OPTIMIZATION OF THE TIME AND TEMPERATURE CONDITIONS FOR THE ROASTING PROCESS OF *CAFÉ DE CAUCA*, TAKING INTO ACCOUNT CONSUMER PERCEPTION

DIEGO ANDRÉS CAMPO CEBALLOS

Tesis de Doctorado en Ciencias de la Electrónica

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PhD. en Automática Avanzada y Robótica

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Departamento de electrónica, instrumentación y control
Línea de Investigación Automática AI
Popayán, Mayo 2023

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Electrónica y Telecomunicaciones de la
Universidad del Cauca para la obtención del
Título de

Doctor en:
Ciencias de la Electrónica

Director:
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Popayán, Mayo de 2023

Nota de aceptación

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Popayán, Mayo 2023

Resumen

Antecedentes: Desde el punto de vista del consumidor, se pueden distinguir varios niveles de calidad: la calidad esperada, la calidad inducida y la calidad efectiva. En esta última, la acidez y el cuerpo son atributos que son percibidos por parte de un consumidor no entrenado e inciden en su preferencia por un producto específico. Para una empresa productora de café tostado el lograr consistencia en la percepción de esos atributos por parte del consumidor habitual, es consecuencia de un riguroso cuidado en la trazabilidad de la cadena de procesamiento del café, que va desde su siembra hasta el café tostado entregado al consumidor. En esa cadena de valor, el proceso de tostado del café es una parte crucial del procesamiento, y se define como la recopilación de transformaciones físicas y químicas dependientes del tiempo y la temperatura, inducidas por el calor. La correcta definición del grado de tueste del café es un área de investigación activa y no trivial, que interviene en la obtención de perfiles de tueste consistentes que se reflejan en la aceptabilidad de las bebidas percibidas por los consumidores. Los perfiles de tueste se registran mediante curvas de temperatura en función del tiempo durante el proceso de tostado del café, y se han publicado diversos estudios que demuestran cómo regiones específicas de los perfiles inciden en la exaltación de los atributos organolépticos del café, al ser evaluados por expertos catadores. Esos estudios correlacionan los perfiles de tueste con la evaluación de atributos realizadas por expertos catadores y con resultados de análisis en laboratorios especializados de las propiedades químicas y físicas de muestras de café tostado o en tasa. Sin embargo, la precepción de los expertos suele ser opuesta a la de los consumidores, es por eso por lo que no sólo se debe rastrear el comportamiento inconsciente de los consumidores de café con pruebas de degustación, sino también su comportamiento consciente. Los hábitos de los consumidores cambian

rápidamente, por lo que las evaluaciones continuas del comportamiento y la sensibilidad sensorial cobran importancia. No se conoce, a la fecha de esta monografía, de evaluaciones sistemáticas que permitan confirmar el grado de incidencia del perfil de tueste en la percepción de acidez y cuerpo, así como en la consistencia en esa percepción por parte de un consumidor no entrenado.

Objetivo: Proponer un esquema de optimización de las condiciones de tiempo y temperatura sobre el perfil de tueste estándar del SCA, que promueva la consistencia en la percepción de la acidez y cuerpo en taza aceptables por los consumidores de café especial en las variedades Castillo y Tabi, cultivados en el departamento del Cauca.

Métodos: En esta investigación se utilizó la metodología de superficie de respuesta (RSM) utilizando el diseño central compuesto (CCD) como herramienta de diseño experimental con 13 experimentos, con el fin de obtener de forma sistemática, un conjunto de muestras de café tostado a través del perfil de tueste. En este diseño se incluyen los puntos críticos del tostado como son la temperatura de carga, el punto de inflexión, la etapa de secado o amarillamiento, el pardeamiento no enzimático, el primer crac, el tiempo de desarrollo y la descarga. El color del grano de café se reportó como punto de referencia transversal de todo el proceso. Se usaron técnicas espectroscopia de infrarrojo cercano – NIR (896-1,684 nm), las imágenes hiperespectrales (400-1,000 nm), para reportar una referencia colorimétrica en el perfilamiento del café, y su respectiva relación con las técnicas industriales KONICA-minolta (La*b*) y los discos SCA (25-95).

Para modelar las respuestas de acidez y cuerpo en la bebida con las muestras de café, fueron seleccionados 104 consumidores de cafés especiales del departamento del Cauca, Colombia, vinculados a procesos de formación trasversal del parque tecnológico del Café TECNiCAFÉ (visitantes, productores, procesadores y comercializadores). Las tazas de café se prepararon con 18 g de café por 250 ml (relación café-agua de 1:14) en una prensa francesa a 93°C. Se tomó como referencia la escala de intensidad 0-15 (0=nada, 2=apenas detectable, 4=Identificable, pero poco intenso, 6=Ligeramente intenso, 8=Medianamente intenso, 10=Intenso, 12=Muy intenso y 15=Extremadamente intenso) del léxico internacional del café, que permite a los consumidores comparar la intensidad del atributo en la muestra con la intensidad en la referencia. Como referencia ácida se usaron soluciones de ácido cítrico de grado alimenticio (0.2 a 2 g/L). Como referencia del cuerpo se prepararon soluciones comerciales de café, con relaciones agua/café de 1:13 hasta 1:20. Los datos de percepción del consumidor se recolectaron, a través de una encuesta directa. Cada uno de los participantes probó 13 tazas de café, reportando su percepción de acidez y cuerpo en la escala de intensidad. Se utilizó el estadístico kappa de Fleiss para mostrar el grado de concordancia entre consumidores en la percepción de intensidad de la acidez y cuerpo, y el alfa de Cronbach para evaluar la consistencia interna de la escala de intensidades.

Las ecuaciones predictivas para la percepción de las respuestas fueron obtenidas usando el modelo de regresión cuadrática, desarrollado para la acidez y el cuerpo y validado antes de los estudios de optimización. Se usó la función de deseabilidad para optimizar numéricamente, a partir de la maximización de las ecuaciones de acidez y el cuerpo obtenidas. Se usó la optimización gráfica para complementar el estudio en las regiones de interés del diseño experimental. Como experimentos de confirmación se tostaron muestras de café Castillo y Tabi con las condiciones optimizadas.

Los cuestionarios CATA (Check-All-That-Apply) fueron utilizados como herramienta de estudio de la percepción de los consumidores de café en relación con los atributos de sabor, acidez y cuerpo de las muestras optimizadas, tanto en bebidas preparadas con granos de café Castillo como en Tabi. Se usó igualmente la prensa francesa como método de preparación y presentación de 6 bebidas, 3 de café Castillo y 3 de café Tabi, tostados con su respectivo perfil optimizado, ante los consumidores. En medio de la contingencia por COVID-19, se contó con la participación de 40 consumidores de Café, los cuales describieron el café mediante una lista de 18 descriptores (Lima, Mandarina, Naranja, Arándano, Plátano verde, Uvas, Cuerpo suave, cuerpo medio, Cuerpo pesado, Amargo, Panela, Piña, Manzana verde, Canela, Chamuscado, Frutos rojos y Chocolate) y una escala hedónica 1-9. Se utilizó el algoritmo CLUSCATA para realizar el estudio de segmentación de los consumidores, según sus preferencias, y así mismo reportar la consistencia de las percepciones del café, basado en los índices de homogeneidad, consenso y similaridad. Igualmente se utilizó el análisis de penalización para evaluar la satisfacción del consumidor ante la presencia o ausencia de algún atributo de los cafés optimizados, revelando así su potencialidades u oportunidades de mejora.

Resultados: En el perfilamiento del café se encontraron referencias para diferenciar el nivel de tostado. La técnica NIR, mostró dos regiones entre 900-1100 nm y 1500-1600 nm. La técnica hiperespectral mostró una región entre 750-1000 nm para diferenciar las muestras con tueste claro, medio y alto. Utilizando el diseño experimental CCD-RSM, se obtuvieron dos modelos cuadráticos significativos para predecir los niveles de acidez y cuerpo del café Variedad Castillo y Tabi, respectivamente. El estadístico kappa de Fleiss reportó una *moderada fuerza de acuerdo* $(\kappa)=0.41< \kappa < 0.60$*”* entre los consumidores y el alfa de Cronbach mostró una *buena homogeneidad* $(CA=0.9> \alpha \geq 0.8)$ en la escala 0-15 para la percepción de intensidad de la acidez y cuerpo. Se maximizó la función de deseabilidad para cada modelo y se obtuvo el perfil de tueste del café Castillo optimizado, en 473 segundos a 192 °C, prediciendo una acidez (9 in la escala 0-15) y un cuerpo (6 in la escala 0-15) en la escala de percepción del consumidor. Por su parte, para el café Tabi, las condiciones optimizadas fueron obtenidas a 540 segundos con 195 °C, prediciendo una acidez (10 en la escala 0-15) y un cuerpo (4 en la escala 0-15) en la escala de percepción del consumidor.

La metodología CATA, reportó la primera caracterización de los cafés Castillo y Tabi tostados con los perfiles optimizados, de acuerdo con 18 descriptores y una escala hedónica. El algoritmo CLUSCATA reportó 3 grupos para segmentar a los consumidores según las preferencias. El índice de homogeneidad=0.647 muestra un “*consenso moderado”* entre los consumidores para discriminar el café según los descriptores de acidez y cuerpo, incluso los atributos de sabor. El método de análisis de penalización fue introducido en esta investigación para presentar una herramienta robusta de análisis e identificación de tendencias potenciales para la mejora del café utilizando un descriptor ideal propuesto por los consumidores. De acuerdo con el análisis de penalización, los cafés optimizados se caracterizaron porque tuvieron percepciones en consenso de acidez frutal a mandarina y naranja, con cuerpo medio.

Conclusiones: Hasta el día de hoy, este es el primer estudio que aborda la inclusión de la percepción del consumidor sobre la acidez y el cuerpo para construir modelos de predicción considerando las muestras de café de especialidad modulando la anatomía de la curva de tueste del café a través de los puntos críticos. Así como la forma en que se validó la percepción de las muestras optimizadas, combinando el enfoque de técnicas sensoriales para obtener perspectivas sobre cómo los consumidores perciben un perfil optimizado de los cafés Castillo y Tabi Cauca.

Se calcularon dos modelos cuadráticos significativos a partir del diseño experimental CCD-RSM para acidez y cuerpo, que los tostadores pueden utilizar para realizar experimentos centrados en la región de tueste óptima para tostar productos de café con una consistencia entre acidez y cuerpo con la calidad deseada, en especial para la variedad Castillo y Tabi del Cauca. La optimización numérica de modelos considerando la percepción del consumidor brinda una herramienta sistemática al tostador para evitar los experimentos comunes de prueba y error cuando se buscan obtener las mismas características del café, con el perfil deseado. Vincular la percepción de los consumidores a modelos matemáticos, permite conocer los puntos de tiempo y temperatura del tueste, genera una ventaja competitiva para que el tostador se concentre en un punto específico del tueste, que generalmente es después del primer crack, y logre un equilibrio entre acidez y cuerpo.

La inclusión de atributos comunes de acidez (lima, naranja, mandarina, arándanos, uvas, manzana verde, plátano verde), cuerpo (agua, ligero, almíbar, mantecoso) y sabor general y defectos (chocolate, canela, piña, panela, amargo, chamuscado), pueden determinar tendencias para la mejora de productos de café, basados en cuestionarios CATA en el desafío de que cada consumidor tiene un sabor y aroma de café ideal y sus preferencias son un tema de investigación actual para cerrar la brecha en las tendencias de productos de café de especialidad.

Palabras clave: Optimización CCD-RSM; Café especial del Cauca; Variedades Tabi y Castillo; Kappa de Fleiss, Alfa de Cronbach; CATA (Check All That Apply), CLUSCATA, Análisis de Penalización.

Abstract

Background: From the point of view of the consumer, the levels of quality can be distinguished: the expected quality, the induced quality, and the effective quality. In the latter, acidity and body are attributes that are perceived by a non-training consumer and affect their preference for a specific product. For a company that produces roasted coffee to achieve consistency in the perception of these attributes by the habitual consumer is a consequence of rigorous care in the traceability of the coffee processing chain that goes from its planting to the roasted coffee delivered to the consumer. In this value chain, coffee roasting is a crucial part of the process. It collects physical and chemical transformations dependent on heat-induced time and temperature. The correct definition of roast coffee grade is an active and non-trivial area of research involved in obtaining consistent roast profiles that are reflected in the acceptability of beverages perceived by consumers. Roast profiles are recorded using temperature curves as a function of time during the coffee roasting process. Several studies have been published that demonstrate how specific regions of the profiles affect the exaltation of the organoleptic attributes of coffee when evaluated by expert tasters. These studies correlate the roasting profiles with the evaluation of attributes carried out by expert tasters and with the results of the analysis in specialized laboratories of the chemical and physical properties of roasted or cupped coffee samples. However, experts' perception is usually the opposite of that of consumers, which is why not only should the unconscious behavior of coffee consumers be tracked with taste tests and their conscious behavior. Consumer habits change rapidly, so continuous evaluations of behavior and sensory sensitivity become essential. Today, no known systematic evaluations confirm the degree of incidence of the roasting profile in the perception of acidity and body, as well as in the consistency of this perception by an untrained consumer.

General Objective: To propose an optimization scheme of time and temperature conditions on the SCA standard roasting profile, which promotes consistency in the perception of acidity and body in the cup acceptable to consumers of specialty coffee in the Castillo and Tabi varieties grown in the department of Cauca.

Methods: In this research, the response surface methodology (RSM) used the central composite design (CCD) as an experimental design tool with thirteen experiments to systematically obtain a set of roasted coffee samples through the roasting profile. This design includes the critical points of roasting, such as the loading temperature, the turning point, the drying or yellowing stage, the non-enzymatic browning, the first crack, the development time, and the unloading. Coffee bean color was reported as a cross-sectional reference point for the entire process. Near-infrared spectroscopy techniques - NIR (896-1,684 nm) and hyperspectral imaging (400-1,000 nm), were used to report a colorimetric reference in coffee profiling. KONICA-Minolta (La*b*) and SCA disks (25-95) with industrial techniques.

To model the responses of acidity and body in the beverage with the coffee samples, 104 consumers of specialty coffees from the department of Cauca, Colombia, linked to transversal training processes of the TECNiCAFÉ coffee technology park (visitors, producers, processors, and marketers) participated. The cups of coffee were prepared with 18 g of coffee per 250 ml (coffee-water ratio of 1:14) in a French press at 93°C. The 0-15 intensity scale (0=not at all, 2=barely detectable, 4=Identifiable, but not very intense, 6=Slightly intense, 8=Medium intense, 10=Intense, 12=Very intense and 15=Extremely intense) of the international coffee lexicon was used as a reference, which allows consumers to compare the intensity of the attribute in the sample with the intensity in the reference. Food-grade citric acid solutions were used as the acid reference. Commercial coffee solutions, with water/coffee ratios of 1:13 to 1:20, were prepared as the body reference. Datasets were collected through a direct survey. Each participant tasted 13 cups of coffee, reporting their perception of acidity and body on the intensity scale. Fleiss' kappa statistic calculates the degree of agreement between consumers on the perception of the intensity of acidity and body. Cronbach's alpha statistic evaluates the intensity scale's internal consistency.

