD-derived predictions. The model achieved high coefficients of determination (R^2 = 0.9292–0.9708), reflecting excellent predictive accuracy across both drying temperatures. These results verify that the proposed CFD model is robust and dependable for estimating cacao bean temperature during drying.

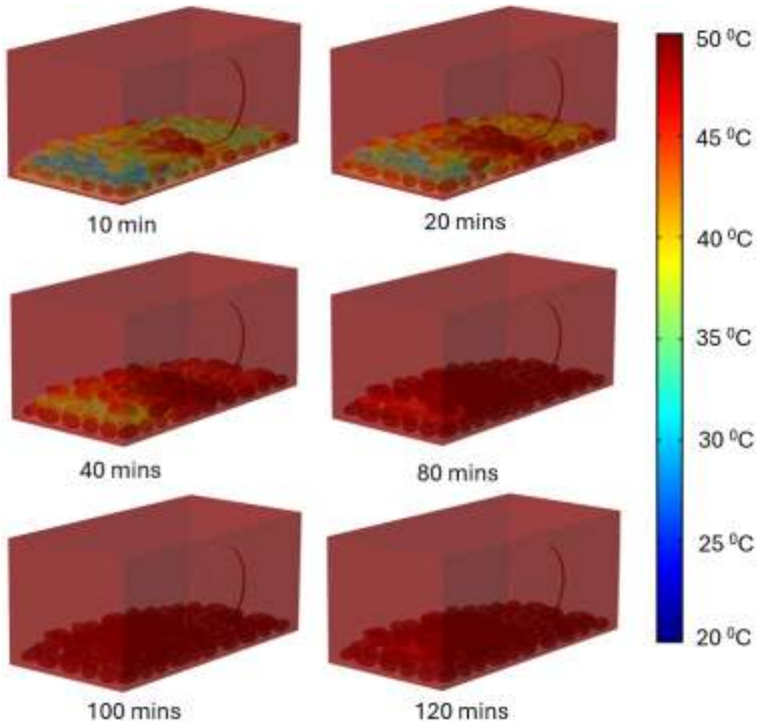
In many food dehydration processes, studying fluid flow and heat transfer in porous media is essential, as these factors influence both product quality and dryer efficiency.

As drying of food and agricultural products often uses heat either from the sun, biomass, or electricity to gradually cause water to vaporize and remove the moisture from the product. In drying the heat raises the temperature of the air that surrounds the product, transferring the heat energy to the surface of the product and further to the inner material of the commodity being dried. The simulated temperature profile of the drying air surrounding the cacao beans is shown in Fig. 6A and 6B. Considerably, the simulated temperature of the air surrounding the cacao beans behaved normally and within the temperature setting. The simulated temperature values are within the temperature range as indicated in the color legend on the right side of the Fig. 6A and 6B. Figure 6B shows the color of the grains from the inside of the rectangular geometry representing the drying air gradually changes from cyan and dark turquoise to yellow orange and finally to ruby red. As can be seen from Fig. 6B, the cacao beans appear cyan and dark turquoise after 10-30 minutes of exposure to the hot drying air.

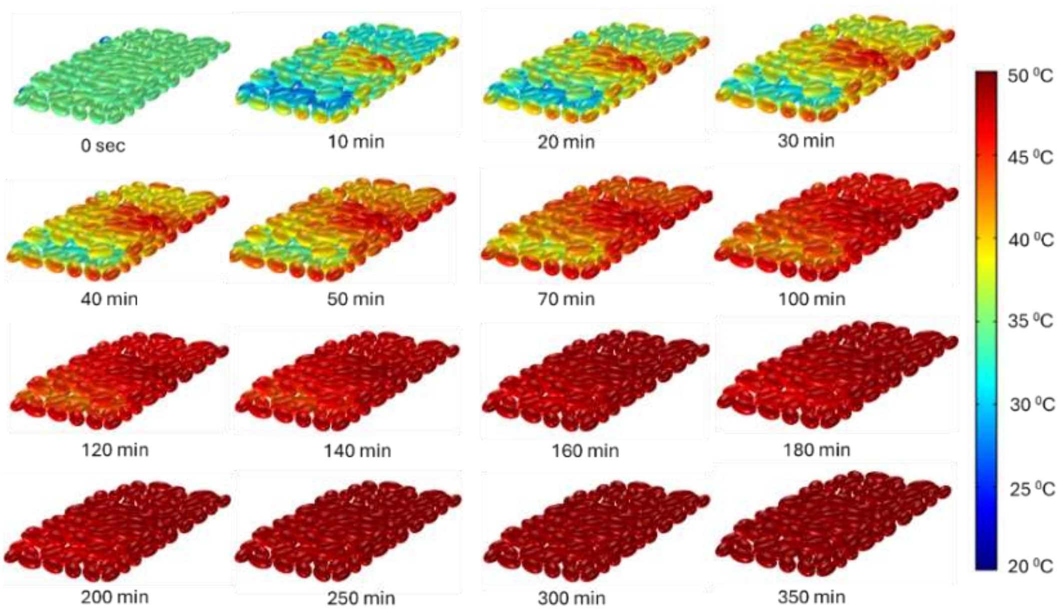
On the other hand, some cacao beans immediately turned dark yellow and ruby red color after a few minutes of exposure to the hot drying air. The color differences in the surfaces of the cacao beans clearly confirm the varying temperature rise in the different domains.

