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ORIGINAL RESEARCH PAPER

MULTIDIMENSIONAL ANALYSIS OF PHYSICOCHEMICAL TRANSFORMATIONS AND SENSORY ATTRIBUTES OF GREEN AND ROASTED COFFEE

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Abstract: This research presents a comprehensive analysis of the physicochemical and sensory attributes of green and roasted coffee beans from Rwanda, Colombia, Ethiopia, and Peru. Advanced image processing tools were utilized for defect analysis. Water activity, *p*H, mass loss, and moisture were determined, and thermal analysis were performed. Substantial variations in physicochemical properties were found among coffee beans of different origins. Utilizing a multi-objective optimization algorithm, Ethiopian coffee emerged as possessing the most optimal physicochemical characteristics. The optimal roasting temperature range for Ethiopian coffee was found to be 216.49 °C to 230.15 °C, with longer roasting times at lower temperatures producing more evenly roasted coffee. This study provides valuable information to coffee producers and processors to optimize the roasting process and improve coffee quality.

Keywords: *coffee, processing, quality, roasting, sensory characteristics*

INTRODUCTION

Coffee is a globally popular and widely consumed beverage, with over 400 million cups consumed annually. In recent years, there has been a growing demand for high-quality beverages and also a demand for health-conscious characteristics, which has led to an increased focus on the production of coffee with superior sensory characteristics [1, 2].
The final product, the coffee drink, is derived from the mixture of roasted and ground coffee beans, mainly from the species *Coffea arabica* and *Coffea canephora* (*Coffea robusta*) [3]. Among them, Arabica coffee is famous for its ability to produce high-quality beverages [4]. However, consistently achieving optimal coffee quality is a multifaceted endeavour that requires a deep understanding of the complicated interplay between various intrinsic and extrinsic factors.
In order to optimise the production process and meet discerning consumer expectations, a thorough understanding of the physicochemical and sensory characteristics underlying coffee quality is imperative. From a physicochemical point of view, coffee is a complex combination of thousands of chemical compounds responsible for its flavour, aroma, and overall sensory attributes. These compounds comprise a wide range of constituents, including carbohydrates, lipids, nitrogenous compounds, vitamins, minerals, alkaloids, and phenolic compounds. Consequently, extensive research efforts have been devoted to exploring the chemical composition, as well as potential beneficial and adverse properties, of green and roasted coffee beans and the resulting beverage [5, 6].
The existing literature on coffee quality emphasises the critical role played by physicochemical and sensory attributes in determining overall coffee quality. Numerous studies have investigated the influence of coffee species [7], processing methods [8] and roasting parameters [9] on sensory and physicochemical profiles of coffee. However, further research is needed to deepen our understanding of the intricate interplay between these attributes and their implications for coffee quality and consumer preferences.
Image processing techniques have emerged as a powerful tool in the food industry, providing a non-destructive method for evaluating and controlling the quality of food products, including coffee. This is a scientific area that aims to develop algorithms that automatically extract and analyse useful information about a certain object or scene from an observed image, a set of images, or a sequence of images [10]. In this regard, the technique extracts quantitative colour information from digital images using image processing and analysis [11]. Moreover, computer vision-based image analysis serves as a useful tool for the automatic inspection of food products in a production line and can be actively involved in the decision-making process where a rapid quality and safety assessment is required [12].
Physicochemical attributes hold significant importance in defining coffee quality and sensory perception [8]. Sensory evaluation, which encompasses aroma, corpulence, and aftertaste, provides invaluable information on the overall coffee experience [13]. Among these sensory characteristics, aroma stands out as an essential criterion in determining coffee quality and is directly influenced by the presence of defective coffee beans [14].
The coffee roasting process is of paramount importance in the formation of aroma compounds and profoundly impacts the composition of biologically active compounds in coffee [15, 16]. The degree of roasting is meticulously controlled by manipulating roasting time and temperature [17]. Initially, at temperatures below 160 °C, drying occurs as the coffee beans dehydrate, releasing steam and initiating the expansion of the

solid matrix [18]. When coffee beans reach temperatures above 180 °C, an exothermic reaction occurs wherein polysaccharides, proteins, chlorogenic acid, and trigonelline begin to form the compounds responsible for the colour, flavour, and aroma of roasted coffee beans [19]. In particular, the roasting process entails the release of CO_2 as a reaction product, contributing to the expansion of the coffee matrix. Subsequently, rapid cooling of the roasted beans is crucial to promptly halt these reactions, thus preventing over-roasting that could compromise the quality of the final product [20].

Efforts to optimise roasting parameters are an ongoing challenge in both scientific research and practical applications. Achieving optimal roasting parameters necessitates the fine-tuning of key variables to obtain the most favourable formula, thus presenting an essential aspect in the development of new coffee products [21]. Response Surface Methodology (RSM), which encompasses techniques such as central composite design and Box-Behnken design, has been extensively used to optimise the physicochemical characteristics of roasted coffee [22]. However, the optimisation of food processes involving multiple responses requires the employment of various conventional and unconventional optimisation techniques. In this context, RSM serves as a conventional optimisation technique used predominantly for optimising processes involving multiple responses [23].

In recent years, considerable research efforts have been devoted to unravelling the physicochemical and sensory attributes of coffee, with the objective of identifying the key determinants of its quality. Based on these efforts, the present study undertakes a comprehensive analysis of both green and roasted coffee, focusing specifically on their physicochemical and sensory characteristics. Furthermore, this study endeavours to elucidate the factors that influence the quality of the final coffee product. By delving into these aspects, we aspire to provide a novel perspective on the factors that influence coffee quality and consumer preferences. The insights garnered from this research are of immense value to coffee producers and processors, facilitating the identification of factors that significantly influence coffee quality and consumer preferences.

Our hypotheses for this study are as follows:

• Different roasting parameters significantly affect the physicochemical properties of coffee. By altering these parameters, we can manipulate these properties to achieve specific quality and flavour profiles.

• The sensory properties of coffee, as perceived by human tasters, are closely related to its physicochemical properties. Therefore, the optimisation of the roasting parameters should also consider the sensory analysis of the coffee.