The predictive equations for perception responses were obtained using the quadratic regression model, developed for acidity and body, and validated before the optimization studies. The desirability function optimizes based on maximizing the obtained acidity and body equations. Graphical optimizations complement the information in the regions of interest of the CCD design. As confirmatory experiments, Castillo and Tabi coffee samples were roasted under optimized conditions.

CATA (Check-All-That-Apply) surveys were used to study coffee consumers' perception of the optimized samples' flavor, acidity, and body attributes, both in

beverages prepared with Castillo and Tabi coffee beans. The French press was used to prepare and present six drinks, three of Castillo coffee and three of Tabi coffee, roasted with their respective optimized profile, to the consumers. In the middle of the COVID-19 contingency, 40 coffee consumers participated and described the coffee using a list of 18 descriptors (Lime, Tangerine, Orange, Blueberry, Green Banana, Grapes, Soft Body, Medium Body, Heavy Body, Bitter, Cinnamon, Pineapple, Green Apple, Cinnamon, Scorched, Red Fruits and Chocolate) and the 1-9 hedonic scale. The CLUSCATA algorithm was used to carry out the segmentation study of consumers according to their preferences and to report the consistency of the perceptions of coffee based on the homogeneity, consensus, and similarity indexes. Likewise, a penalty analysis was used to evaluate consumer satisfaction with the presence or absence of some attribute of the optimized coffees, thus revealing their potential or opportunities for improvement.

Results: Using the CCD-RSM experimental design, two significant quadratic models were obtained to predict Castillo and tabi coffee's acidity and body levels, respectively. Fleiss' kappa statistic reported "moderate strength of agreement $(\kappa)=0.41< \kappa < 0.60$" among consumers, and Cronbach's alpha showed "good $(CA=0.9> \alpha \geq 0.8)$" homogeneity on the 0-15 scale for the perceived intensity of acidity and body. The desirability function was maximized for each model, and the roasting profile of the optimized Castillo coffee was obtained in 473 s at 192 °C, predicting acidity (9 in 0-15 scale) and body (6 in 0-15 scale) on the consumer perception scale. For Tabi coffee, the optimized conditions were obtained at 540 s at 195 °C, predicting an acidity (10 in 1-15 scale) and a body (4 in 0-15 scale) on the scale of consumer perception.

The CATA methodology presented the first characterization of Castillo and Tabi coffees roasted with optimized profiles according to 18 descriptors and a hedonic scale. The CLUSCATA algorithm reported 3 clusters to segment consumers according to preferences. The homogeneity index=0.647 shows a "moderate consensus" among consumers to discriminate coffee according to acidity and body descriptors, including flavor attributes. The penalty analysis method was introduced in this research to present a robust tool for analyzing and identifying potential trends for coffee improvement using an ideal descriptor proposed by consumers. According to the penalty analysis, the optimized coffees were characterized in that they had consensus perceptions of fruity tangerine and orange acidity with medium body.

Conclusions: To this day, this is the first study that addresses the inclusion of consumer perception of acidity and body to build prediction models considering the specialty coffee grade samples modulating the anatomy of the coffee roasting curve through the critical points. As well as the way in which the perception of the optimized samples was validated, combining sensorial techniques approach to get insights on how consumers perceive an optimized profiles of Castillo and Tabi Cauca coffees.

In practical terms, two significant quadratic models were calculated from CCD-RSM for acidity and body, that can be used by roasters to conduct experiments focusing on the optimum roasting region for roasting coffee products with an acidity/body consistency with the desired quality properties of Cauca coffees, especially for the Castillo and Tabi variety. Numerical optimization of models considering the consumer's perception is to provide a systematic tool to the roaster to avoid the common, trial and error experiments when seeking to obtain the same coffee characteristics, with the desired profile. Linking consumers perception to mathematical models, allows to know the roasting time and temperature points, generates a competitive advantage for the roaster to concentrate on a specific point of roasting, which is generally after the first crack, and to achieve consistency between acidity and body.

The inclusion of common attributes for acidity (lime, orange, tangerine, blueberries, grapes, green apple, green banana), for body (water, thin, syrup, buttery) and for overall flavor and defects (Chocolate, Cinnamon, pineapple, panela, bitter, Scorched), can determine tendencies for the improvement of coffee products, based in CATA surveys on the challenge that each consumer has an ideal coffee flavor and aroma and their preferences are a matter of current research for close the gap in specialty coffee product trends.

Keywords: CCD-RSM optimization**;** Cauca specialty Coffee; Tabi and Castillo Varieties; Fleiss kappa, Cronbach alpha; CATA (Check All That Apply), CLUSCATA, Penalty Analysis.

I dedicate my thesis work
to Angela María, my wife, partner, and friend.
I fell in love with a world through her eyes.
To my son Andrés Gabriel,
a gift from God and the purpose of my existence.
To my parents Margarita and Harold my guidance and strength.
To my siblings Mónica and Adrián,
examples of perseverance and discipline.
To the Cauca peasant, indigenous and afro communities
whose tireless efforts have supported the
quality of Cauca coffee as a powerful tool for
implement the total peace in Colombia.

Acknowledgment

I am grateful to the Universidad del Cauca, especially to the professors of the Ph.D. program in Electronic Sciences, for contributing all their experience so that the doctoral program is a research space in context with the needs of the department of Cauca. I thank my director Carlos Alberto Gaviria López, for his direction and excellent support so that the work could fulfill the objectives and realize the research contributions from different engineering points of view in the coffee challenges. Thanks to the Corporación Universitaria Comfacauca, Unicomfacauca, for its financial support, within the scope of Acuerdo 005 of 2016 - sponsorship of master and doctoral degrees. Likewise, to the mechatronics engineering teamwork, with whom we developed a space to promote Cauca Coffee growing research in cooperation with the Universidad Politécnica de Madrid-UPM and the group LPF-TAGRALIA: Técnicas Avanzadas en Agroalimentación, directed by Prof. Belen Diezma Iglesias. Thanks to Professor Marcelo Becker, Associate Professor at University of São Paulo-EESC (Escola de Engenharia de São Paulo, São Carlos) - USP, Brazil. Mechatronics Group - Mobile Robotics Lab, for the professional learning experience in the internship and acquire knowledge in designing experiments and statistical tools for sensory data analysis. Also, to continue managing joint research in engineering applied to the agricultural sector. Thanks to Professor Nelson Gutiérrez, associate professor of the Universidad Sur Colombiana - USCO, director of the Centro Surcolombiano de Investigación en Café - CESURCAFÉ, Neiva -Huila, and his teamwork; Pilar Cortés for the management and coordination of tasks within CESURCAFÉ, Ricardo Cortés, for the support throughout the process of optimized roasting of the samples in PRISMA roaster, Nicolas and other fellow expert tasters, for the sensory analysis and valuable contributions in the coffee descriptors.

Special thanks to TECNiCAFÉ, INDESTEC, Slowcoffee, Café del Campo Orgánico, Identidad Cafetera, Asociación Campesina en Agricultura Limpia de Morales ASOCALM and Café RICO for their support in allowing visits to their commercial establishments, the use of their equipment, their constant accompaniment, and providing coffee samples for the tests conducted in this work

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GLOSARY

Acidity /Bright: The acidity flavor in coffee is described as bright, it is quite common in Central American Coffees such as Guatemala, Colombia, Costa Rica, Kenia, and Ethiopia. This acidity or bright can be tasted at the tip of the tongue.

Bitter: Bitterness on coffee is a characteristic of the flavor which is harsh and not sweet. The first descriptor of commercial coffee

Body: The body of the coffee is intended to explain the texture of the beverage, it ranges from thin, delicate, juicy, syrupy, and heavy.

CATA: Check-All-That-Apply multiple choice questions in which respondents are presented with a list of words. CATA binary data can be analyzed with algorithm such as CLUSCATA (clustering data) and penalty analysis (Mean-drop)

CCD-RSM: Central Composite Design (CCD) for Response Surface Methodology (RSM)

Immersion: As its name implies immersion is an extraction method which consists of immersing the coffee grounds in water and letting the water extract the flavors and aroma. One well-known immersion coffee maker is the French press.

Maillard: Non-enzymatic browning complex reactions between free amino acids and reducing sugars, and contribute to the brown color of coffee, bittersweet taste, aromas, and flavor.

Pyrolysis: Thermal decomposition of materials at elevated temperatures

Roasting: The process of heating the beans to lose their humidity they then start getting brownish and depending on the roasting time the darker they will get. This process is vital to the development of the flavors that will then be extracted on a cup.

Roast profile: A roast profile represents the effects of how the airflow and the heat are controlled during the roasting which determines how quickly the beans arrive at a roasting degree.

Specialty coffee: coffee that is graded eighty points or above on a 100-point scale by a certified coffee taster (SCA)

SCA: Specialty Coffee Association of the world. It is an America and Europe temporal association.

SCA Coffee Standard: High-quality recommendations based upon scientific testing, that are agreed upon by qualified industry professionals (committee) which set values and/or ranges of values for coffee.

CHAPTER 1

1. Introduction

1.1. Context

Cauca, Nariño, and Huila departments have formed the new coffee axis of specialty coffee in Colombia. On August 10, 2011, the *Federación Nacional de Cafeteros de Colombia* managed the denomination of origin Café de Cauca. Its outstanding characteristics have taken it as a coffee of powerful and caramelized fragrance and aromas, presenting a high acidity, medium body, a balanced global impression as clean, and smooth with some sweet and floral notes. Due to the diversity of the territory and its own cultural, climatic, and social conditions, there are four Cauca coffee regions. The center region of Cauca produces the Popayan coffee. Up of 43,000 coffee-growing families in 11 municipalities in the center of the Cauca Department, including the Popayán Plateau, belonging to peasant, Afro-descendant, and indigenous Nasa, and Misak communities, cultivating close to 44,500 hectares of coffee reported in 2021. This coffee is recognized for high-altitude coffees because, on average, they are located at 1,700 meters above sea level and cultivated in soils derived from volcanic ashes, sun, and semi-shade. Its cup profile contains a unique character with a pronounced fragrance and aroma, medium-high acidity, medium body, and balanced cup, with caramel and floral notes (Federación nacional de Cafeteros, 2022). In total, there were close to 93,000 hectares of coffee in Cauca at 2021, where 99% of coffee growers are small producers (less than 5 hectares), which promotes the work in micro batches, guaranteeing traceability throughout the process and allows the development of differentiated specialty coffees (Solis et al., 2021).

Coffee is considered a specialty product when it is perceived and valued by consumers for the characteristic that differentiates it from conventional coffees, for which they are willing to pay a higher price. For this coffee to be a compelling specialty product, the higher value that consumers are willing to pay must represent a benefit for the producer (Federación nacional de Cafeteros, 2022). The Specialty Coffee Association of America (SCA) has generated a list of qualification parameters to classify coffee. In this protocol, coffees that obtain more than 85 points out of 100 are classified as "Specialty", those that obtain a score between 84 and 80 are called "Premium"(SCAA, 2009). Specifically for green coffee, the Special grade is achieved when the beans have no more than five complete defects in 250 grams of coffee. Primary defects are not allowed (SCAA, 2009). A maximum of 5% above the sieve size is tolerated. A specialty coffee must possess at least one distinctive attribute in body, flavor, aroma, or acidity. It must be free of blemishes and stains. Unripe beans are not allowed. (SCAA, 2009). Moisture content should be between 9-13%. Premium grade is achieved when the grains have no more than eight complete defects in 250 grams. At this point, primary defects are allowed (SCAA, 2009). A maximum of 5% above or below the sieve size for coffee bean size is tolerated.

A Premium coffee must possess at least one distinctive attribute in body, flavor, aroma, or acidity. The coffee should also be free of blemishes and stains and could contain up to three immature beans. Moisture content should be between 9-13%. (SCAA, 2009). The coffee industry is interested in obtaining procedures that enhance and potentiate the attributes of coffee to satisfy the requirements of consumers of pure coffees (Bustos-Vanegas et al., 2018). The inclusion of these procedures would make it possible to generate new markets, as well as to verify the authenticity of the raw material.

Cup profile of Cauca coffee was described as one of pronounced fragrance, intense and caramelized aromas, a cup of high acidity, medium body, balanced overall impression as clean, smooth, and with sweet and floral notes. Achieving consistency in the perception by consumers of these outstanding characteristics is not an easy task. In the coffee value chain, several critical points go from the seed to the preparation of the coffee. One of these is the roasting process, which is a procedure that generates the most significant impact on the value addition of coffee (Fadai et al., 2017).

From a science focus and scope, roasting is the compilation of time and temperature dependent physical and chemical transformations induced by heat (Gloess et al., 2014). It converts a hard, spongy bean with an herbal green aroma into a dark brown, intensely fragrant, brittle, and extractable bean (Bottazzi et al., 2012). During the roasting process, chemical reactions, such as hydrolysis, polymerization, and pyrolysis, contribute to the chemical and physical changes in the beans. These chemical reactions produce volatile and non-volatile compounds that compose the organoleptic properties of the beverage, such as aroma and flavor, and are also responsible for the change in color of the coffee beans (W. Sunarharum et al., 2014).

The change in coffee beans' color during roasting is due to the formation of melanoidins. They are dark, high molecular weight compounds resulting from complex chemical transformations of the Maillard and the caramelization reaction. Both chemical reactions are closely related to the sensory properties of coffee (W. Sunarharum et al., 2014). In this way, the correct definition of the degree of roasting of coffee, through the study of the time-temperature profile, is an active and non-trivial area of research, which intervenes in the obtaining of consistent roasting profiles with effects in the acceptability of the beverage perceived by consumers.

The first indicator of roasted coffee quality is the color of the bean, although there is still a gap in determining its relationship with the development of the organoleptic properties in the process (Leme et al., 2019). However, different tones of brown color are possible for the same sample or batch of coffee beans after the roasting process (Schenker & Rothgeb, 2017).

On the other hand, acidity is one of the key attributes within the organoleptic profile of coffee. This characteristic depends on the origin of the coffee, the variety, and the processing method of the coffee cherries (Puerta Quintero, 2016). Although compounds responsible for the acidity developed in coffee beans are still being identified, it is known that citric, malic, acetic, quinic and mainly chlorogenic acids are the most abundant acid species in coffee beans and may be responsible for this organoleptic characteristic (Osorio et al., 2021). Coffees grown at higher altitudes or subjected to a post-harvest wet treatment have a higher acidity. The perceived acidity depends on the final quantity of acids present and extracted, which is mainly related to the degree of roasting. A very acidic perception can be considered as a defect of the coffee (Osorio et al., 2021).