Fig. 6C illustrates the distribution of moisture content inside the cacao domain for several times. Depicted in the figure are the slices of the 3D ellipsoid geometry representing cacao beans with varying colors in the different drying times.

It is clearly seen that all the profiles are symmetrical as expected since all external surfaces of the sample are subjected to the same boundary conditions. This is because the cacao beans geometry is assumed to be a homogeneous and isotropic condition. Using the model, the average moisture content of the cacao beans can be computed from the drying conditions under study. The simulated data closely matched the experimental results, showing minimal deviation. The root mean square errors (RMSE) between the simulated and experimental data for the moisture content are 2.538 and 2.221 g water/g dry matter, respectively. The simulated distribution of moisture within the cacao bean kernel provides valuable insight into the concept of the moisture gradient. The critical moisture content of the beans dried at 60 °C was determined to be 15% (dry basis), occurring after approximately 420 minutes (Fig. 3A). During this period, the simulation results indicated that the surface moisture content decreased to about 10% (dry basis), whereas the centroid of the nib was predicted to retain a moisture content of up to 60% (dry basis).



A



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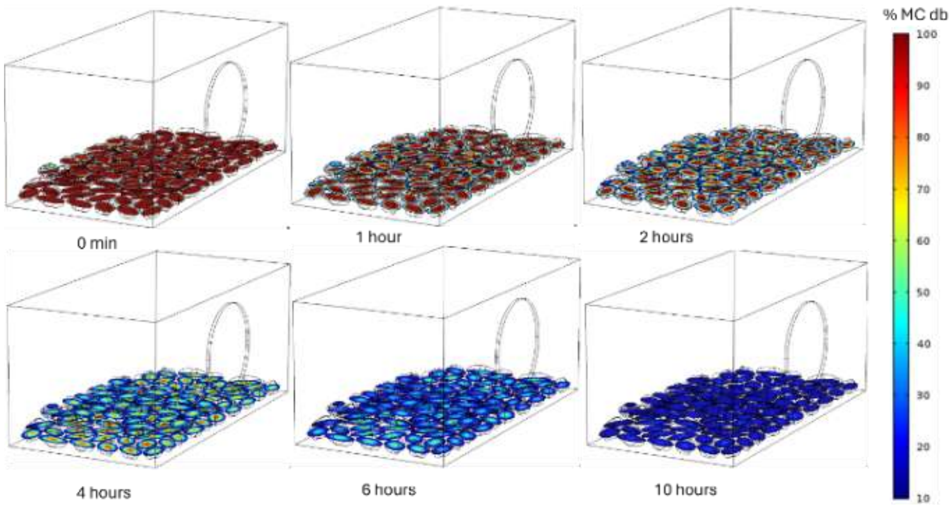