Through this research, we aim to highlight the factors that influence the quality of the final product and provide a novel perspective on the factors that influence coffee quality and consumer preferences. The insights garnered from this research are of immense value to coffee producers and processors, facilitating the identification of factors that significantly influence coffee quality and consumer preferences. Confirming or disproving these hypotheses will have crucial implications for both coffee science and the global coffee industry.

MATERIALS AND METHODS

This study employed a systematic approach to delve into the complexities of coffee. The methods were crafted to ensure the reproducibility of the experiment; additionally, all chemicals adhered to the conventions of the International Union of Pure and Applied Chemistry (IUPAC). All measurements were recorded in accordance with the International System of Units (SI). Moreover, the methods utilised in this study were chosen based on their relevance and accuracy for the analysis of the physicochemical properties of coffee beans. Through a combination of these methods, we garnered a comprehensive understanding of the factors that influence coffee bean quality, and how these factors can be optimised for enhanced quality control in the coffee industry.

The coffee samples

Five hundred grams of green coffee beans from four different origins were sampled. The coffee beans were sourced from the following regions and farms: Rwanda (Muganza farm), Colombia (El Paraiso farm in Cauca region, owned by Jose Gabriel Velasco), Ethiopia (Adado farm in Yirgacheffe region) and Peru (Jumarp farm). The coffee beans were meticulously selected through visual inspection to ensure the uniformity in size. These regions were chosen due to their significant contributions to global coffee production and the distinct characteristics of their coffee varieties.

Preparation of coffee samples

Sampling was performed in line with ISO 4072:1982 [24]. Prior to the roasting process, approximately 200 g of green coffee beans were selected and placed into containers. The samples were stored in a cool, dark environment until chemical determinations were conducted. The coffee samples encompassed four distinct categories of labelled green coffee samples (Colombia, Ethiopia, Peru, and Rwanda). Additionally, Ethiopian coffee samples underwent a roasting process under varying roasting conditions using a BESCA BSC-05 coffee roaster (BESCA, Turkey). The roasting process was monitored and controlled to achieve a medium roast level, which is typically preferred in taste tests. Roasting time and temperature were ascertained from the roaster output data, which provided graphs of roasting temperature and time. The roasting temperatures utilised in our study ranged from 188 to 282 °C, with the roasting time adjusted between 8 to 10 minutes. The roasted coffee was labelled (P1, P2, P3, P4). Sample P1 represents green coffee roasted for 8.2 minutes, sample P2 represents green coffee roasted for 8.5 minutes, sample P3 represents green coffee roasted for 9.04 minutes, sample P4 represents green coffee roasted for 9.3 minutes. The roasted coffee subjected to physicochemical analysis was compared with a standard of Ethiopian green coffee named "M". This sample served as a control group, enabling us to evaluate the effects and implications of the roasting process in a rigorous manner. We also considered factors such as batch size, airflow, and bean density, as these variables have been documented to significantly influence the roasting process [25].

Defect analysis

Determining the defects in green coffee was accomplished using a MATLAB script. This script utilized a web camera to capture images, which were then processed to identify individual coffee beans. The process employed a variety of digital image processing techniques, as detailed in works by Gonzalez and Woods [26], Otsu [27], Serra [28], Vincent and Soille [29], using the MATLAB image processing toolkit. This determination, involved two main components: image acquisition and image processing.
Image Acquisition: A web camera, configured with a resolution of 640x480 pixels, was utilized for continuous image capture. The images obtained served as primary sources for further digital processing and analysis of coffee beans.
Image Processing: The image processing workflow comprised the following steps:
Color Conversion: The captured RGB (red, green and blue) images were converted to the color space. This step was crucial for isolating the Luminance (L) layer, providing a more effective channel for subsequent segmentation than the original RGB channels.
Image Binarization: The luminance component (L) underwent normalization using Otsu method, resulting in a binary image [27]. This process was essential for distinguishing the coffee beans from the background.
Morphological Operations: The binary image was inverted, followed by the application of morphological closure using a disc-shaped structuring element (radius: 5 pixels). This procedure helped to eliminate small holes within the identified coffee beans.
Size-Based Filtering: Objects identified as smaller than a predefined threshold (3000 pixels) was eliminated. This step was necessary to remove image noise and small debris.
Watershed (Image Processing): The inverse distance transform of the binary image was subjected to the watershed technique. This allowed for the effective separation of adjacent coffee beans.
Boundary Extraction: The contours of the coffee beans were extracted and overlaid on the original image. This step ensured the successful identification of defects.

Determination of water activity

For green coffee and roasted coffee, water activity was measured by equilibrating the liquid-phase water in the sample with the vapour-phase water in the headspace of a closed chamber and measuring the equilibrium relative humidity (ERH) in the headspace using a Lab MASTER-aw instrument (Novasina, Switzerland).

Determination of *p*H

The *p*H of coffee was determined by extracting 5 g of coffee powder in 50 mL of hot water. The extract was then cooled to room temperature and the *p*H of the extract was measured using a S400 SevenExcellence *p*H-meter (Mettler-Toledo, Australia).

Determination of humidity

Moisture determination was performed according to the ISO 11294:1994 method [30]. This method consisted of determining the mass loss of the sample at 103 °C until a constant mass was achieved (A&D Company, Limited, Japan).

Differential Scanning Calorimetry (DSC) and Thermogravimetric Analysis (TG)

DSC and TGA for green coffee beans were performed using the SDT Q600 (TA Instruments, USA) calibrated using indium and zinc. Between 15 and 20 mg of sample were taken for analysis. This was obtained by cross-sectioning the green coffee bean so that the samples contained all parts of the bean in the ratio in which they naturally exist in the green bean. The experiments were carried out by heating the samples in platinum cups, open, in a nitrogen atmosphere, at a heating rate of 10 °C·min^{-1}, in the range of 30 - 600 °C. The Universal Analysis 2000 software from TA Instruments was employed to interpret the curves. For a better interpretation of the results, derivatives of the thermogravimetric curves (DTG) were also obtained

Sensory analysis

Sensory analysis was conducted according to the procedures delineated in ISO 5496:2006 [31] and ISO 8586-2:2008 [32]. The exercise comprised a systematic and objective assessment of the sensory characteristics of the coffee. Coffee was prepared using roasted beans in accordance with previously described methods. The coffee was then served at a uniform temperature in a standardised cup with no added milk or sugar. Sensory analysis was executed by a panel of ten individuals. Participants were chosen based on their regular coffee consumption and their willingness to engage in the analysis. Before the sensory analysis, the panellists underwent a 30-minute training session led by a trained sensory analyst. The session aimed to familiarise the panellists with the sensory attributes of the coffee they would be evaluating, such as intensity of aroma, acidity, corpulence, and aftertaste. This training ensured that all panel members had a consistent understanding of the sensory attributes and evaluation process, thus enhancing the reliability of the sensory data collected. The data garnered from this evaluation was then analysed to ascertain the sensory profile of the coffee.