In the chemical composition of the green coffee bean, the lipid fraction constitutes an important part and is reflected in the body of the beverage. Most of the fatty components, saturated and unsaturated, contained in the coffee beans are not degraded during the roasting process, and become part of the mouthfeel of the beverage (Echeverri-Giraldo et al., 2020). In this sense, the industry has been using sensory consumer tests both in the optimization of existing coffee roasting processes and in the development of new products (Poltronieri & Rossi, 2016). Process optimization methodology in the food industry is used to model consumer responses, generating predictive equations that relate consumer response to the variables studied in the process (Malaquias et al., 2018). These mathematical models can optimize the process and to estimate the expected consumer response to combinations of factors not directly tested (Malaquias et al., 2018). After parameterization, mainly given by obtaining a polynomial, the desired responses of the variables are calculated for each phase of the roasting profile: the Time, Temperature, and consumer sensory perception (Malaquias et al., 2018). The systematic way to make this calculation is to use a constrained optimization algorithm based on the dynamics of the standard roasting process curve of the association of specialty coffees. Some complex relationships can be explained by relating optimal time and temperature terms that seek consistency in the final product (Bozkurt Keser & Buruk Sahin, 2021; Lin et al., 2017).

1.2. Motivation

Motivation of this project is to contribute to the understanding of the processes that lead to generating consistency in the characteristics perceived by consumer of the denomination Café de Cauca, specifically, the acidity and body attributes which are related with temperature and time profiles of the toasting process. This research proposes the definition of a scheme to optimize the conditions of time and temperature of roasting of coffee to enhance the distinctive and consistent characteristics in the attributes of acidity and body acceptable to consumers of specialty coffees.

For this purpose, multiple data could be explored, among which variables that could be of greater relevance to determine the quality of the coffee were evaluated. There are uncontrolled variables in the coffee process related to the genetics of the bean, the variety, its height, the processing, its green density, the homogeneity in size, and the water and humidity activity that affect the beginning of the profiling and subsequent methodological scheme proposed. This way, collecting and structuring a large amount of data on the coffee process could be implemented in and used to improve the coffee supply chain.

On the other hand, according with (Gastón Ares, Tárrega, et al., 2014), 60 to 80 perception CATA data of consumers can be regarded as a reasonable minimum compromise to get stable sample and descriptor configurations. In this experiment, 40 participants evaluated 6 cups of coffee of both, Castillo, and Tabi varieties. However, a stable configuration could be achieved to evaluate the optimized samples in this experimental setup, striking a balance between the costs of the practical scheme and the number of consumers that can adequately participate in achieving consistency in the evaluation. The scope of this studio is limited to the Castillo and Tabi varieties and try to isolate the experimental data from other factors influencing the acidity and body attribute considering a precise protocol taking into account the traceability of the coffee samples studied, the description of their physical properties, the profile in time and temperature of the roasting of the coffee beans, the perception of intensity and sensory attributes through CATA surveys of perception of the consumers of specialty coffees in the department of Cauca.

1.3. Problem statement

In the coffee industry, the roasting process develops the unique organoleptic properties of coffee and generates high-quality conditions in the beverage acceptable to consumers. These conditions present the variables of time and temperature of roasting, known as the roasting profile, which involves instrumental factors such as the type and technology of the roaster, the degree of roasting required, the kind of heat source, etc., and aspects of the raw material such as the variety of coffee, its bean size, density, humidity, and water activity, among other characteristics of the origin, its altitude, the harvest and post-harvest processes of the specialty coffee (de Melo Pereira et al., 2019; W. Sunarharum et al., 2014). Coffee research authors report a correlation between the degree of roasting and the flavor attributes perceived by the consumer. Its elements indicate that using inadequate combinations of time and temperature during the roasting of coffee beans can cause quality defects, such as burnt flavor, dark color, deficient flavor, and unpleasant acidity, among others that are not acceptable to consumers (Giacalone et al., 2019).

One of the open problems in the coffee roasting process is determining the optimum conditions of time and temperature to obtain consistent and replicable profiles according to the attribute sought to be enhanced. Consistency is the object of study of specialty coffees, which implies providing consumers with the same expression of coffee flavor, despite the variations in the raw material. Coffee roasting levels are established based on time-temperature profiles, but these are not uniform from batch to batch. These profiles generate a change in the perception of the flavor of the coffee to the final consumer (Giacalone et al., 2019). Computer-based approaches for sensory analysis have been reported in the literature, including optimal design approaches for sensory experimental designs, and the incorporation of nonlinear modeling methods such as artificial neural networks; but only in the analysis of the results (Yu et al., 2018). Classical techniques such as fractional factorial designs and partial least squares regression have been used in studies related to flavor and sensory perception of foods. Still, these techniques may be inadequate to fully describe a complex and potentially nonlinear system found in the roasting process due to the many variables involved in the system. Machine learning and artificial intelligence methods seek to integrate all the variables of the coffee roasting process, but they are still under development since they require an adequate data set, which due to its structure, is complex to obtain, given the impossibility of systematically recording all the magnitudes of the variables involved in the process (Yu et al., 2018). Thus, it is crucial to explore easily adaptable methods and contribute to showing the relationship between the perception of the organoleptic attributes of specialty coffee and the roasting process, documented in its critical phases (Loading Temperature, Turning Point, Dry, First Crack and Drop).

The importance of generating systematic measures to define categorical data from subjective, objective, and hedonic scales as input information to include consumer preferences has also been highlighted (Birwal P & BK, 2015; Li et al., 2019). Rapid sensory profiling techniques have also been identified (Gastón Ares et al., 2010; Dehlholm et al., 2012; Liu et al., 2018; Narain et al., 2004) and dynamic sensory methods such as the temporal dominance of sensations (TDS) (Charles et al., 2015). On the other hand, it has been shown the direct affectation of the consumer's sensory perception when the shape of the cup where a coffee beverage is served is changed (Spence & Carvalho, 2019), and analysis methods based on binary questionnaires known as CATA (Check-All-That-Apply) have been introduced to contribute to studies of consumer perception concerning attributes, finding complex relationships that, for example, depend on psychological and cultural aspects (G. Ares & Jaeger, 2015; Oliver et al., 2018). These latest techniques offer a positive outlook for proposing the fusion of the information already available on the traceability of specialty coffee with the roasting process and consumer perception.

Although sensory analysis has relied on classical experimental designs and linear multivariate analysis techniques, it incompletely addresses the complexity of coffee flavor due to the lack of information between the roasting process and the consumer's perception, coupled with a large number of variables in the process (Chung et al., 2013). Coffee research authors have contributed to the optimization methods based on response surfaces (RSM) using central composite design (CCD). These methods integrate polynomial models, which report effective results correlating coffee's several physical and chemical characteristics; such as sensory quality, antioxidant activity, caffeine content, total sugar, phenolic compounds, and pH; to affective relationships in the drink (Anisa et al., 2017; Chung et al., 2013; Ku Madihah et al., 2013; Malaquias et al., 2018; Riskiono Slamet & Darsef, 2014).

In Colombia, the research on the effect of numerical optimization of roasting conditions of specialty coffee genotypes based on consumer preferences and affective data is still limited. Only one study has been reported to optimize the roasting of blends of healthy and roasted coffee as a function of the temperature of the process and slaking water, where no significant differences in quality between healthy and roasted beans were obtained (Castrillón Castaño & Quintero Sánchez, 2001). Considering those research gaps, this study drives to answer the question: How to modulate the time and temperature conditions of the SCA standard roasting profile to maintain consistency in the perception of acidity and body in the cup acceptable to coffee consumers, with the Castillo and Tabi varieties of Cauca coffees?.

1.4. Research objectives

1.4.1. General objective

To propose an optimization scheme of time and temperature conditions on the SCA standard roasting profile, which promotes consistency in the perception of acidity and body in the cup acceptable to consumers of specialty coffee in the Castillo and Tabi varieties grown in the department of Cauca.

1.4.2. Specific objectives

- Identify the physical variables involved and the methods required to obtain the SCA standard roast profile for the Castillo and Tabi varieties grown in the department of Cauca.
- Calculate a mathematical model for optimization, which correlates the perception of acidity and body in cupping test by consumers of specialty coffee with the conditions of time and temperature in the roasting profiles.
- Evaluate the performance of an optimization algorithm for time and temperature conditions in roasting profiles, taking as a criterion the consistency in the perception of acidity and body perceived by coffee consumers.

1.5. Main contribution and relevance

This work proposes an optimization scheme based on experimental design methods using physical properties data, harvest and postharvest information, time and temperature profiles, and assessment of final consumer perception, which for the first time reports the consistency and homogeneity of non-expert consumers assessment of samples of the Castillo and Tabi varieties grown in the department of Cauca, as input for the roasting coffee strategies. This work contributes to solve the lack of an integration scheme between the roasting profile data and the perception of the final coffee consumer, providing a valuable tool for the premium and specialty coffee market, as a baseline for subsequent studies in Origin Coffees in Colombia.

The main contribution is the consequence of a series of original contributions in critical aspects of the coffee roasting process, which can be summarized as:

- The adjustment of the roasting curves has traditionally been conducted based on the concept of expert tasters seeking the enhancement of the organoleptic properties of coffee in the cup. The most systematic investigations like those of this work have correlated the roasting profiles with the analysis of samples of roasted coffee or coffee in cup. This work presents a methodology that allows the systematic evaluation of the development of important attributes for the final consumer such as acidity and body through the roasting process, which is an important input for the specialty coffee value chain.

- Mathematical models developed in this research show a way to predict consumer preferences about acidity and body attributes of coffee on cup, from design parameters of the roasting profiles. This result allows to roasters to maximize the consumer acceptance and reducing the needed time to produce new specialty coffee denominations having a differentiable consumer perception.
- It is known that acidity and body perception and consistence is strongly determined by the roasting profiles. However, not systematically research has been performed until now analyzing large volumes of information to understand patterns, making forecasts, and proposing a tool to make decisions considering the assessment of consumer perception by signatures around of their preferences.

1.6. Scope and limitations

The scope of this research is to study the consumer's acidity and body perception of specialty coffee, by modulating the points of the roasting curve, within an experimental space designed with RSM-CCD. By obtaining predictive equations a region in the experimental space was constructed to optimize the coffee samples aiming at maximizing consistency in acidity and body as perceived by consumers. To include analyzing the experimental confirmation samples, alternative methods to the classical descriptive analysis were integrated, such as CATA (Check-All-That-Apply) questionnaires, including the CLUSCATA algorithm and penalty analysis, with the advantage of flexibility, speed, and suitability to be performed both by experts and directly by untrained consumers. These methods contribute rigorously to the task of consumer preference training, as well as in cupping, by directly capturing consumer perception, finding that both variations in bean selection, genetics, and grading, as well as differences in the roasting and brewing process can lead to a change in consumer perception.

Some limitations of the methods used in this research are:

- The criteria used to measure the quality of coffee include the genetic, origin, size and shape of the green beans, the post processing as well as the absence of defects. The coffee profiling process is fed by the physical data of the selected and classified coffee sample, including traceability data. Therefore, a limitation for working with specialty coffees is that each specialty coffee laboratory has a structure to build and manage the massive data of the coffee to be studied.

- The first indicator of roasted bean quality is measured by visual color scoring on a scale. In this work this bean color reading usually occurs by visual inspection process or by using traditional instruments in the 25-95 agtron scale with scope limitations. Two roasted coffee samples could have the same color but could have been roasted by different time and temperature profiles, generating significant differences in their aroma and flavor expression. For this reason, the color of the roasted coffee should always be accompanied by its respective roasting curve as a measure of the transparency and follow up of the process.

- To achieve better precision in the prediction acidity and body equations, RSM-CCD requires evaluating the fitness of the experimental values of the model. In the present study, R^2 values of all responses fall within the acceptable range ($R^2 \geq 0.80$) revealing the effects of Time and Temperature variables on the acidity and body parameters with good reliability. However, to achieve these levels, in this work washed, selected, classified and defect-free process coffee, carries the cost associated with each sample. When experimental costs are low, planning and optimizing the number of runs to be carried out is not critical. However, as the number of experiments increases, process costs may increase, and therefore, it could generate missing data. The presence of missing data in an experiment causes the loss of the original structure of the experimental design and consequently the loss of the orthogonality of the design.

- Cup quality is determined when samples are submitted to professional coffee tasters who evaluate body, acidity, flavor, and overall level, trained to determine both good attributes and off-flavors. Coffee experts cannot necessarily estimate whether a consumer will accept the product that was brewed. For example, acidity and body is highly valued by SCA experts and is a profiling objective attribute for roasters to accentuate, however, the number of consumers who like this experience has not been studied. The untrained consumer has difficulties in distinguishing quality levels of coffee compared to an expert. The role of familiarity with the product is important in the assessment of its quality. Consumer perceptions of the acidity and body of Cauca coffee could drive, with the methods present in this work, a different consumption behavior. A limitation of this study was that it was conducted in COVID-19 pandemic, and the sample of forty coffee consumers reached 66% of the range recommended by Ares et al. (60-80 respondents) for CATA analysis to obtain a better view of the perceptions of Cauca coffee Consumers. Despite, this work presents adequate consistency related with consensus among consumers and report the possibility of the implement an untrained panel of consumers to differentiate coffees.

- The results of this research show that the analysis of optimization validation data through CATA surveys and analyzed with CLUSCATA algorithms, and penalty analysis measures could effectively predict the sensory evaluation of experts to save time and money. For the information gathering strategy, one must also consider one's own resources, including the number of consumers, the availability of selected green coffee samples, the preparation of the roasting profiling, and the time in which the tests are performed. It is often more efficient to use these standardized tests for sensory science, as they are well known, easy to explain, and come with defined statistical procedures for analyzing the data. However, these prediction models are only valid within the limits of the sensory space of the samples and the selected conditions.

1.7. Thesis structure

The document has been organized as follows.

Chapter 1 presents the research topic's introduction, context, motivation, the problem statement, the research objectives, main contributions and relevance and the scope and limitations of methods.

Chapter 2 presents the background and state-of-the-art related to the quality of specialty coffee. This chapter introduce the physical evaluation of the coffee samples, approaching the roasting process from the instrumental perspective and the anatomy of the roasting curve, integrating it with the fundamental concepts to understand the elements of optimization and sensory perception of the consumer, and the research gap and proposition of this work.

Chapter 3 presents the experimental development of the roasting process of the samples, detailing the materials and methods used for the investigation considering four main axes: First, the evaluation of the raw material, second the coffee roasting process, third the RSM-CCD methods, to obtain the mathematical models for acidity and body. Fleiss Kappa and Cronbach Alpha statistics were used for the strength of agreement and consistency of the descriptors scale, having as input the consumers' acidity, body, and color perception. In fourth place, the document presents the experimental development to study the relationship between the roasting curves and the categorical variables of consumer preferences, using the CATA (check all that apply) methodology as a sensory description instrument. The CLUSCATA algorithm was used to analyze the homogeneity of perception among consumers. Due to consumer assessments, penalty analysis was used to identify potential directions to improve coffee products from sensory and affective data.