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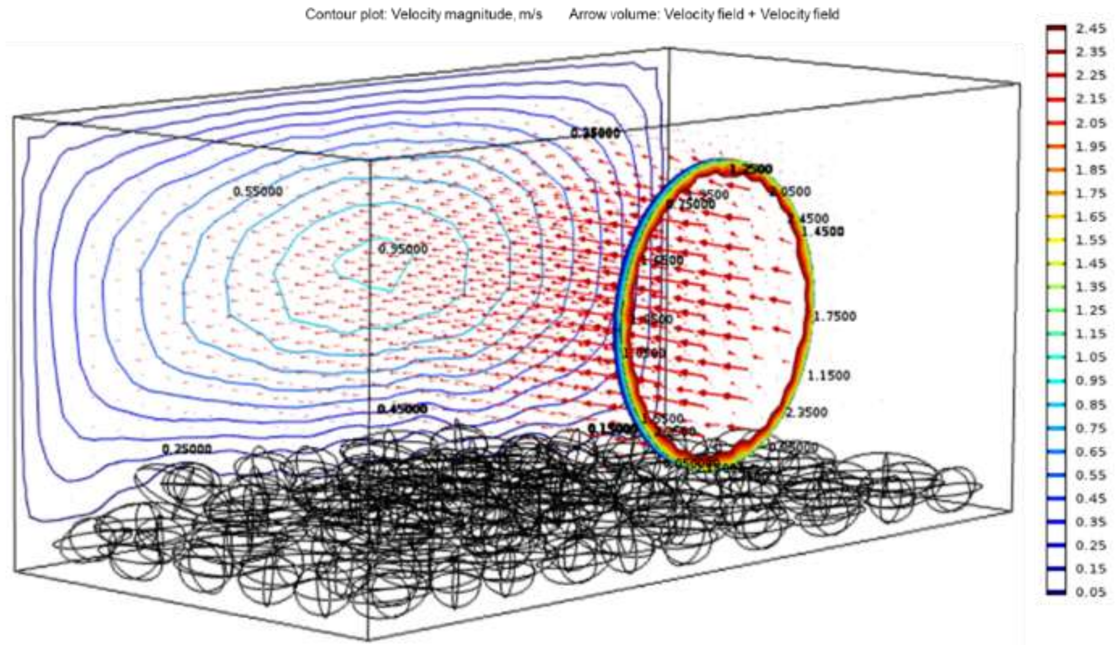

D

Figure 6. Simulated results of the temperature and velocity profile. A) temperature inside the drying air chamber; B) surface temperature profile the cacao beans at 50 ºC; C) moisture distribution inside the cacao beans; D) contour plot of the velocity magnitude and the velocity vector field

Effect of cacao bean location in the drying tray to temperature

The temperature of a medium near a heat source decreases as the distance from the source increases, following principles of heat transfer like conduction, convection, and radiation. However, for a food item in which the source of heat is surrounded by calm air, then the process of heat transfer from the object to the surrounding air is dominated by the radiation process (Novák 2020; Rahayu et al. 2023). During drying, where a mechanical dryer is used where a blower or fan is integral to the dryer, the heat transfer is a combination of all three modes of heat transfer. However, in mechanical dryers, particularly those using hot air, heat transfer is primarily dominated by convection, where warm air is circulated around the medium to facilitate evaporation and drying (Donoso-García et al. 2024).

The temperature in any food material dried in a mechanical dryer is dependent on proximity to the heat source as well as the direction of the flow of the heated air. Spatial distributions of

Table 2.
Root Mean Square Error (RMSE) for the simulated temperature at the different location in the drying tray

Drying temperature (ºC)	RMSE (ºC)			
	Right	Left	First layer	Second layer
50	2.64	2.19	2.84	3.30
60	3.62	3.15	3.52	2.78

airflow significantly affect temperature increase in the material, thus affecting the drying kinetics (Khan et al. 2022). Shown in Fig. 4C-4D, the temperature profiles of select cacao beans are relative to their position in the drying tray as well as its location away from the blower. In Fig. 4B, cacao bean 58 is located just one centimeter away from the blower, while cacao beans 16 and 93 are located around 8 centimeters away from the blower. Nonetheless, bean 98, despite being 8 centimeters away from the blower is directly along the flow of the hot air. Thus, the temperature profile of bean 93 is comparatively higher than bean 16. Assessing the performance of the model in validating the simulated data against the experimental data revealed that the RMSE values shown in Table 2 ranged from 2.19–3.30 °C at 50 °C and from 2.78–3.62 °C at 60 °C, respectively. The values of the RMSE for both temperatures remained within an acceptable range.

Simulated air flow

In the field of Computational Fluid Dynamics (CFD), contour plots and velocity vector fields are essential tools for visualization and analysis. A contour plot provides a clear and intuitive representation of the spatial distribution of scalar quantities within the flow field, while velocity vector fields are crucial for interpreting the flow patterns and directions. As shown in Fig. 6D, the contour of the velocity magnitude and the corresponding velocity vectors of the present 3D model are presented, illustrating the airflow characteristics analyzed in this study.