Multi-objective optimisation

The multi-objective optimisation was carried out using a MATLAB script. The script was crafted to read the outcomes of the physicochemical analysis for the four green coffee samples (Colombia, Ethiopia, Peru, and Rwanda). Equation (1) was defined in the script that calculated the sum of the squared differences between the data and a certain input value x. The optimisation function was defined as follows:

$$minimize: f(x) = \sum_{i=1}^{n}(w_i - x_1)^2 + (p_i - x_2)^2 + (m_i - x_3)^2 + (c_i - x_4) \quad (1)$$

where: w_i, p_i, m_i and c_1 represent the values of water activity, *p*H, mass loss and coffee defects, respectively.

x represents the vector of optimization variables, with x_1, x_2, x_3, and x_4 corresponding to the optimal values of water activity, *p*H, mass loss, and coffee defects, respectively. The optimization problem sought to find the values of x that minimize the objective function f(x) subject to constraints defined by lower and upper bounds on the given x. To identify the optimal sample of roasted green coffee, we used a multi-objective optimization algorithm implemented in MATLAB. This algorithm was designed to minimize the sum of squared differences between observed data and predicted values based on a set of four variables: water activity, *p*H, mass loss, and coffee defects.

Statistical interpretation

Statistical analysis was performed to evaluate the significance of the results obtained from the different determinations. Descriptive statistics were calculated for each variable, and test statistics, such as t-tests or analysis of variance (ANOVA), were used to determine whether there were significant differences between groups or treatments. In addition, a correlation analysis was performed to investigate the relationships between the variables. Regression analysis was used to develop predictive models and identify key factors influencing coffee quality and consumer preferences. All statistical analyses were performed using MATLAB 2022a. The confidence level for all statistical tests was set at 95 %. The results of the statistical analysis were interpreted in the context of the research objectives and used to draw conclusions and make recommendations.

RESULTS AND DISCUSSION

The physicochemical characteristics of green coffee beans are crucial in determining the quality of the final product. Analysis of defects, water activity, *p*H, moisture, and thermal properties (DSC and TGA) provide a comprehensive understanding of the quality of the green coffee beans used in this study.
The values obtained for green coffee bean defects, water activity, moisture, and *p*H for the four samples of green coffee beans from different regions shown in Figure 1 provided valuable information. However, the study has limitations that should be acknowledged. For example, we analysed only four coffee samples from different regions. A larger study involving more samples from each region could provide a more comprehensive picture of the physicochemical characteristics of green coffee beans from those regions.

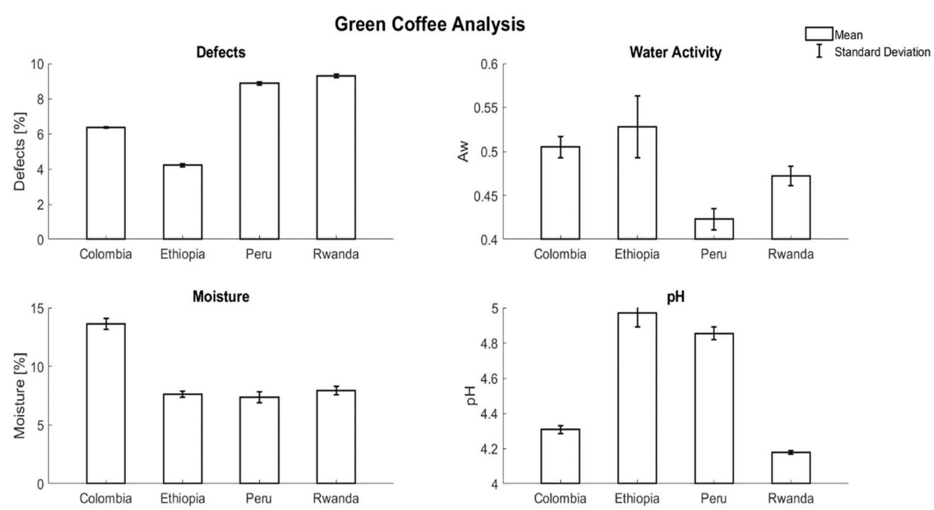


Figure 1. *Values obtained for green coffee bean defects, water activity, moisture and pH for the four green coffee bean samples from different regions*

Defects in green coffee beans

The MATLAB script, described in the Materials and Methods section, was utilized to capture and process images of green coffee beans in real-time. The process, illustrated in Figure 2, enabled the effective identification and quantification of defects in the coffee beans.

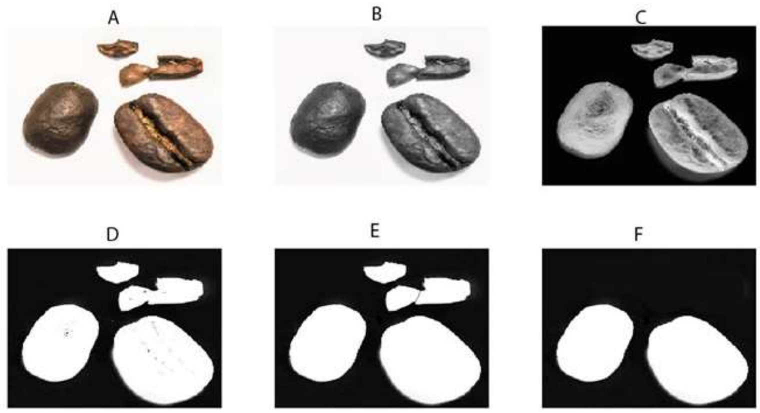


Figure 2. *Identification of defects in coffee beans using digital image processing: (A) original image, (B) L-channel, (C) binarized image, (D) filled image, (E) removed small objects, (F) after watershed transformation*

The obtained results demonstrate that our system of continuous image capture and processing allows the instantaneous detection and quantification of defects in coffee beans. This real-time processing facilitates the immediate identification of defective beans, significantly simplifying the quality control and selection process. The system's ability to quickly and accurately process large quantities of coffee beans ensures prompt detection of any defects, allowing for more efficient sorting and grading.