Chapter 4 presents results and discussion. First presents the experimental setup from RSM-CCD modulating points for roasting specialty coffee. Second and third section present the roasting process and perception of acidity and body for Castillo and Tabi coffees results. Here we present, for each one, the correlation analysis between roasting profiles and the perception of acidity and body from consumers. The Fleiss kappa and Cronbach´s alpha analysis, also the mathematical models for acidity and body and the numerical and graphical optimization results. Forth section present the sensory characterization with consumers by using CATA data analysis. CLUSCATA and penalty analysis for both Castillo and Tabi coffees. Five section reports final consideration for the results.

Chapter 5 presents the conclusions and future work, with the optimization of the time and temperature conditions of the roasting coffees considering consumers perception.

CHAPTER 2

2. Background

The objective of this chapter is to establish the conceptual basis of the research proposal of this research. For this purpose, is necessary to establish a theoretical framework allowing the understanding of the diversity of aspects involved in the coffee roasting process and in the assessment of the sensory perception of the final coffee consumer, and then to specify the research gap that originates the proposed solution that will be developed in the following chapters.

This chapter is divided in two sections. The first one presents a conceptual framework which provides the fundamental concepts addressed throughout the coffee roasting process as support for the development of the research. Initially, a review of coffee quality and its assessment mechanisms is presented. Next, the concepts that contextualize the coffee aroma triangle are presented. Genetics, roasting (profiling, machines, defects, and anatomy of the s-curve), optimization techniques focused on acidity and body, closing with the concepts for sensory analysis based on consumer perception. The second section summarize the research gap and proposal of this research work.

2.1. Conceptual framework

2.1.1. Assessment of roasted coffee attributes

Cup quality of coffee depend on critical factors such as geographical origin, environmental and genetic factors, and others related to agricultural practices, its storage and the preparation of the drink (Cheng et al., 2016; Mestdagh et al., 2014; Puerta Q et al., 2016). Significant differences have been found in the taste and aroma of coffee that are related to the physical, chemical, and physiological alterations that occur in the beans during the stages of their processing. Colombian coffee has a quality recognized worldwide and has been appreciated by roasters as one of the best within Arabica coffees and are the subject of constant study to generate quality control strategies in the coffee value chain (Bosselmann et al., 2009; Liang Wei Lee et al., 2015; Moroney et al., 2015; Puerta Quintero, 2016; W. Sunarharum et al., 2014). The most important roasters in the United States, Brazil, Germany, and Switzerland, for example, have different preferences regarding the characteristics of coffee and have made great progress in roasting and sensory analysis of selected coffee batches. The best known methods for the quality control of coffee roasting have been the visual, olfactory and flavor comparison made by a panel of tasters duly trained under an assessment protocol, demonstrating expertise and experience with the diagnosis of the quality of the sample of previously roasted and prepared coffee (Correa et al., 2011; Diezma & Cristina, 2011). This assessment is contrasted with the quality format of both roasted coffee and beverage according to the Specialty Coffee Association (SCA), taking into account the lexicon of flavors and aromas defined by The World Coffee Research Organization (Chambers IV et al., 2016).

2.1.2. Assessing roasting by experts

Traditionally, a panel of trained experts evaluate coffee quality parameters to identify, define and understand the sensory characteristics that determine that quality (N. Gutiérrez & Barrera, 2015) The method of quality assessment based on human sensory inspection relies heavily on the senses of vision, smell and taste, to define and identify the parameters of appearance, color, aroma, acidity, bitterness, body and taste of the drink, respectively, and tend to be subjective, despite the training provided, as this assessment may contain perceptions or omissions of the operator by not being able to confirm any abnormality in the coffee, the use of inadequate statistical techniques, or the misinterpretation of the data. This fact has generated disadvantages related to the costs of their training, the time invested to analyze the samples, and the discrepancies that may occur between each taster (intra-observer perception) and between the cupping panel (inter-observer perception), due to tiredness, fatigue, stress, and some non-pre-existing diseases that experts may suffer and that generate subjectivity in the process of quality assessment and expression the flavor of roasted coffee. This problem has been addressed since the calibration of the taster panels using the SCA protocols and their respective calibrations and recalibrations that must be performed annually (Brudzewski et al., 2012). Currently there is no complete technological approach that allows to contribute instrumentally to this aspect.

2.1.3. Assessing roasting by color properties

Roasting is key step in coffee processing, responsible for the chemical, physical, structural and organoleptic changes in the bean (Wang & Lim, 2015a). During this process, the green and dry grains are subjected to a treatment characterized by applied temperatures in the phases over time, which will determine the final characteristics of the product. The bean color is the parameter to establish the level of roasting of the coffee, a relevant aspect to assess the quality of the final product. For color measurement in coffee, there is specific instrumentation such as commercial colorimeters developed exclusively for this application (Puerta Quintero, 2016). Experimentally, the type of light, medium or dark roasting has a definitive impact on quality and is also associated with consumer preferences (Gloria Puerta, 2009). The darker the roast, the less pronounced the acidity and different flavor aspects (and defects) of the drink, but the more consistent the body (Gloria Puerta, 2009). The lighter the roast, the more pronounced the acidity and taste (and defects), but the body is lighter. Thus, it has been detected that in the roasting industries, where green coffee beans are required, several parameters can be used as quality indicators of the degree of roasting: the aroma, flavor, temperature of the bean, pH, chemical composition, loss of mass, and fundamentally the color and hue (Ruiz-Altisent et al., 2010; Vargas-Elías et al., 2016; Wu & Sun, 2013).

The relationship of color and organoleptic characteristics of cup coffee is established by expert tasters, who define the color descriptors according to the SCA protocol for each relevant quality attribute. The Agtron Gourmet Scale of the SCA corresponds to the measure of light reflected off roasted coffee and ranges from 25 (#25, the darkest common roast) to 95 (#95, the lightest roasting) at intervals of 10 (SCAA, 2015) (Gloria Puerta, 2009). The AGTRON system uses eight numbered color discs corresponding to the Agtron Scale, with which the sample of finely ground and roasted coffee, usually crushed on a Petri disc, is compared. In this way, roasted coffee is assigned the approximate number on the SCA scale. This information is highly subjective, despite the preparation and experience of the roaster, and is used to generate the roasting curves, manually or automatically, and thus achieve the desired coffee. The most relevant question in research for this field has been: What is the optimal tone and intensity level of a roasted coffee?. This question has admitted several answers depending on the habits and tastes of the market to which the final product is directed. Different manufacturers roast coffee in different ways, they must know what kind of roast their buyers need, and this is how the expressions “light”, “medium’’ and “dark" mean different things to different people and therefore are subjective terms (SCAA, 2015)(Gloria Puerta, 2009).

The AGTRON/SCA scale allows producers and roasters to use the same language when talking about the “roasting” of a coffee. However, this language incorporates subjectivity, especially when in the assessment of a roasted brown machine the lighting is not controlled and two different shades can be found for the same coffee, which causes a difference in the color perception of that coffee sample. The latest studies in colorimetry have striven to integrate the measurement of color and hue parameters, both of roasted coffee, and of the SCA Agtron measurement discs, in their standardized scale, contributing to the quantification of the levels of roasting that they throw and their corresponding instrument. The colorimetric study has focused on quantitatively determining the level of roasting of coffee based on color, however, the study of the variability that exists in the final assessment of coffee quality is not addressed, given that there are nuances, for example, between the middle colors, No. 55 or No. 65, of the discs of the Agtron/SCA scale, generating fluctuation in the assessment of the expert taster in account of the perception of color in an uncontrolled lighting environment (Diezma & Cristina, 2011). Meanwhile, the determination of the color of the middle tones, where the best organoleptic attributes of coffee has been obtained, is currently a subject of research in this field.

Table 2.1, shows some relations between colors in Agtron disks and parameters of some color spaces for computer vison analysis and spectral reflectance spectrum analysis, which has been some approaches studied to give answers to the subjectivity problem in assessment of roasted coffee samples.

Table 2.1. Agtron discs of the SCA gourmet scale related to parameters of some common color spaces and spectral reflectance spectrum

COLOR	Agtron disc # tile	SCA	L	a*	b*	HUNTERLAB spectral reflectance (650 nm)	RGB	%C, M, Y, K
	25	Very Dark	14,7	4,31	4,41	2,54	(45, 35, 31)	(0,23,32,82)
	35	Dark	14,85	6,15	5,87	2,43	(49, 34, 29)	(0,30,40,81)
	45	Moderately Dark	18,23	8,77	9,71	3,66	(61, 39, 31)	(0,35,49,76)
	55	Medium	22,07	10,94	13,01	6,58	(74, 46, 34)	(0,37,54,71)
	65	Light Medium	25,45	12,31	17,59	8,19	(85, 53, 34)	(0,38,60,67)
	75	Moderately Light	28,1	13,1	20,53	9,71	(93, 58, 35)	(0,38,62,63)
	85	Light	30,15	13,55	22,86	11,28	(100, 62, 36)	(0,38,64,61)
	95	Very Light	32,45	13,04	23,48	12,81	(105, 68, 40)	(0,36,62,59)

Although modeling studies of physical properties such as grain size, density, humidity and water activity have been carried out in relation to heat transfer processes, the chemical mechanisms that give way to color variability throughout grain volume are still unknown (Fabbri, Cevoli, Alessandrini, et al., 2011). From a quantitative point of view, the color of roasted coffee is not yet a quantifiable indicator of quality, because, although the coffee seems roasted on the outside, it could be raw inside; this is due to the density of the bean and its homogeneity in size at the time of roasting.

Currently, the color of roasted coffee can be offered to the consumer as a measure of transparency of the entire roasting process and currently colorimeters are used that show values associated with the experience and taste of consumers in the process of making beverages (Fabbri, Cevoli, Alessandrini, et al., 2011).

2.1.4. Attributes of coffee: acidity and body

Acidity perception in coffee brewing's

The acidic taste is felt most intensely at the middle lateral edges of the tongue and also at receptors located on the mucosa of the lips and on the veil of the palate (Gupta et al., 2010). The salty taste is felt in all parts of the tongue and especially in the lateral and front areas of the tongue (Gupta et al., 2010). Other taste sensations are freshness, spiciness, astringency, metallic and umami (Monosodium glutamate) (Sung et al., 2017). Thus, the subjectivity in the sensory perception of a taste is high and is technically related only to a person's experience when a food is tasted, and a memory of the sensation is engraved in your memory.

Coffee contains several alkaloids and other components that contribute to the bitter taste of coffee such as caffeine, trigonelline and others in lower concentration such as paraxanthine, theobromine and theophylline. On the other hand, chlorogenic acids correspond to many hydroxycinnamic phenolic acids, chlorogenic or caffeoylquinic (CQA) which is the most abundant in coffee and is also found in blueberries and apples; and the dicaffeoylquinics (di-CQA) of artichoke and sunflowers. The components that present the most variability in roasted coffee and coffee drink are chlorogenic acid and caffeine. These two compounds have been the subject of various studies to evaluate their quality and authenticity, through the chemical composition of a cup of coffee (Mendez, 2016; G Puerta, 2011). It is evident that there is a large field of research in this area, given the variety of characteristics and attributes that are assigned to the sensory perception of coffee, which makes it possible to study the complex components of coffee remains to be investigated of each of the factors that affect the coffee quality assessment (W. Sunarharum et al., 2014).

Body perception in coffee brewing's

Coffee body refers to the consistency and density that is perceived when a consumer experiences a coffee beverage (Echeverri-Giraldo et al., 2020). The body describes the physical properties - heaviness or mouthfeel - of coffee when it settles on the tongue; that is, the sensation of coffee coating the tongue. The body is characterized by soluble and insoluble elements in roasted coffee (Seninde & Chambers, 2020).

Soluble elements in roasted coffee: reducing sugars, caramelized sugars, amino acids, ashes(oxides), non-volatile acids (chlorogenic, caffeic, quinic, oxalic, malic, citric), volatile acids, trigonelline, caffeine, phenols, water soluble acids such as caffeine which gives bitterness, acids (some of them create sour and/or sweet flavors), lipids (viscosity), sugars (sweetness, viscosity) and carbohydrates (viscosity, bitterness) (Osorio & Pabón, 2022; G Puerta, 2011).

Insoluble elements in roasted coffee: protein molecules, coffee fibers and oils. Coffees with a washed process are associated with a more delicate body, they are more appreciated for their clarity and cleanliness than for their mouthfeel. As for natural coffees, a larger and rounder body can be expected (Puerta Quintero, 2016). In a coffee beverage you can find descriptors for the body such as: Oily - oily (HEAVY), Grainy - sandy (HEAVY), Water (LIGHT), Milky (MEDIUM), Juicy (MEDIUM), Thick (HEAVY) or Honey (HEAVY) (Rao, 2008, 2014).

2.1.5. Sensory Lexicon: World Coffee Research Organization

Considering the need to generate a transversal vocabulary to define the characteristics, descriptors, and attributes of coffee, since 2012 the World Coffee Research Organization was founded, generating a compendium of descriptors or lexicon for coffee. The following is a brief description.

The objective of the World Coffee Research Sensory Lexicon was to use for the first time the tools and technologies of sensory science to understand and name the main sensory qualities of coffee and to create a replicable way of measuring these qualities (World Coffee Research, 2017). Although several tools are currently available to evaluate coffee, such as the rigorous SCA cupping protocols, none of them are suitable for scientific research (World Coffee Research, 2017). This lexicon is characterized by three fundamental elements for its use in research.

1. It is descriptive: It does not have categories of "good" and "bad" attributes, nor does it allow to classify the quality of the coffee. It is a purely descriptive tool that allows us to say with a high degree of confidence that a coffee tastes or smells of a certain characteristic (World Coffee Research, 2017).

2. It is quantifiable: It allows not only to say that, for example, a certain coffee has blueberries in its flavor or aroma, but that it has blueberries in an intensity of 4 on a scale of 15 points. This makes it possible to compare the differences between coffees with a significantly higher degree of precision (World Coffee Research, 2017).

3. It is replicable. When properly used by trained sensory professionals, the same coffee evaluated by two different people, no matter where they are, what their previous taste experience is, what culture they come from, or any other difference between them, will always achieve the same intensity score for each attribute (World Coffee Research, 2017).

The functional elements of the lexicon are the name of the attribute, its definition, the reference, the 0-15 points intensity scale, and the preparation instructions. The 0-15 intensity scale used in this research is detailed below.

Intensity scale 0-15 points

References have been given an intensity score on a scale of 0 to 15 and labeled as an aroma or flavor reference. The intensity score allows evaluators to compare the perception of the attribute in the sample with that of the reference and thus, assign the appropriate score to the sample. In Figure 2.1, the lexicon intensity scale is presented.