As indicated, the contour profile of the magnitude of the velocity of the drying air, the center of the radial fan has the highest velocity magnitude. Along the direction of the airflow, the magnitude of the velocity is higher near the fan. This is because the radial fan increases the speed of the air flowing through it. The fan imparted energy to the airflow. As the radial fan rotates its blades, the imparted energy increases the air's stagnation pressure, the pressure at which the fluid velocity is zero and all kinetic energy has been isentropically converted into pressure energy. Even along the direction of the flow, the pressure energy reduces as it goes farther away from the fan. Hence, the magnitude of the flow has reduced from 2.5 m/s to about 0.95 m/s at about 10 cm away from the fan. Theoretically, the velocity vector field shows the length of the arrows indicates the strength or magnitude of the vector, while the direction shows which way the vector is pointing. The sizes of the arrows that represent the vector field agree with the magnitude reflected in the contour lines.

CONCLUSIONS

In conclusion, a theoretical model that coupled the heat and mass transport phenomena involved in the convection drying of fermented cacao beans was developed and presented. The model used mathematical relationships, particularly piecewise and analytic functions, for the physical properties of the drying air. In a similar manner, constant physical and thermal properties of the cacao beans were used. The result of the 3D simulations accurately predicted the general trend of the experimental temperature curves. The simulation results closely correspond with the experimental moisture content data at both drying temperatures. The temperature rise in the cacao beans located in the different positions inside the drying tray obtained from the experiment was also similar to the simulated data in both temperatures. The magnitude of the velocity of the drying air inside the drying chamber was similar to the experimental data. The 3D model showed higher airspeed near the radial fan, which was consistent with experimental observations. The mechanical energy of the rotating fan blade pushes the mass of hot air forward into the drying chamber. The presented model can be used to simulate and predict the convection drying of cacao beans. The drying time and temperature in the drying chamber were modelled adequately. Furthermore, the present 3D model represents an improvement over earlier studies that primarily utilized single-seed models, as it incorporates a multi-bean configuration consisting of 108 beans. However, it remains a challenge to incorporate the shrinkage of the geometry. Future experiments and 3D modeling studies are encouraged so that they can be used further in optimizing the convection drying conditions, processes, and design of mechanical dryers in the pursuit of controlling the cacao beans' quality and safety.

AUTHOR CONTRIBUTIONS

Conceptualization, visualization, data analysis, curation, writing original draft, review and editing, supervision, validation, project administration, J.H.P.

DATA AVAILABILITY STATEMENT

The datasets generated and/or analyzed during the current study are available within the article.

ACKNOWLEDGEMENTS

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

CONFLICT OF INTEREST

The author declares that there are no conflicts of interest related to the preparation of this manuscript and confirms having read and agreed to all information reported herein.

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MODELOVANJE PRENOSA TOPLOTE I MASE TOKOM SUŠENJA FERMENTISANIH KAKAO (*THEOBROMA CACAO L.*) ZRNA

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Sažetak: Trodimenzionalni model konačnih elemenata, koji se sastoji od 108 zrna kakaoa, razvijen je radi simulacije prenosa toplote i mase tokom sušenja prinudnom konvekcijom. Model je procenjivao raspodelu temperature unutar komore za sušenje i pojedinačnih zrna pod uticajem strujanja vazduha, dok su fizičke i termodinamičke osobine izračunate i primenjene u simulaciji. Performanse modela su eksperimentalno validirane, pokazujući dobro slaganje između simuliranih i posmatranih profila vlage i temperature. Podaci o sadržaju vlage dali su RMSE vrednosti od 2.538 i 2.221 g vode/g suve materije, dok se RMSE temperature kretala od 2.19–3.30 °C pri 50 °C i 2.78–3.62 °C pri 60 °C, što ukazuje na prihvatljivo odstupanje. Rezultati su pokazali da zrna pozicionirana na ivicama tacne i gornjim slojevima imaju više unutrašnje temperature od onih u donjem sloju. Ova saznanja sugerišu da preraspodela zrna tokom 60–90 minuta nakon početka procesa sušenja može poboljšati ujednačenost sušenja i kvalitet proizvoda. Predstavljeni 3D model sa više zrna predstavlja značajan napredak u odnosu na tradicionalne pristupe modelovanja pojedinačnih semena i pruža koristan alat za optimizaciju procesa sušenja kakaoa, sa potencijalnom primenom na industrijskom nivou.

Ključne reči: *prerada kakao zrna, konvektivno sušenje, model konačnih elemenata, prenos mase, prenos toplote, numerička simulacija*

Received: *12 November 2025/* ***Received in revised form:*** *08 December 2025/* ***Accepted:*** *15 December 2025*

Available online: *February 2026*