The presence of defects in green coffee beans can have a significant impact on the quality of the final product. According to ISO 4149:2005, the quality of green coffee beans is assessed based on the presence of foreign matter and defects [33]. According to the results in Figure 1, each green coffee sample (Rwanda, Colombia, Ethiopia, and Peru) has a different number of defects per 100 grams of coffee. Defect percentages varied among green coffee samples, with Rwanda having the highest percentage of defects (9.29 %) and Ethiopia the lowest (4.21 %). Many defects may indicate poor harvesting or processing methods, as well as problems with storage or transportation. Colombia also has a defect count of 6.36 %, which is lower than Rwanda but higher than Ethiopia. This may indicate that the coffee has been affected by pests, diseases or other environmental factors that could affect its quality. Ethiopia has the lowest number of defects at 4.21 %, indicating that it may be of better quality compared to the other samples. These results suggest that the quality of green coffee beans can vary significantly depending on origin and processing methods, which aligns with previous research [34]. However, future research should include a more diverse range of coffee bean varieties to increase the generalisability of the results.

Water activity

Water activity is a critical parameter for determining the storage stability and flavour of green coffee. Water activity in green coffee beans is influenced by storage time, the packaging in which it is stored, the temperature at which it is stored, and the humidity of the air in the storage [35]. The water activity results (Figure 1) indicate that green coffee samples from Rwanda and Peru have lower water activity compared to those from Ethiopia and Colombia. A water activity of 0.472 for the Rwandan sample suggests that it has a relatively low moisture content and is therefore less susceptible to mould growth during storage. Similarly, the Peru sample has a water activity of 0.423, suggesting that it has the lowest moisture content of all the samples. On the other hand, samples from Ethiopia and Colombia have a higher water activity, indicating a higher moisture content, which can lead to the development of moulds and a decrease in coffee quality during storage. However, the range for water activity in green coffee ranged from 0.45 - 0.55 and was similar to 0.45 to 0.53 as reported by Aung Moon *et al*. [36]. A value lower than 0.45 is likely to affect the quality of green coffee beans, while a value higher than 0.9 is likely to cause moulds [37]. Consequently, water activity is an important parameter for maintaining the physical properties of coffee beans during storage.

The moisture content of green coffee

In general, the moisture content of green coffee beans should be around 10-12 % and may vary depending on the origin and processing method of the coffee [38]. In the present case, the humidity varied between 7.37 % and 13.62 %. In this study, the Colombian coffee sample had the highest moisture content at 13.62 %, suggesting a different harvesting or processing method compared to the other samples such as Rwanda with 7.95 %, Ethiopia with 7.64 % and Peru with 7.37 %. These values suggest that the Colombian coffee samples were likely harvested or processed differently than the other samples, resulting in a higher moisture content. Moisture content can affect coffee quality in various ways; that is, a high moisture content can lead to the growth of moulds [39], the diminution of flavours, and the decrease of the shelf life [36].

The *p*H of green coffee beans

The *p*H of green coffee beans is another important factor that influences the taste, aroma, and overall quality of coffee. The *p*H values ranged from 5.2 to 6.0, the lowest *p*H observed in Colombian coffee samples. In general, Arabica coffee beans are known for their higher and more pleasant acidity compared to Robusta coffee beans. The acidity of coffee can also vary depending on the altitude, soil type, and climate in which the coffee plants are grown [40]. The *p*H of coffee in all samples is slightly acidic, typically ranging from 4.85 to 5.10. All four samples of green coffee beans in this study were within this range, suggesting that they have the potential to produce high-quality coffee. Also, the *p*H values match the values reported in the literature [41].

These findings are consistent with previous studies that reported significant variations in the physicochemical properties of coffee beans of different origins [42]. Variations in physicochemical properties can be attributed to differences in the genetic structure of coffee plants, growing conditions, and post-harvest processing methods [43].

DSC, TG and DTG thermal analysis

Following the thermal analysis, DSC, TG, and DTG curves presented in Figures 3 and 4 were obtained, and the determined values are indicated in Tables 1, 2, and 3.

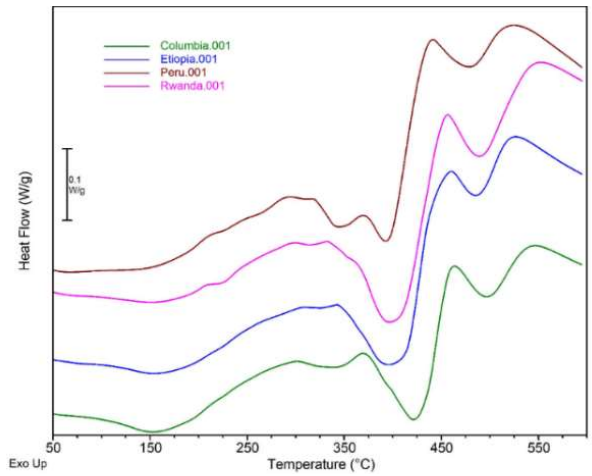
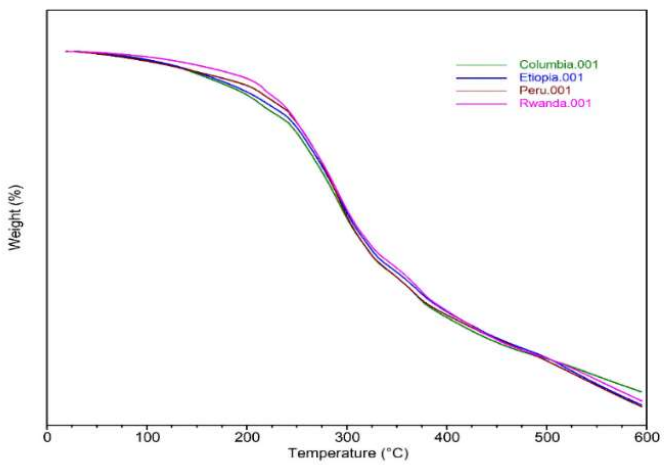