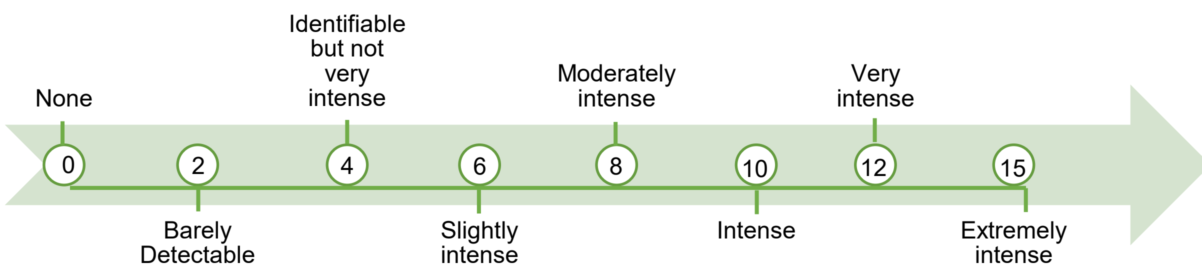


Figure 2.1. Intensity scale 0-15 point from eight categorical levels (World Coffee Research, 2017).

2.2. The coffee aroma triangle

Coffee aroma is a concept that has been developed from different points of view in recent years (Giacalone et al., 2019). Figure 2.2, shows the concept of the coffee aroma triangle to explain the primary variables involved in the aroma and flavor expression of the coffee. One of the perspectives that addresses this complex relationship is called the coffee aroma triangle (P. R. A. B. De Toledo et al., 2016). It consists of relating the genetics of the coffee bean, the activities carried out to beneficiate or process the coffee and finally with roasting as an enhancer and generator of the aromatic profile of coffee (W. Sunarharum et al., 2014).

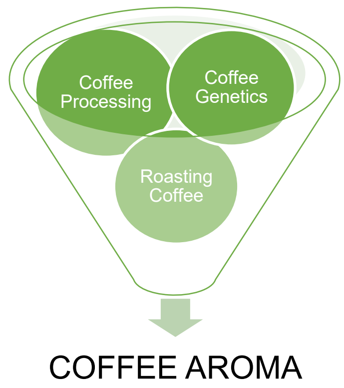


Figure 2.2. Coffee aroma triangle.

Coffee beans had in their interior water, sugars, proteins, fats, minerals, and vitamins. Figure 2.3, shows some relevant data on coffee beans.

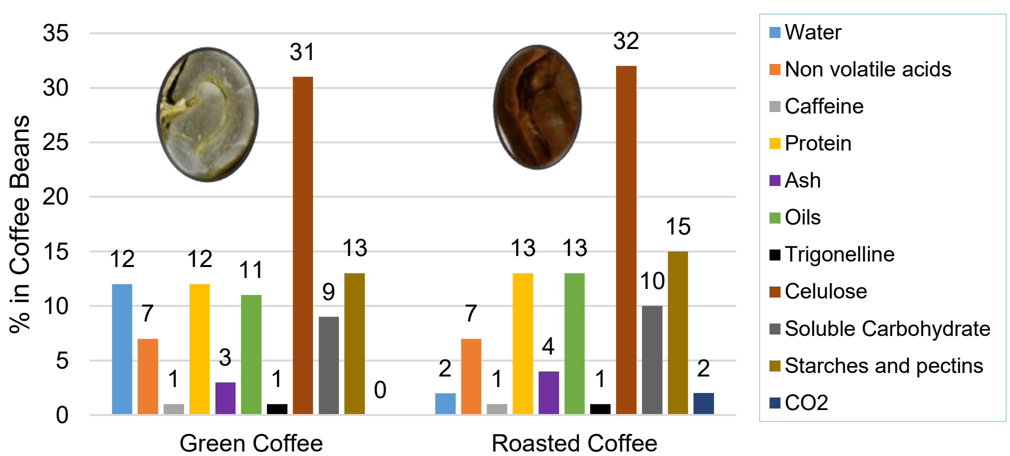


Figure 2.3. General composition of a coffee bean. Adapted (Rao, 2014).

The quality and quantity of these elements varies depending on the quality of the bean, the type of roasting and other factors such as origin, processing, and selection.

2.2.1. Coffee bean genetics

One of the first elements to consider in the study of specialty coffee is the genetics of the coffee bean. In this item are grouped the set of variables related to the physical properties, variety, humidity, density, size and shape of the bean (Leroy et al., 2006). On the other hand, the characteristics related to the origin of the coffee bean are also considered. Figure 2.4 shows the relationship between these variables.

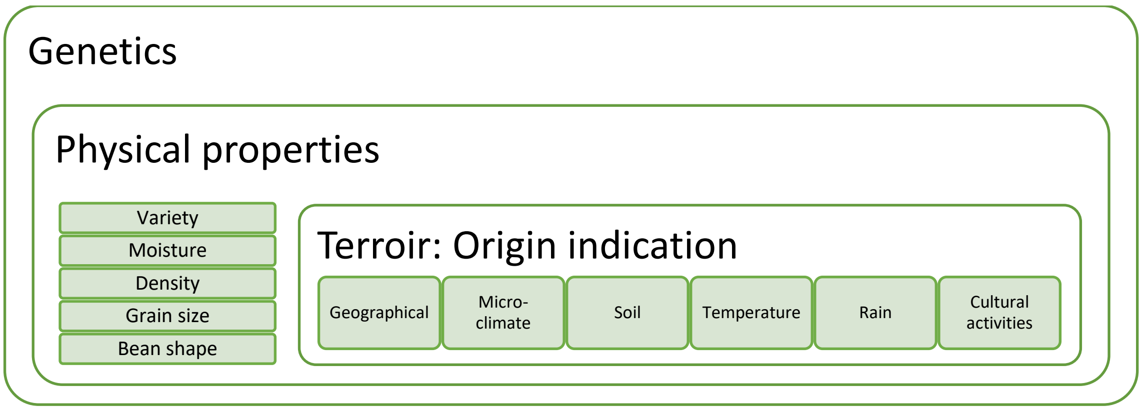


Figure 2.4. Coffee variables taking into account bean genetics. Adapted (Giacalone et al., 2019).

Terroir is a term used in the coffee industry to refer to the denomination of origin of a crop, and is reflected in a set of variables associated with the geographical position, the microclimate of the coffee crop, the quality, properties and characteristics of the soil, the temperature and rainfall conditions of the crop and even with the cultural work in the region where the specialty coffee bean is grown (Giraudo et al., 2019).

2.2.2. Coffee varietals in the study

Tabi

Tabi in Guambiano means good. Towards the decade of the 70's, the National Coffee Research Center (Cenicafé) initiated a program to develop high bearing varieties with resistance to coffee rust. In order to fulfill this purpose, crosses were made between the Timor Hybrid, resistant to coffee rust, and plants of the Típica and Borbón varieties, from which the Tabi variety was developed, with high growth and resistance to coffee rust (Farfán Valencia et al., 2000). These varieties are preferred by coffee growers in areas with some climatic limitations such as high temperatures, low rainfall and high solar radiation, among others, in agroforestry systems (Farfán Valencia et al., 2000).

Castillo

The Castillo variety was developed at Cenicafé from the cross between the Caturra and the Timor Hybrid as a Colombian variety resistant to coffee rust. This variety is recognized for its high production and excellent cup quality (Alvarado-Alvarado et al., 2005; Rincon-Jimenez et al., 2021). Its properties depend on the geographical origin and type of species, as well as multiple factors such as climate, harvesting methods, coffee cherry processing and roasting. There are regional varietal: Naranjal, Paraguaicito, Santa Barbara, Pueblo Bello, El Rosario, La Trinidad and El Tambo (Federación nacional de Cafeteros, 2022).

2.2.3. Moisture and water activity

Water activity (aw) is a measure of the strength of the bond between water and dry material in a coffee bean or other food product (Rao, 2014). The level of the aw variable indicates the probability of moisture entering or leaving a bean, which in turn affects how beans interact with their storage environment and how quickly they degrade in storage. Water activity is different from moisture content, which is defined as the percentage of water in green coffee. Recent studies address the computer modeling of adsorption isotherms in order to describe the influence of water activity and temperature on equilibrium moisture content (Collazos-Escobar et al., 2022). The unbound water present inside the grain is of great importance as the vehicle for the chemical reactions involved in roasting. Water activity and moisture correlate, although this relationship may decrease when the moisture content exceeds 12%. (Rao, 2014). For this reason, coffee samples are worked with moisture between 9% and 12%. Both characteristics influence the quality of the cup, considering the rate of degradation of the green coffee during storage and the risk of microbial growth during storage.

2.2.4. Density, size, and shape of the coffee beans

From the physical point of view, these properties depend on the variety and the height of the crop. The greater the height, the smaller the size and the greater the density. Small coffee bean sizes tend to contain a greater amount of more concentrated flavor precursors. Homogeneous roasting facilitates roasting uniformity. Differences in bean size and shape react differently to the application of heat, which is why it is important to know the particle size distribution. Table 2.2 presents the classification of coffee beans according to density. Cauca coffee represent the hard coffee beans.

Table 2.2. Density of specialty coffee beans

Characteristic	Density	Overall Value(g/L)
Hard Coffee	High	> 720
Semi-hard coffee	Medium	680 - 710
Soft Coffee	Low	< 670

2.2.5. Denomination of origin: CAFÉ DE CAUCA

The geographical area delimited for production and processing is between 1100 and 2100 meters above sea level in the municipalities of Popayán, Almaguer, Argelia, Balboa, Buenos Aires, Cajibío, Caldono, Caloto, El Tambo, Inza, Jambaló, La Sierra, La Vega, Miranda, Morales, Páez (Belalcázar), Patía (El Bordo), Piendamó, Puracé, Rosas, San Sebastián, Santander , Sotará, Suárez, Sucre, Timbío, Toribio and Totoró in the Department of Cauca (Superintendencia de Industria y Comercio, 2012).

Café de Cauca is characterized for being a coffee of the arabica species, with a very strong and caramelized fragrance and aromas, and in the cup it presents high acidity, medium body, balanced global impression, soft clean with some sweet and floral notes, which is produced in the delimited geographical area, through homogeneous processes of selective manual harvesting, wet milling, threshing and manual classification (Superintendencia de Industria y Comercio, 2012).

2.3. The roasting process

Coffee roasting involves processes in which variables of diverse nature intervene. Figure 2.5 presents the general variables considering the whole roasting process. In the coffee roasting process, the kind of heat transmission to the coffee bean has a direct relation with its organoleptic properties and of course in the final beverage. In this process the heat can be transferred by the methods of conduction, radiation, or convection; therefore, the variables involved in this process have to do with the type and technology of the roaster and likewise, with the temperature that the coffee beans will reach as well as the time of duration of the roasting process. Each item of the roasting process is presented below.

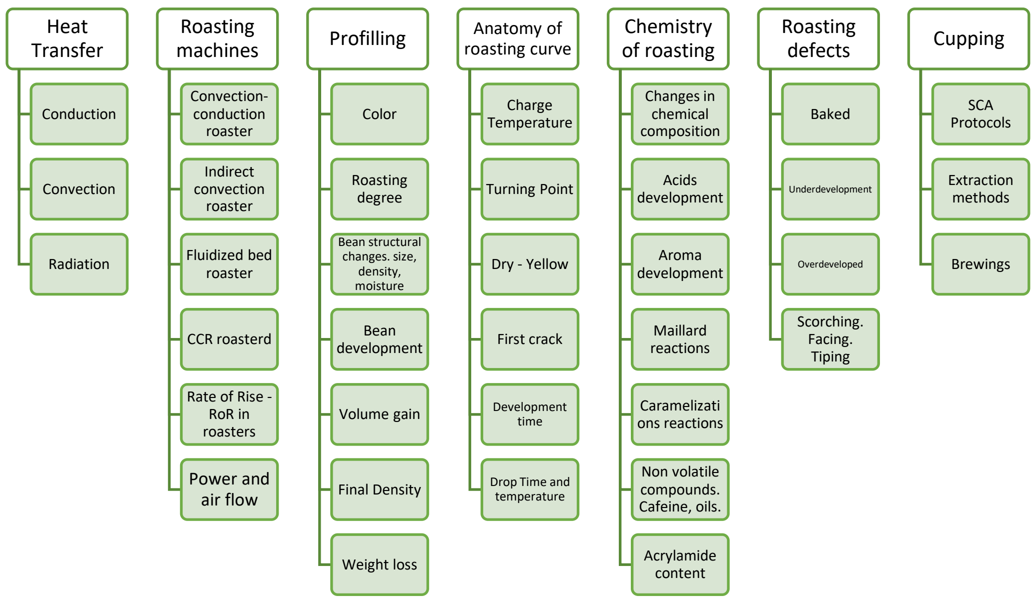


Figure 2.5. General variables considering the roasting process (Rao, 2019).

2.3.1. Heat transfer in the roasting process.

To introduce the roasting processes from a scientific approach, the heat and mass transfer equations that govern the behavior inside the coffee bean can be studied. The work of (Fabbri, Cevoli, Alessandrini, et al., 2011) also presents a numerical model, based on a 3D geometry, that describes the heat and moisture transfer inside a coffee bean during the roasting process. The model refers to a rotating cylinder roaster under natural convection conditions and shows the importance of moisture, bean shape, density, and size in bringing a green coffee bean to a state of development of volatile and non-volatile organic aromatic components.

Figure 2.6 shows the comparison between digitized shape of coffee bean and the three common roasting levels. Bean Color is not always linked with the heat transfer (Fabbri, Cevoli, Alessandrini, et al., 2011).

(a) (b)Light (c) Medium (d) Dark

Figure 2.6. Coffee beans with (a) digitized shape (Fabbri, Cevoli, Alessandrini, et al., 2011) and (b) at three levels of light, medium, and dark roast.

Other numerical models for coffee bean roasting address the above phenomena under different assumptions. These techniques identify that the total amount of heat transferred to the beans and the rate of heat transfer are the main factors in the roasting process (Bottazzi et al., 2012). Numerical models can predict the performance of the coffee roaster in terms of pressure, temperature, mass flow rate in the process stages and gas injection. In addition, the temperature profile of the coffee beans inside the roaster drum is evaluated as a function of the working conditions of the system. Therefore, different roasting machine control strategies can be compared and the effects on the coffee roasting profile including the size and shape of the coffee beans can be analyzed.

On the other hand, researchers (Fadai et al., 2019) introduced a model that explains deformations that are created and controlled by moisture content, temperature, and gas pressure within the roasted coffee bean. The model combines previously derived mass and heat transfer models for roasting coffee beans to determine when and where surface deformations are likely to occur. Starting at the outermost layer of a coffee bean, moisture evaporates during roasting and causes an evaporation flow, which moves toward the center of the bean. The cellulose structure inside the bean, being relatively cold, remains intact and traps the moisture in the center of the bean. The heating of this trapped water produces water vapor, increasing the pressure inside the coffee bean, leading to the expansion of its structure. This pressure, estimated by several researchers to peak as low as 5.4 atmospheres (550 kPa) to 25 atmospheres (2,533 kPa), increases until the stresses are great enough to break the cellulose structure, at which point the first crack, crackle or crackle occurs (Fadai et al., 2019). Figure 2.7 shows the green coffee bean and the roasting stage. the coffee bean absorbs heat and becomes a spongy, voluminous, brittle, and aromatic element.