Figure 3. *DSC curves obtained for the four types of green coffee beans*

a)



b)

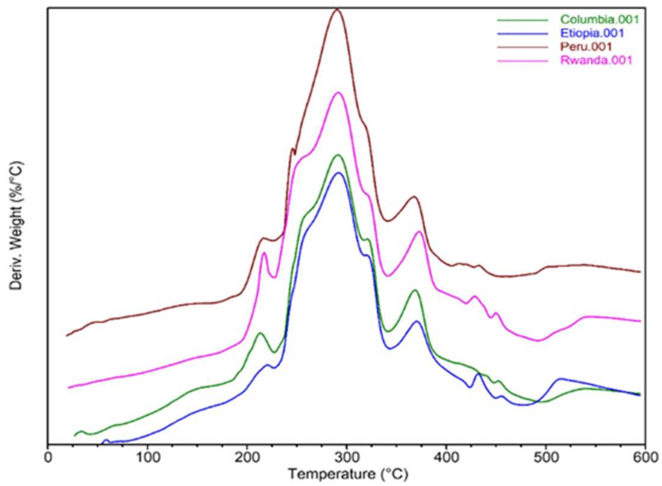


Figure 4. *TG curves (a) and DTG curves (b) obtained for the four types of green coffee beans*

From the thermal analysis in the presence of nitrogen, as the temperature increases in the range of 50 - 600 °C, several thermal events are observed. The first two are endothermic processes also observed by other researchers. At temperatures between 58.18 °C and 74.56 °C, the DSC curves indicate endothermic phenomena for all samples, mainly due to the elimination of water. Following the thermogravimetric analysis of coffee silver skin, observed, in this temperature range, a significant decrease in mass due to the drying process. The authors also show that disaccharides such as sucrose, maltose, trehalose, and lactose show glass transitions at temperatures higher than 58.96 °C [44]. A second endothermic phenomenon was observed at temperatures higher than 100 °C, as can be seen from Table 1.

Table 1. *The values determined on the DSC curves for the four green coffee samples*

Sample		**Colombia**		**Ethiopia**		**Peru**		**Rwanda**
Endothermic peak 1	Ton [°C]	48.83		63.20		42.21		nd
	Tp [°C]	58.44		74.56		58.18		60.56
	ΔH [$J \cdot g^{-1}$]	0.04		0.16		0.45		0.58
Endothermic peak 2	Ton [°C]	107.92		120.34		105.24		104.79
	Tp [°C]	153.27		162.99		145.04		155.49
	ΔH [$J \cdot g^{-1}$]	6.37		3.90		1.23		3.84
Exothermic peaks 3 and 4*	Ton [°C]	216.49	320.38	230.15	328.61	268.65	315.60	199.05
	Tp [°C]	285.19	327.38	271.2	347.78	284.97	327.77	212.46
	ΔH [$J \cdot g^{-1}$]	51.26		69.69		35.91		0.81
Exothermic peak 5	Ton [°C]	350.85		nd		354.10		316.52
	Tp [°C]	371.21		nd		371.44		341.22
	ΔH [$J \cdot g^{-1}$]	5.84		nd		5.28		1.85

Note: Ton - the temperature at which the thermal phenomenon begins, Tp - the temperature at which the thermal phenomenon reaches its maximum, ΔH - the enthalpy of the thermal process.
* Exothermic processes 3,4 overlap; nd- not determined

In this case, the removal of water by evaporation continues but, as shown by de Carvalho Neto *et al*. [45], there is also a loss of volatile substances such as alcohols, aldehydes, and organic acids. Yeretzian *et al*. [46] monitored the emission of volatile components and showed that these volatile compounds are not products of the Maillard reaction.

Table 2. *Values determined on the TG curves for the four green coffee samples*

Sample	Mass loss at 100 °C [%]	T1 [°C]	T2 [°C]	Mass variation [%]	The final mass of the sample (at 600 °C) relative to the initial one [%]
Colombia	1.94	257.47	325.90	48.84	18.06
Ethiopia	2.02	249.84	347.78	57.86	14.93
Peru	2.33	253.07	329.27	61.22	14.52
Rwanda	1.28	251.91	332.79	63.38	15.91

Table 3. *Values determined on DTG for the four green coffee samples*

Sample	Peak 1		Peak 2		Peak 3	
	Ton [°C]	Tp [°C]	Ton [°C]	Tp [°C]	Ton [°C]	Tp [°C]
Columbia	195.22	212.11	234.99	290.10	346.95	369.32
Ethiopia	198.87	217.61	235.31	291.31	349.04	371.08
Peru	200.49	214.05	237.61	290.21	346.46	368.97
Rwanda	208.64	216.33	232.08	291.43	348.73	373.24

Note: Ton - the temperature at which the thermal phenomenon begins, Tp - the temperature at which the thermal phenomenon reaches its maximum

Brondi *et al*. [47] coupling DSC analysis with chemometric analysis showed that between 175 and 250 °C, the melting of some components such as amino acids, lipids, and carbohydrates takes place. Amino acids also react with carbohydrates to form brown compounds following the Maillard reaction [47]. This phenomenon can also be observed during the roasting of coffee beans, as can be seen in Figure 3.

It is believed that during the heating of the coffee beans to a temperature of about 160 °C, the drying of the green beans takes place (Figure 4). The most important stage, which influences the characteristics of the future coffee, begins after the first "crack", i.e., at a temperature higher than 190 °C. Most of the water is already removed, and the coffee bean increases in size. It seems that this first "crack" can best be observed in the results presented for the DTG curves, more precisely it corresponds to the first peak (Table 3). A second "crack" appears at temperatures between 200 °C and 240 °C [48]. This is observed in the DTG curves in the second peak, which is the widest, and the temperature range is between 232.08 °C (Rwanda) and 237.61 °C (Peru).