Figure 2.7. Samples of green coffee beans and their final states when roasted.

Moisture content within the beans has a more complex influence on roasting. A higher moisture content has three main effects on heat transfer within a coffee bean (Rao, 2014).

- Increased heat transfer because moisture increases the thermal conductivity of the grain.
- Increases the specific heat capacity of the grain, since the grain requires more thermal energy to raise its temperature by a given amount.
- Generates greater transfer of evaporated moisture out of the grain, which inhibits heat transfer into the grain (Rao, 2014)

The effect commonly found is that temperature rises more slowly in wetter grains than in drier grains (Rao, 2014). Considering the above, knowing the technologies in roasting machines in the process of heat transfer to the coffee bean will allow the development of strategies for its drying and subsequent development, according to its physical and chemical characteristics contained within the bean. Appendix D reports the warmup roaster protocol.

2.3.2. The roasting machines

To conduct the roasting process of a coffee bean, an instrument known as a roaster is used, which implements the combination of two or more of the heat transmission phenomena. Drum roasters are characterized by the transfer of heat to the bean through convection originated by the hot air that circulates due to the hot surfaces. Heat transfer is also generated by conduction, when the beans come into contact with these surfaces (Gancarz et al., 2022; Resende et al., 2017).

Convection roasters transfer heat to the beans using a rotating drum that heats the air and then this is supplied to the coffee sample. This system maintains a speed in its drum so that the coffee does not meet the hot surfaces. In spite of this, conduction is inevitable, but it manifests itself in smaller quantities (Fabbri, Cevoli, Romani, et al., 2011; Gancarz et al., 2022).

Fluidized bed roasters are a combination of drum and convection roasters, in which the heat is transferred to the beans by pressurized hot air, causing the coffee beans to float inside a container (Campo-ceballos et al., 2020; Gancarz et al., 2022)

One of the critical situations in roasters is the instability of the roasting process. For example, a roasting drum that relies solely on conduction heat will not guarantee a uniform temperature distribution in the coffee beans due to the non-homogeneous contact with the hot surface. On the other hand, in the fluidized bed roaster, the coffee beans are constantly moving due to the pressure of the hot air, the speed of which is not controlled or its control is complex (Campo-ceballos et al., 2020; Gancarz et al., 2022) . Hence, fluidized bed technology is expensive on a large scale.

It has also been noted that in drum roasters, adjusting one variable can cause countless variations in other parameters. For example, varying the gas or air inlet and the speed of the rotating drum does not evenly distribute the heat around the drum, and therefore generates hot and cold spots that affect the roasting performance of the coffee (Gancarz et al., 2022). Roasters have now been developed with technology that implements the combined phenomena of conduction, convection, and radiation as the key element of heat transfer. Radiant heat is caused by the cast iron materials.

Quality materials used in the manufacture of the roaster cause high consistency during roasting. Some worldwide and local manufacturers are Probat, Giensen, Stronghold, Quantik, Prisma, among others. In spite of this, coffee roasters must be configured since their instrumentation is diverse and combinations of instrumental variables can be generated that do not guarantee an accurate control of the air flow through the drum containing the coffee beans during the roasting process, which normally causes defects in the roasting process. (Gancarz et al., 2022; Giacalone et al., 2019). Appendix D reports the warm-up roaster protocol.

2.3.3. Roasting and Profiling of High-Quality Coffee

A coffee profiling is a process to analyze the variables that are determinant to obtain a consistent product and, in this way, establish typologies to be reproduced at any moment. Figure 2.8 shows the scheme of the objectives of roasting profiling.

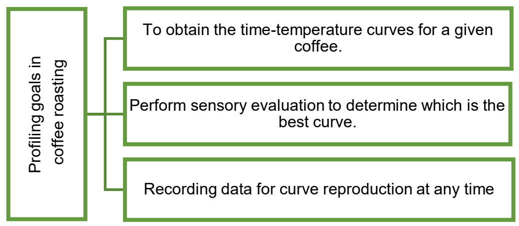


Figure 2.8. Goals of coffee profiling (Rao, 2014; Schenker & Rothgeb, 2017).

Every roasting process has an objective, which can be to highlight, enhance or on the contrary reduce the attributes of the flavor expression of the coffee (Seninde & Chambers, 2020). This process integrates the collection of time and temperature data, the cupping of the coffee and its respective registration for subsequent reproduction. The quality of coffee is reflected by extrinsic and intrinsic characteristics of the process. Figure 2.9 shows the scheme of the determining factors for the profiling of specialty coffee.

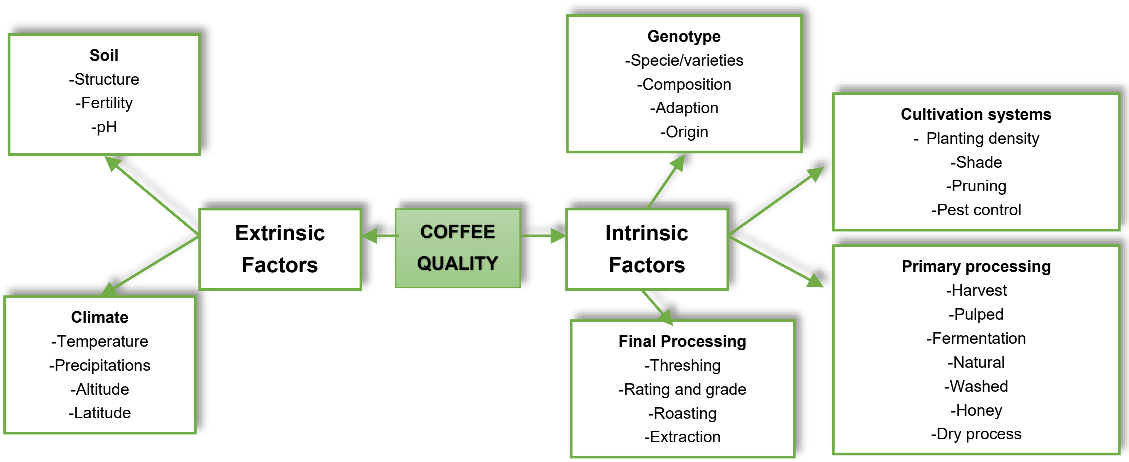


Figure 2.9. Factors that determine coffee profiling and cup quality. Modified (Seninde & Chambers, 2020).

A roasting curve typology is the systematic procedure between the intrinsic and extrinsic characteristics of the bean with the content of the coffee beverage. Roasting profiles take into account genetic characteristics (variety), physical characteristics (density, humidity, size), soil characteristics (soil, cultivation techniques, microclimate, altitude, harvesting technique, post-harvest and drying processes) and stabilization (time, temperature, locality and % of ambient moisture) (Puerta Q et al., 2016; Rao, 2019).

Figure 2.10 presents the standard scheme for defining the roasting profile through a time and temperature curve in a roasting machine. After roasting the samples, sensory tests are performed in the cupping process to determine the characteristics of the profile and finally define the roast typology and report the finding in a recipe or register (Seninde & Chambers, 2020).

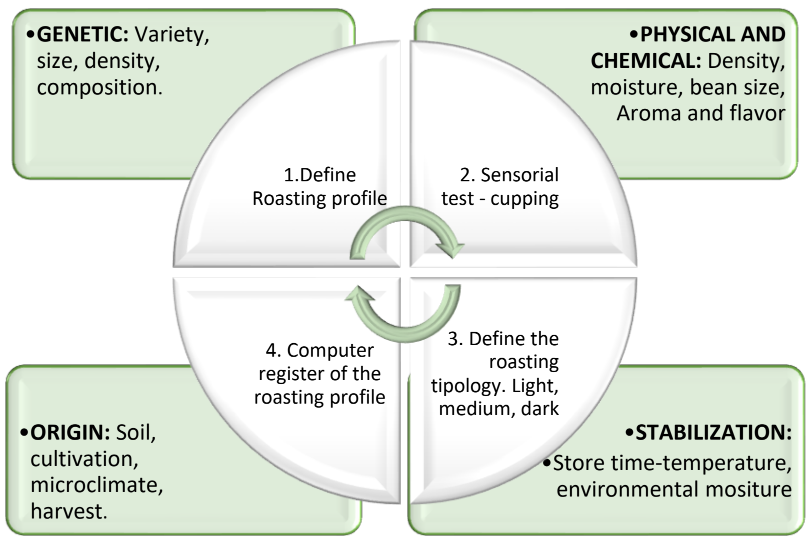


Figure 2.10. Standard scheme of a coffee roasting profiling system (Osorio et al., 2021; Seninde & Chambers, 2020).

To define a roasting profile, it is necessary to measure and record process data, taking into account times, temperatures, flame power and air flow (Rao, 2019; Schenker & Rothgeb, 2017). A representative schematic is shown in Figure 2.11.

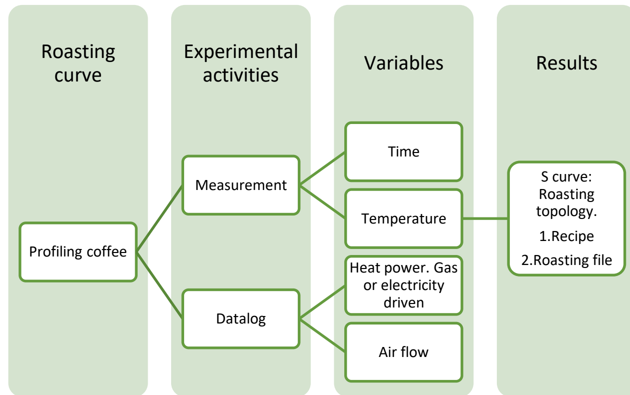


Figure 2.11. Scheme for the construction of a roasting curve (Rao, 2019)

The result of a coffee profiling will then be the roaster's recipe, with the roasting curve graphing tool and a computer file.

Physical and chemical changes in coffee

In coffee roasting two key processes are identified that guarantee the follow-up of the development of the flavor expression of the bean. Physical and chemical changes (Gloess et al., 2014; Seninde & Chambers, 2020). These phenomena can be grouped as shown in Figure 2.12.

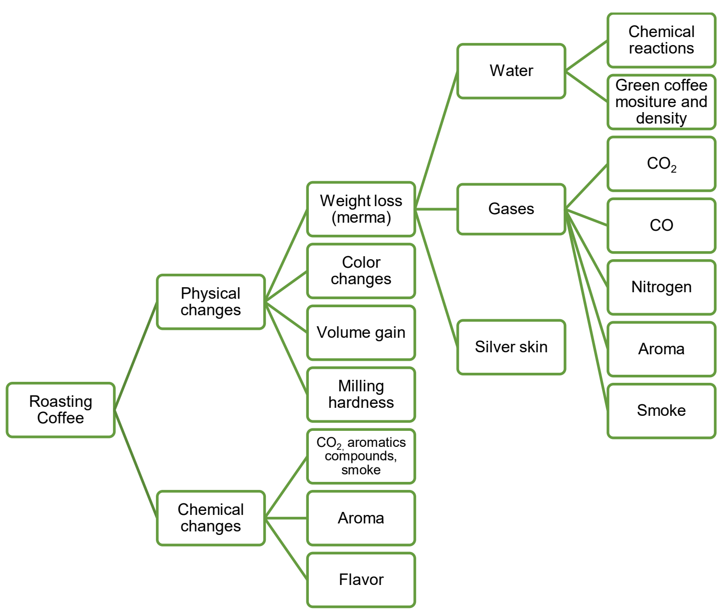


Figure 2.12. Roasted coffee profiling variables

According to Figure 2.12, the following concepts can be explored.

Physical changes:

Physical changes have to do with weight loss due to dehydration of the grain during the process, color change, which is a non-enzymatic browning, volume increase due to internal pressure increase phenomena, and hardness, which has to do with the homogeneity of the internal structure of the grain (Puerta Quintero, 2016).

Weight loss is included as an indicator to follow up the development of flavor expression in the coffee bean. It can be used as evidence of water loss, gas generation and detachment of the silver film. All this information is key for the traceability of the roasting process; however, it should be analyzed together with the color and roasting temperature.

Chemical changes:

On the other hand, chemical changes, related to the generation of aromatic components due to the internal composition of the coffee bean. These can be volatile, contributing to the characteristic development of the aroma, and others can be non-volatile, which contribute to the flavor of the coffee beverage (Zakidou et al., 2021).

The aroma and flavor of coffee are entities that are still being explored from different points of view (Poisson et al., 2017; Seninde & Chambers, 2020; Zakidou et al., 2021). The acidity and the body of coffee present an interesting relationship to study the character of coffee (Lingle & Menon, 2017).

Acidity:

The acidity of coffee has been recognized as one of the main quality attributes and is generated to a certain extent by aliphatic carboxylic acids. Green coffee of the arabica species contains 0.5% citric acid, 0.5% malic acid, 0.2% oxalic acid and 0.4% tartaric acid (Osorio et al., 2021).

The formation of aliphatic acids, small in quantity, in the order of 1.5%-2.5%, depends on the roasting level (Osorio et al., 2021). It has been found that the total content of organic acids remains constant in light to medium roast grades and changes from medium to dark roast grade. The content of quinic and lactic acid increases with darker roast grade, as well as the decrease of citric, malic, and formic acid. Chlorogenic acids (CGA) are the most representative compounds in coffee kernels (Osorio et al., 2021). Roasting causes their degradation associated with the formation of new antioxidants as products of the Maillard reaction.

The main representative of the CGA is 5-caffeoylquinic acid (5-CQA), which contributes to quality, but there is a wide variation in the content for coffees with a similar roasting degree (Osorio et al., 2021). Total AGC content may vary according to species, degree of maturity, agricultural practices, climate and soil (Osorio et al., 2021).

Body:

The body in coffee means the contribution of non-volatile compounds that are generated in the Maillard process, caramelization, and pyrolysis in general. It is made up of lipids. Most of the lipids contained in coffee beans are not degraded during roasting, although some fatty acids release oxidation by-products, mainly aldehydes, that mix with the products of the Maillard reaction to give way to aromas and flavors characteristic of coffee (Echeverri-Giraldo et al., 2020; G Puerta, 2011).

Roasting Curve Anatomy:

Roasting curves are instruments that are constructed by measuring and recording the roasting profile. Normally there are two variables: roasting time and roasting temperature (Rao, 2019). These instruments are based on monitoring points focused on key temperatures for your study (Okamura et al., 2021).

T_i: Charge temperature

T_{tp}= Turning Point temperature

T_{dry}= Dry or yellow temperature

T_{fc}= Fist crack temperature

T_{drop}= Drop temperature

Considering these points and the temporal tracking of the roasting processes, a record called the S-curve can be constructed.

The S-Curve:

Figure 2.13 shows the standard S-curve of a coffee roasting process.