In the same temperature range, between 216.49 and 230.15 °C, DSC analysis shows that exothermic processes start for the samples: Colombia, Rwanda, and Ethiopia, while for the Peru sample, the process only starts at 268.65 °C. These exothermic peaks are very broad and may comprise an overlap of several exothermic phenomena. Górska *et al*. [44] found for the "silver skins" two exothermic events with maxima at 265 °C and 340 °C.

In the range 249.84 - 257.47 °C, the results of the thermogravimetric analysis (Table 2) indicate the start of degradation with a significant change in the mass of the samples. These degradations continue up to 325.90 - 347.78 °C, with a reduction in the mass of the samples between 48.84 - 63.38 %. Muñoz Neira *et al*. [49] obtained in their study a loss of 68 % for the berry endocarp and considered this to be due to the depolymerisation of hemicelluloses or the breakdown of pectin and cellulose.

Degradative processes continue, and at the temperature of 600 °C only ash remains.

Data optimisation

The optimisation algorithm was applied to the results of the physicochemical analysis of four green coffee samples from Colombia, Ethiopia, Peru, and Rwanda. The optimisation problem sought to find the values of x that minimise the objective function f (x), subject to constraints defined by lower and upper bounds on the given x.

The identification of the optimal physicochemical characteristics for the green coffee samples was achieved by using an optimization algorithm and defining a feasibility region, which is shown in Figure 5.

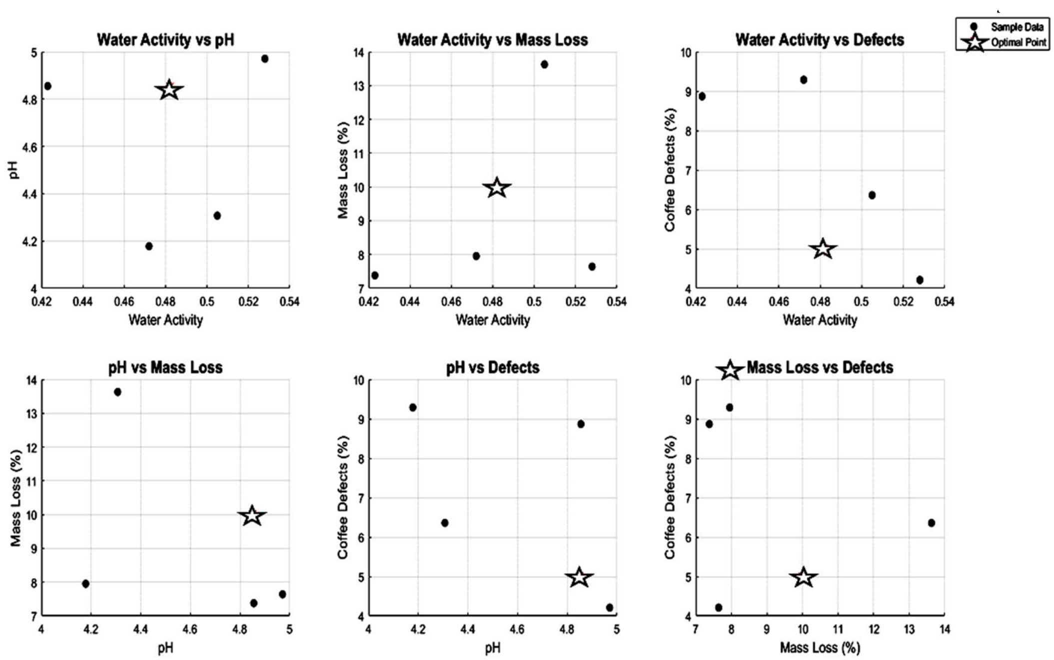


Figure 5. *Feasibility region for identifying optimal physicochemical characteristics of green coffee*

The feasibility region constitutes all potential points that meet the constraints of the optimization problem. Constraints in our analysis were determined by the lower and upper limits of the investigated variables: *p*H, water activity, mass loss at 103 °C, and coffee defects. Thus, the optimization algorithm considered the optimal values for coffee as reported in the literature, i.e., water activity of 0.450 - 0.550, *p*H of 4.81-5.1, mass loss 10 - 12 %, and defects of coffee between 0 - 5 %. Our data set came from green coffee samples, each characterized by a distinct set of measurements such as water activity, *p*H, mass loss, and coffee defects. On the scatterplots illustrated in Figure 5, each of these samples is represented by a black dot. Applying an optimization algorithm led to the determination of an optimal point in the feasibility region, which is represented by a red star on the scatterplots. This point is the result of the 'fmincon' function in the MATLAB programme which minimises the objective function. The location of the optimum points on the graph provides vital information on the theoretically ideal characteristics of the coffee sample according to the established model. For example, the black star in the Water Activity vs. *p*H suggests an ideal combination of water activity and *p*H value. Similar interpretations can be drawn for the remaining plots.

By comparing the location of the optimum point to the sample data points, we can measure the closeness of our samples to these theoretical optimum conditions. Insights derived from this comparison could guide quality control efforts or facilitate the improvement of coffee processing techniques.

Following simulations of the optimization algorithm, it was found that the Ethiopian green coffee sample represented an optimal coffee sample from a physicochemical perspective. These results position Ethiopian coffee as a potentially ideal model for the roasting process.

Selecting the roasting process

Comprehensive examination of the roasting process and its impact on the physicochemical properties of coffee beans provides valuable findings. A deeper exploration of how these changes might affect the taste and overall quality of coffee can provide valuable additional insights. In our research, Ethiopian coffee had an optimal roasting temperature range between 216.49 °C and 230.15 °C. This finding is in line with the work of Sanchez-Bridge *et al.* [50], who also reported a similar optimum temperature range for Ethiopian coffee beans. Also, these parameters can be influenced by factors such as roaster size and coffee variety.

In terms of roasting time, the study showed that longer roasting times at lower temperatures tend to produce a more evenly roasted coffee. This could translate to a more balanced flavour profile in the cup, as it allows the heat to penetrate deeper into the green coffee beans, promoting more even flavour development. On the other hand, shorter roasting times at higher temperatures can lead to a more complex flavour profile with increased acidity, a phenomenon attributed to the rapid development of volatile flavour compounds [51].