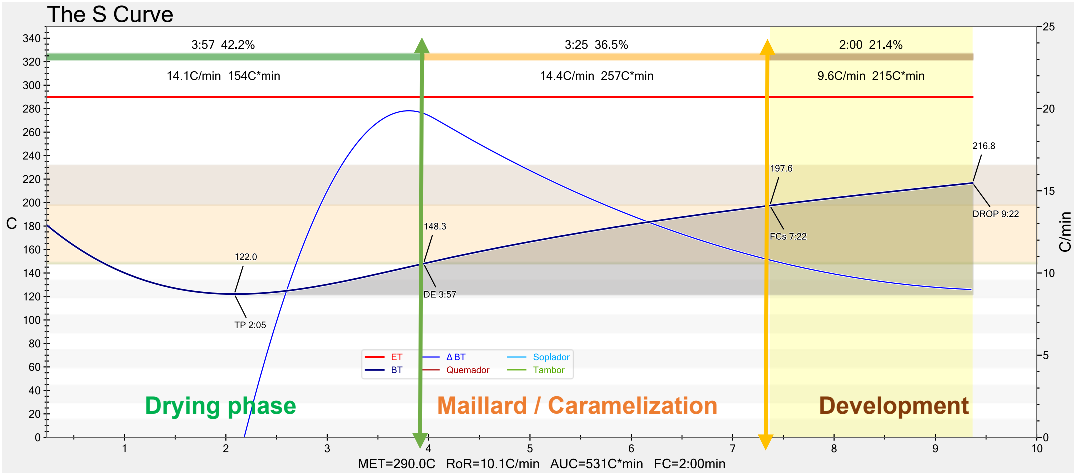


Figure 2.13. Anatomy of the S-curve in a roasting process. Adapted (Münchow et al., 2020).

The S-curve is the standard representation of the temperature progress readings inside the drum of a coffee roaster. After the coffee is loaded into the drum, the temperature drops due to the transfer of heat to the batch of coffee. Subsequently an equilibrium point called "Turning point" is registered, from where the temperature readings, at the beginning increase rapidly and then in a progressive and controlled manner they decrease until the end of the roasting process (Rao, 2019). Temperature readings are recorded at two locations. One for the drum, where the bean temperature (BT) is measured and the other for the hot air leaving the drum or ambient temperature (ET).

Three standard areas of study are highlighted. The drying area, including Maillard and caramelization processes, the first crack, including the development time of the bean, and finally the discharge or end of roasting (Okamura et al., 2021). With the time and temperature records, the rate of rise of temperature (ΔBT) can be calculated, which corresponds to an indicator that measures the rate of temperature rise (RoR) (Rao, 2019).

Drying, Maillard and Caramelization:

As can be observed in Figure 2.14, the color of the bean, which initially is light green, undergoes color changes due to the dehydration process.

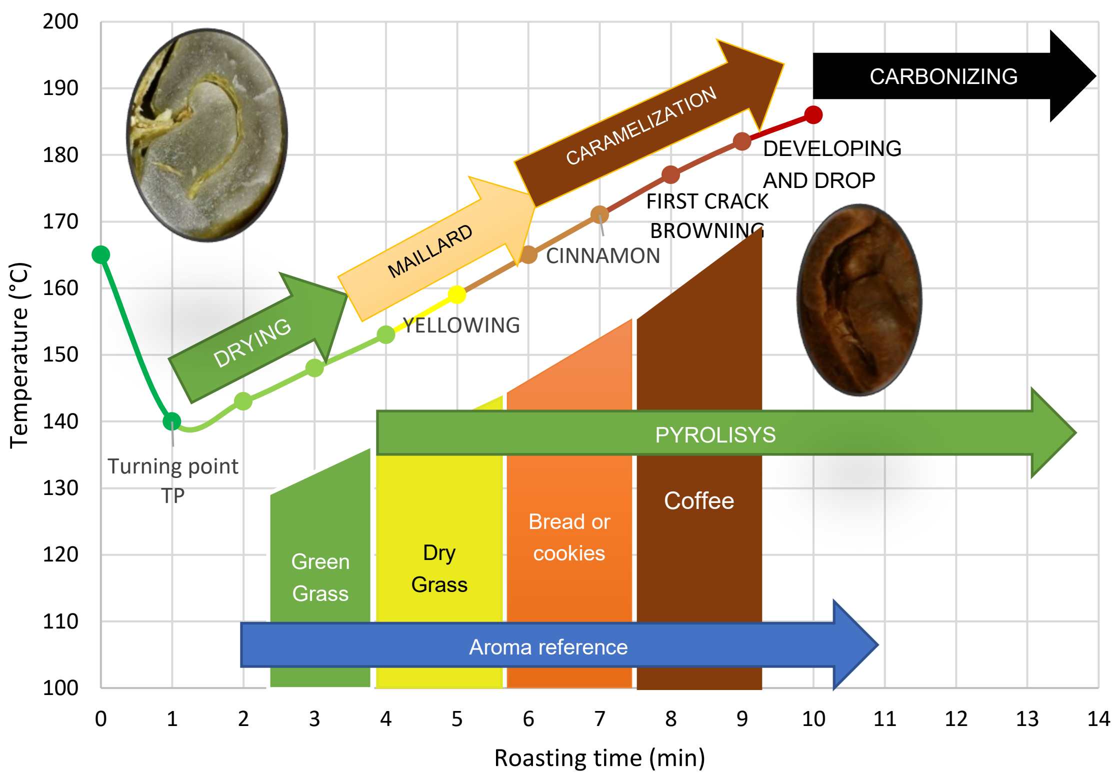


Figure 2.14. Aromatic in the roasting curve. Adapted (Caporaso, Whitworth, Cui, et al., 2018; Ciaramelli et al., 2019; Okamura et al., 2021).

Subsequently the Maillard and caramelization processes generate non-enzymatic color changes and volatile and non-volatile chemical compounds in the coffee, transforming the color of the coffee bean to yellow, cinnamon, brown and finally, through pyrolysis, or degradation of the material by the effect of heat, carbonization is observed, defined by its black color (Caporaso, Whitworth, Cui, et al., 2018; Ciaramelli et al., 2019; Okamura et al., 2021).

One of the indicators used to monitor the roasting curve is the color of the coffee bean. This color changes from green to brown after the dehydration processes due to the action of heat. Initially, after the coffee mass is balanced with the temperature of the roaster, a drying process can be observed that leads the coffee to lose water. In this phase, a characteristic green grass aroma is perceived. The Maillard reaction involves the interaction between reducing sugars and amino acids or peptides of low molecular weight present inside the coffee bean, leading to the formation of compounds such as pyrroles, thiophens, oxazole and thiazole (Seninde & Chambers, 2020; Velásquez et al., 2019). The color at this stage changes to yellow and cinnamon and an aroma of dried grass and cookies or baked bread is perceived. Caramelization, on the other hand, which consists essentially in the pyrolysis of monosaccharides, disaccharides, oligosaccharides and polysaccharides, which by dehydration form more complex molecules of a brownish color, with a typical caramel aroma (Seninde & Chambers, 2020; Velásquez et al., 2019).

The first crack:

The first crack represents the release of accumulated water, vapor pressure and CO_2 from within the grain, due to pyrolysis processes induced by excess heat (Schenker & Rothgeb, 2017). When this happens, the surface of the grain cracks and expels water in the form of steam, generating a noise and a drop in the roaster temperature (Poltronieri & Rossi, 2016). For this reason, this point is a critical point and is taken as a reference to calculate the development time of the bean and enhance its flavor expression. Normally a specialty coffee develops between the first crack and the unloading time, without reaching a second crack. Specialty coffees never reach the carbonization stage, due to the fact that what is desired is to highlight the attributes of the coffee and not to hide them with the smoke and the degradation of the material (Poltronieri & Rossi, 2016).

The bean development:

There is a consensus for the optimal development of the coffee bean, which should be between 20-25% of the total roasting time (Rao, 2019). Figure 2.14 shows the processes that occur in the roasting curve and the aromas commonly perceived by bean development. Metrics of a good profile include consistency in coffee batch size, between batch protocols, loading temperature, bean time-temperature curve, air time-temperature curve and fuel power (gas or electricity), rate of rise in bean temperature (RoR) and final temperature and time (Rao, 2019; Schenker & Rothgeb, 2017). An analysis and comparison of the time spent in the drying phase (from loading to the color change to yellow), the Maillard phase (from the yellow color change to the beginning of the first crack) and the development phase (time from the beginning of the first crack to the end of roasting) can show consistency batch by batch. However, the records of these data have shown that the coffee bean can be taken to the same point, but by different paths (Schenker & Rothgeb, 2017). Figure 2.15 shows how, through three different roasting curves, the same final discharge point is reached.

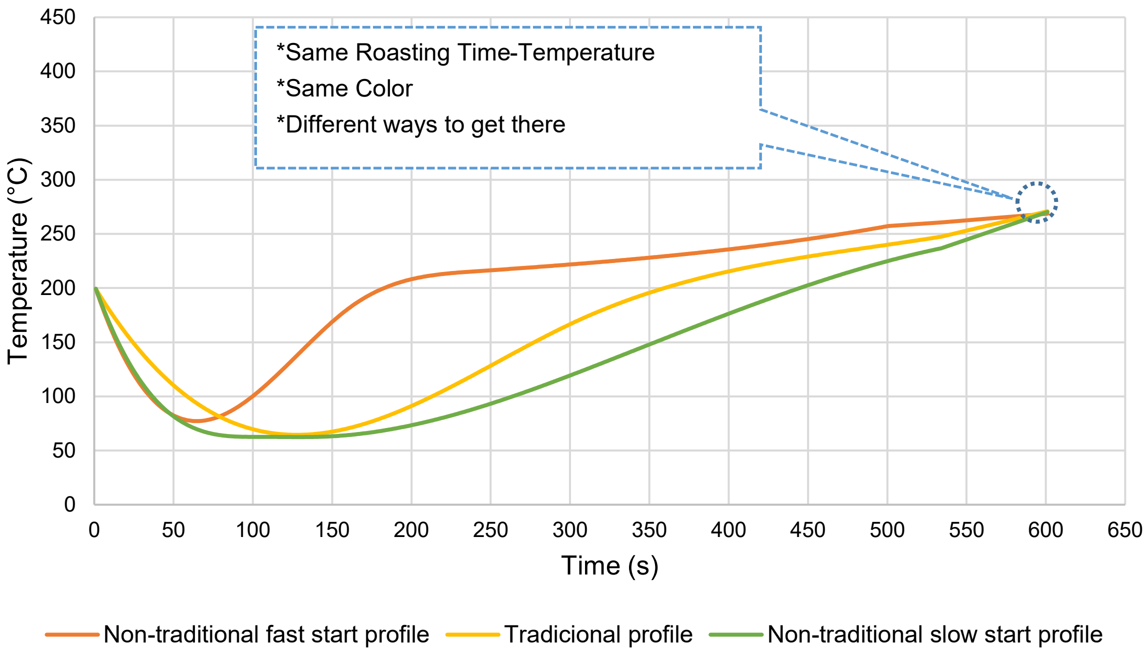


Figure 2.15. Obtaining a roasting point from three different paths. Adapted (Schenker & Rothgeb, 2017).

At that point the coffee beans will have the same color, the same temperature and final roasting time, but since it was obtained through different paths in the roasting curve, it will probably have considerable differences in its flavor expression or roasting defects. For this reason, there are other indicators of traceability of the consistency of coffee and the effects of the action of heat, such as loss of mass, increase in volume and hardness. Several authors have studied these indicators focusing on weight loss, especially in the detection, classification and quantification of gases produced by the roasting process. Aroma in particular has been extensively studied, identifying up to 1000 potent odorants characteristic of coffee (Zakidou et al., 2021).

The authors (Giacalone et al., 2019; Yang et al., 2016) generated a conceptual framework that allows navigating through the identification of coffee defects as a product of the roasting process. The following section introduces the most common defects in the roasting process related to both the instrumentation and the raw material.

Defects and Consistency in coffee roasting:

Today, roasters can be found with technology that implements the combined phenomena of conduction, convection and radiation as the key element of heat transfer (Fadai et al., 2017). Particularly, the radiant heat is generated by the cast iron materials. These materials used in the manufacture of the roaster guarantee a high consistency during roasting (Rao, 2019). In spite of this, coffee roasters must be configured since their instrumentation is diverse and combinations of instrumental variables can be generated that do not guarantee an accurate control of the air flow through the drum containing the coffee beans during the roasting process, which normally causes defects in the roasting process (J. S. Cho et al., 2017; Giacalone et al., 2019). The most common roasting defects are:

Baked coffee:

It is a coffee defect that occurs when coffee beans are subjected to a long-time profile at a low temperature (Low Temperature Long Time LTLT-profile), which results in coffee samples that never reach the first crack. This defect, called "stagnation" of roasting, cannot be easily perceived with the color, but the roasted beans have a flat taste like baked bread or cookie flavor (J. S. Cho et al., 2017; Giacalone et al., 2019).

Under-development coffee:

This defect is generated when roasting is conducted at high temperatures and with short times (High Temperature Short Time HTST-profile), so that the bean does not develop its attributes. Underdeveloped coffee beans have an herbaceous perception (grass) and lack the caramelized sugars, since, although the heat initiated the caramelization processes, these were abruptly suspended by the very early unloading of the sample (J. S. Cho et al., 2017; Giacalone et al., 2019).

Over-development Coffee:

This defect is produced when the temperature is high and at the same time the roasting time is generously prolonged (High Temperature Short Time HTST-profile). The beans will have a dark aspect with oils on their surface, as an effect of excessive heat during an extended time. The taste of coffee beverages prepared from overdeveloped beans will have a burnt and bitter perception, with notes of smoked charcoal (J. S. Cho et al., 2017; Giacalone et al., 2019).

Scorching coffee:

Coffee scorching occurs when the loading temperature, i.e., the initial temperature is too high, and the drum speed is too slow. This roasting defect appears in dark burnt spots on the surface of the coffee beans, and the coffee has an oily, smoky flavor, with a sensory perception of roasted chicken. Certain beans may also present a defect associated with burning known as tipping, where the bean does not burn completely, but experiences a burn at its tips. This can usually be corrected by synchronizing the speed of the drum and the amount of coffee in the drum (J. S. Cho et al., 2017; Giacalone et al., 2019).

2.4. Optimization techniques

The RSM response surface methodology is a multivariable statistical tool that consists of a group of mathematical and statistical techniques based on the adjustment of empirical models to experimental ones. The use of RSM in process optimization leads to the need for an experimental design, which can generate many samples for consumer assessment in a short period of time and, therefore, testing at the laboratory level is more efficient (Mendes et al., 2001; Y. Zhang & Wu, 2021). The CCD is the most useful design for estimating the multifactorial response surface, which minimizes the number of experiments, while allowing simultaneous assessments of the variations of all the experimental factors studied and distinguishing the interaction between them (Madihah et al., 2012). Optimization methods based on multifactor response surfaces (RSM), using composite central design (CCD), have been used in several studies for the determination of various physical and chemical characteristics of coffee (sensory quality, antioxidant activity, caffeine content, total sugar, phenolic compounds, pH, etc.)(Amdoun et al., 2018; Anisa et al., 2017; Chung et al., 2013; Erdogdu, 2008; Mendes et al., 2001), integrating polynomial models. The step-by-step execution of an optimization process at this level is shown in Figure 2.16.