In the case of sample P2, which was roasted for 8.5 minutes, the sensory analysis showed that it received the highest average flavour profile score. This suggests that the roasting conditions used for P2 resulted in the development of the desired flavours.

Moreover, the analysis revealed significant mass losses during roasting, which could be attributed to the evaporation of water and the decomposition of organic compounds. The process is essential for the development of aromas in coffee beans, as they result in the formation of numerous aromatic compounds that define the taste of coffee. Therefore, the degree of roasting, which influences the extent of these transformations, can have a significant impact on the taste and overall quality of the coffee.

Results of physicochemical analyses of roasted coffee

The roasting process significantly alters the physicochemical properties of the coffee beans, thus influencing the quality of the final product. Analysis of water activity, *p*H, mass loss, and moisture content furnish a comprehensive understanding of the quality of the roasted coffee beans utilised in this study (Figure 6). Moisture content decreased, whereas total acidity, total soluble solids, and caffeine content increased [16].

Water activity

The water activity of roasted coffee is a critical parameter for determining its storage stability and flavour. Water activity values decreased during roasting compared to sample M (unroasted green coffee), likely due to the reduction in moisture content during the roasting process. Water activity appears to diminish progressively with P4, demonstrating the minimum value of 0.144. It is plausible to attribute this tendency to the roasting intensity, which induces greater dehydration of the coffee beans, thus decreasing their water activity. This trend could be attributed to the degree of roasting, as more roasted coffee beans tend to have lower water activity values due to increased dehydration. The optimal range for water activity in roasted coffee is below 0.7 [52]. In this study, all four roasted coffee samples fell within this optimal range, indicating good storage stability and high-quality flavour potential.

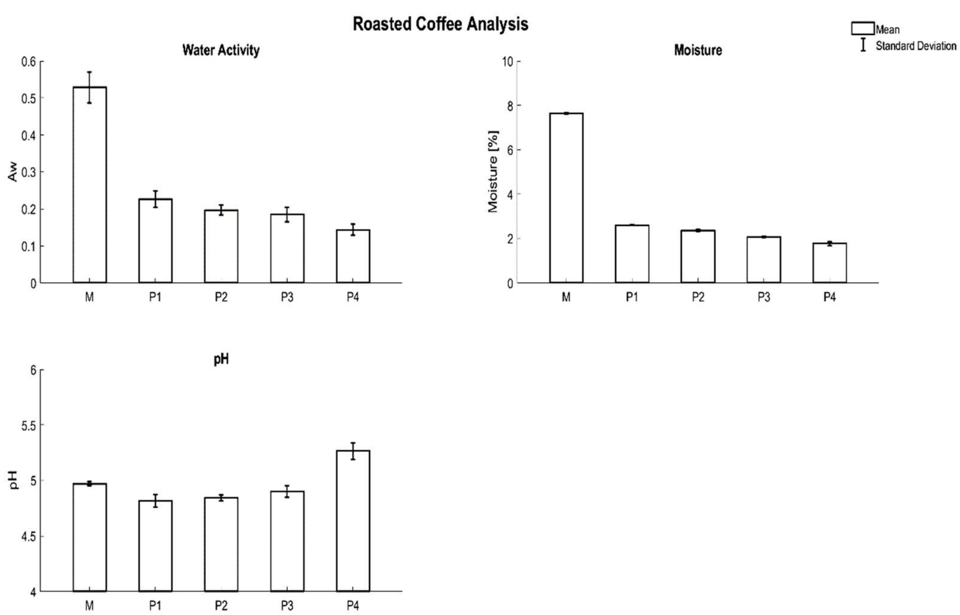


Figure 6. *The values of the physicochemical determinations obtained for water activity, humidity, and pH for the four samples of roasted coffee beans (P1, P2, P3, P4) and for the control (M)*

pH values

The *p*H values decreased, indicating an increase in acidity [42]. The acidity level of coffee, indicated by its *p*H, plays a vital role in its sensory characteristics and overall quality. Our data suggest that the *p*H of the coffee was slightly acidic, ranging from 4.85 to 5.10. This aligns with observations made by Batali *et al*. [53], who observed significant variations in *p*H with different levels of roasting. The roasting process seems to have a profound impact on the *p*H and acidity of the coffee. As Rao *et al*. [54] pointed out, *p*H tends to increase with the degree of roasting, suggesting that roasting significantly influences coffee acidity. This *p*H value reflects the acids present in the coffee. Among the different acids found in roasted coffee, acetic acid is frequently observed [55]. Moreover, the *p*H of coffee is largely attributed to the formation of aliphatic acids during the roasting process, as demonstrated by Ginz *et al*. [56]. This formation process depends on precursor compounds such as sucrose, highlighting the complex chemistry involved in coffee roasting.

Mass loss and moisture

The results of the analysis of mass loss and moisture suggest that the coffee samples [P1, P2, P3, and P4] exhibited a significant reduction in mass compared to the control sample [M] after roasting. The difference in mass and moisture loss among different coffee samples may reflect variations in the roasting process or the composition of the coffee beans [57]. In general, mass loss during roasting is an important indicator of the degree of roasting and can affect the flavour and overall quality of the coffee. The moisture content of roasted coffee beans can significantly impact the quality of the final product. During the roasting process, the coffee beans lose mass.

Sensory analysis

The global appreciation of coffee is mainly determined by its sensory attributes, which can be represented by complex interactions of factors such as coffee variety, geographical origin, land, processing, roasting and preparation methods. These factors contribute to a sensory profile through aromatic compounds, carbohydrates, acids, lipids, proteins, antioxidants, and volatile aromatic compounds [58].

Our sensory analysis (Figure 7) showed that sample P2 obtained the highest average flavour profile score (7.0), followed by P3 (6.6), P1 (6.3) and P4 (6.2). These data suggest that P2 has a more pronounced or taste-appealing flavour profile compared to the other samples, possibly due to the unique combination of origin, processing, and roasting parameters [59]. This information is invaluable to coffee roasters and producers as it provides insights into the sensory properties of different coffee samples, allowing them to make more informed decisions about roasting techniques to achieve desired sensory attributes.

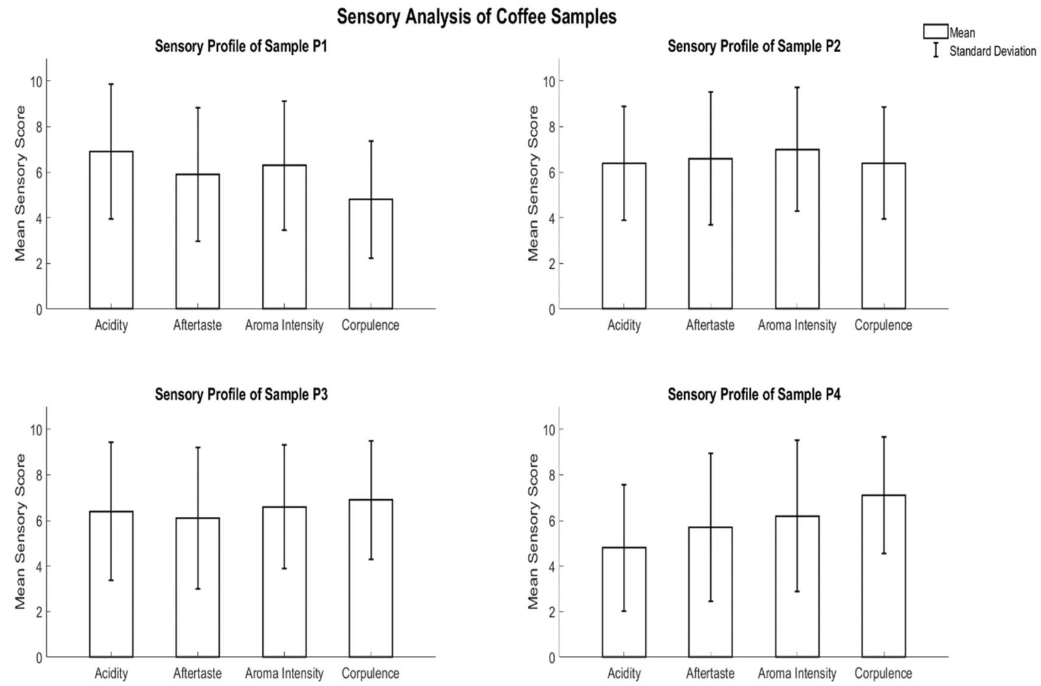


Figure 7. *Mean values of sensory scores for samples P1, P2, P3, P4*

Interestingly, P4 presented the highest average score for corpulence (7.1), followed by P3 (6.9), P2 (6.4) and P1 (4.8). The corpulence of a coffee, often described as texture or mouthfeel, is a critical sensory attribute [60, 61]. Our analysis suggests that the four coffee samples (P1, P2, P3 and P4) show distinct corpulence profiles, with P1 having the lowest score, indicating a lighter corpulence compared to the other samples.

Acidity, another key component contributing to the overall sensory properties of coffee, was highest in P1 (6.9), followed by P2 and P3 (6.4) and lowest in P4 (4.8). This suggests that factors such as coffee bean variety, roasting process and brewing method can significantly influence the perceived acidity of coffee [62].

In terms of aftertaste, P2 scored the highest (6.6), followed by P3 (6.1), P1 (5.9) and P4 (5.7). This indicates that the roasting method used for P2 may have resulted in a more pleasant tasting coffee, a critical factor in overall coffee satisfaction [63].

Our results suggest that P2 presents the most balanced sensory profile, with high scores for aroma intensity, aftertaste, acidity, and corpulence. P4, while having the most well-rounded flavour profile, scored lower for flavour intensity and aftertaste. P1 and P3 showed high levels of acidity but had lower corpulence and aftertaste scores. Also, these data are in accordance with previous studies that reported significant variations in the sensory attributes of coffee beans of different origins. Variations in sensory attributes can be attributed to differences in the genetic structure of coffee plants, growing conditions, post-harvest processing methods and roasting parameters [59].

From a consumer perspective, the variations in sensory attributes between coffee samples from different origins suggest that consumer preferences for coffee may vary depending on the origin of the coffee beans. Therefore, to satisfy diverse consumer preferences, it is crucial to offer a variety of coffee products that cater to different sensory preferences.

CONCLUSIONS

The results of our physicochemical and sensory analyses of green and roasted coffee samples provide invaluable information on the factors that influence coffee quality and sensory properties. Different coffee samples exhibited unique physicochemical properties, largely attributed to origin, harvesting, and processing methods. Understanding these factors is critical for coffee industry stakeholders such as coffee producers, roasters, and retailers when selecting coffee samples and formulating various coffee products.

The degree of roasting significantly affected the physicochemical properties of coffee, such as water activity, *p*H, and moisture, and also influenced the sensory properties. Therefore, fine-tuning the roasting process for each sample is essential to achieve the desired flavour profile and consistently high-quality coffee. The knowledge gained from our research can provide coffee producers and roasters with valuable data to optimise their roasting processes and create new, unique coffee products.

Furthermore, the practical implications of our findings extend to the retail sector. Retailers can use this information to better inform their customers about the unique characteristics of different coffees, improving the buying and consumption experience. In addition, coffee storage recommendations can be adjusted based on our findings related to water activity and other physicochemical properties, helping to ensure maximum flavour retention and quality preservation.

However, it is important to note that the optimal roasting parameters may differ for different types of coffee beans. Therefore, each type of bean requires a customised selection of parameters to achieve the optimal flavour profile.

We recognise that this research presents a small snapshot of the vast spectrum of coffee varieties and processing techniques available globally. In this regard, future research could deepen the analysis of different coffee processing methods on the chemical composition and potential health impact.

Additionally, exploring the interactions between the various chemical compounds in coffee and their collective impact on human health could be a promising area for future investigation. Given the popularity and daily consumption of coffee worldwide, understanding these aspects has far-reaching implications for public health and the global coffee industry.

In conclusion, our study underlines the integral role of physicochemical and sensory analyses in understanding the influence of different roasting parameters on the quality and sensory properties of coffee. The data presented in our study could serve as a valuable resource for stakeholders in the coffee industry, guiding efforts to optimise roasting processes and assisting in the creation of diverse, high-quality coffee products.

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