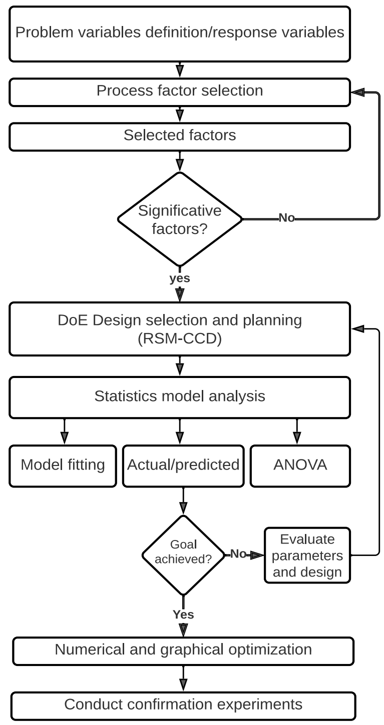


Figure 2.16. Flowchart of an optimization process based on CCD central composite design. Modified (Asghar et al., 2014).

The experimental phase of the project is to obtain an objective function, defined by the physical and chemical parameters from the roasting curve. The time and temperature parameters included in the roasting process can be optimized to show consistency in two selected attributes of coffee: the acidity and body. Figure 2.16 shows that the optimization process must guarantee the design and planning of the experiment, to iterate consecutively until the desired objective is achieved.

2.5. Sensory assessment and consumer perception

Sensory analysis groups together a set of techniques, which are used to measure the responses of the five human senses to characteristics of foods and beverages (Birwal P & BK, 2015). There are three fundamental challenges in sensory analysis: discrimination, characterization, and typology. Sensory methodologies based on consumer perceptions have become popular and widely used by industries in recent years to replace classical methods (Dunkel et al., 2014; Lestringant et al., 2018). These methods require no training, have a low financial impact, optimize time and resources within companies, and provide information that is highly correlated with traditional methods. Among the rapid methods used that have been highlighted to capture consumer perceptions and categorical variables are the intensity scales, the Check-all-that-apply (CATA) (G. Ares & Jaeger, 2015), the Flash Profiling (Liu et al., 2018), similarity-based methods (Projection Mapping and Classification) and reference-based methods (Polarized Sensory Positioning - PSP, Polarized Projective Mapping - PPM and Pivot Profile) (Dehlholm et al., 2012). Coffee flavor profiles could be evaluated to understand how roast grade and changes in coffee aroma affect the flavor characteristics perceived by consumers. Consumer assessments would be necessary to identify key attributes that could affect acceptability. Consumers and experts are opposed, the use of these tools is still the subject of study and the literature still has gaps to show techniques to help bring them closer (Thomas et al., 2017).

2.6. Optimization in roasting coffee process: literature review

The methodology of systematic mapping of the literature has been taken as a reference (Petersen et al., 2015) in order to establish a linking point around to emphasize how the roasting process can be approached from Electronic Sciences topics like optimization, data science and parameterization including consumers perception data. This section establishes a procedure consisting of five stages: (i) Define the research questions. (ii) Conduct the literature review. (iii) Select studies. (iv) Classify items. (v) Extract and perform data aggregation. To implement the search strategy, keywords related to the topic were used, mainly in the english, spanish and portuguese languages. The search strings used were used in the Science Direct, IEEE, EBSCO, and SCOPUS databases.

Inclusion criterion

In this review, the inclusion criteria relate of documents records by origin, language, topics, and year of publication. We considered peer-reviewed articles for scientific and technical sources. Therefore, the types of documents included were those marked as originals and review articles written in English, Spanish or Portuguese, and published between 2010 and 2021.

Exclusion criterion

As in the inclusion criteria, the types of documents, the population sample, the stimuli, and the experimental design were considered. Documents with opinions, views or anecdotes were discarded.

Logical operators and search equations in the title, abstract and keyword fields, the documents were searched using selected databases. Table 2.3 present the research questions concerning to coffee samples, their origin, harvesting and post-harvest processes, beverage preparation methods, consumers perception and data analysis tools.

Table 2.3 Resarch questions for the literature review

Research questions	
RQ1: What techniques have been used to identify and classify coffee according to its origin, variety, benefit, value addition and sensory profile?	RQ1.1: Which methods are used to identify the physical variables in the standard roasting profile of the SCA? RQ1.2: How the perception of coffee attributes by consumers of special coffee are validated?
RQ2: What is the relationship and importance between the degree of roasting of coffee and the sensory attributes of fragrance, aroma, acidity, bitterness, body, and overall flavor?	RQ2.1: How to modulate (optimize) the time and temperature conditions of the SCA standard roasting profile? RQ2.2: How to maintain consistency in the perception of acidity and body in the cup acceptable to coffee consumers?
RQ3: What techniques have been used to identify the aroma and flavor components of roasted coffee?	RQ3.1: What are the consumers non-trivial techniques for determining smell and taste of roasted coffee, applied to the quality assessment process?

Searching with boolean operators

Table 2.4 shows the keywords and boolean operators to write the search strings used to select the relevant works within the research questions of this study.

Table 2.4. Classification of information found in selected databases.

Keywords/Connector Combinations/strings		DATABASE	# Found papers	Selected # papers	Precision
roasting coffee quality assessment electronic instrumentation data analytics sensors consumers	 *AND* *AND* *AND* *OR* *AND/OR* *OR/AND* *OR/AND* *OR/AND*	SCIENCEDIRECT	157	100	63.7%
		IEEE	27	10	37%
		SCOPUS	120	71	59.2%
		EBSCO	30	14	46.7%
subtotal			334	195	
Duplicate				-23	
Total				172	100%

Figure 2.17 shows the flowchart of the systematic literature review process.

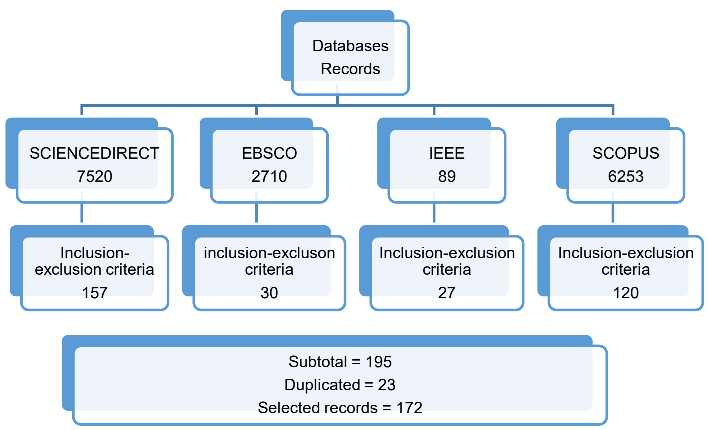


Figure 2.17. First step results

From 195 papers and removing the duplicates, systematic review obtained a total of 172 articles. Five topics of interest were created, described in Table 2.5.

Table 2.5. Cluster information for review in topics of scientific interest

Topics	# papers	weight %
Physicochemical characteristics of roasted coffee	80	46.5%
Cupping evaluation for quality control purposes	32	18.6%
Sensors and systems for quality assessment	40	23.3%
Optimization of roasting profiles conditions	14	8.1%
Coffee consumers perceptions	6	3.5%
Total	172	100%

Network concepts in coffee quality analysis

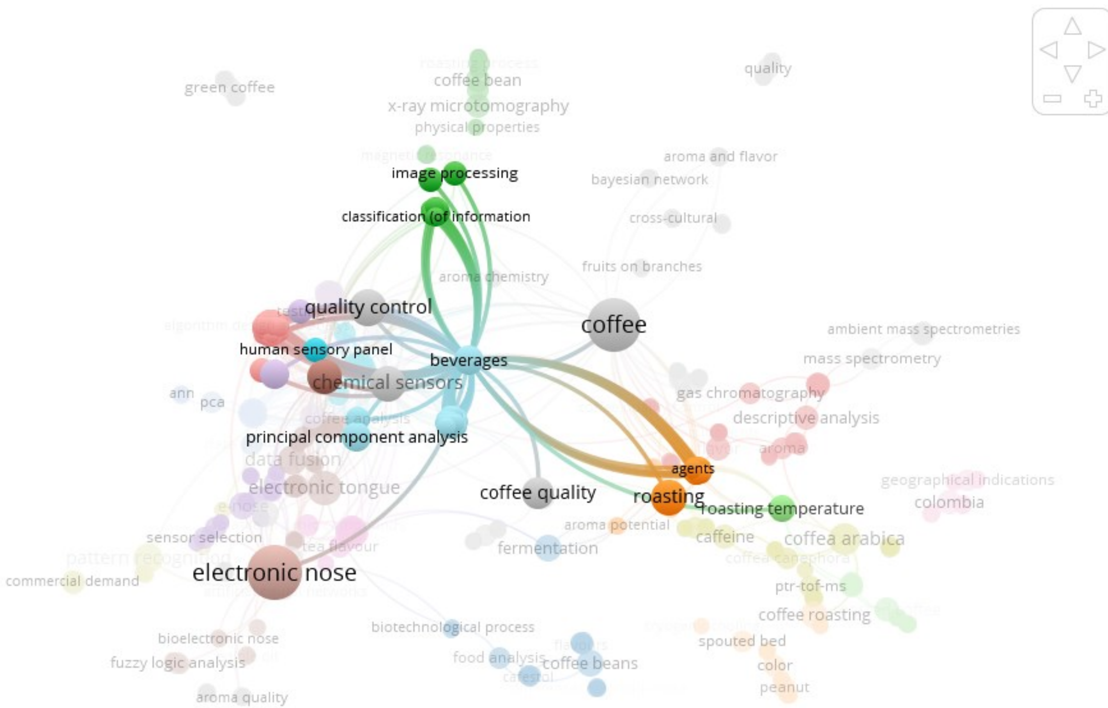


Figure 2.18 Bibliometric maps for coffee quality control in literature review.

Currently, advances in food quality inspection, assessment, and analysis systems have focused on Industry 4.0 for food products (Afoakwa, 2016; Costa et al., 2015; Dunkel et al., 2014; J. Gutiérrez & Horrillo, 2014; Jackson, 2008; Le Quéré, 2010; Nolvachai et al., 2017; Steinhart et al., 2000). Literature proposes that the ideal coffee production process, should be a predictable and continuous process, similar to that of the automotive industry; this is not possible for the coffee industry, since each process of harvesting, processing, roasting and storage is different, and influences the quality of the final product (Neuhaus, 2017). The industrial automation of the coffee process is being interrupted by sensory analysis, which must be done by an expert human taster or even consumers, before and after the roasting process, to assess, and monitor quality. The coffee roasting process is the focus of current research and development, as this is where the greatest added value to coffee is generated (Neuhaus, 2017). Literature reports previous studies and research to optimizing odors, identify the volatile compounds of coffee, determine its roasting level, decode its flavor and reconstruct its aroma (Borém et al., 2013; Castro et al., 2013; P. de Toledo et al., 2017; Ferreira et al., 2016; Puerta Quintero, 2016; J. S. Ribeiro et al., 2012; Rodrigues et al., 2012; Santos & Ribeiro Da Silva, 2011; Toshio et al., 2009) and it still represents a challenge to integrate these instrumented systems for sensory analysis (vision, smell and taste), as a support tool for the human panel of experts cuppers and the consumers. In general, the information on what would be the contribution of consumers to the definition of coffee quality is still limited.

The traditional way of optimizing the roasting process and obtaining consistency requires carrying out numerous experiments that imply costs of green coffee and time that do not make it viable in the industry because coffee has its own characteristics considering for quality control, such as origin (Puerta Q et al., 2016), bean size, yield, density, humidity, water activity, color (Borém et al., 2013; Correa et al., 2011; De Oliveira et al., 2016; Suslick et al., 2010; Wang & Lim, 2015b), texture (Guevara Barreto & Castaño Castrillón, 2005), roast profiles, roasted coffee color, fragrance, aroma, flavor, body, acidity, clean cup and uniformity (Alessio et al., 2016; Brudzewski et al., 2012; S Buratti et al., 2017; Mendez, 2016; Romani et al., 2012; Sberveglieri et al., 2014; Várvölgyi et al., 2012, 2013). The figure 2.19, presents the bibliometric map detail of research papers including consumers perception and the optimization procedures for time and temperature in coffee roasting process.

Considering these limitations of traditional optimization approach, multivariate statistical optimization techniques such as response surface methodology (RSM) should be employed for modeling and optimizing the coffee roasting process (Amdoun et al., 2018; Anisa et al., 2017; Chung et al., 2013; Erdogdu, 2008; Esposito et al., 2020; Ku Madihah et al., 2013; Riskiono Slamet & Darsef, 2014), since it is necessary to consider that coffee roasting is a complex process that significantly impacts the flavor, aroma, and quality of the final product (W. Sunarharum et al., 2014). Achieving the desired flavor profile requires careful optimization of various parameters during the roasting process.

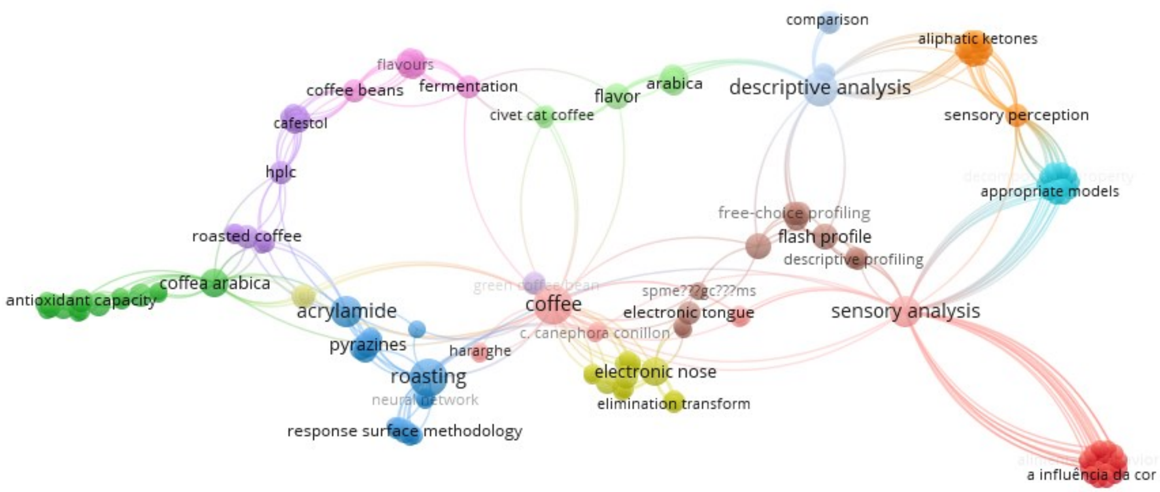


Figure 2.19. Bibliometric maps detail on consumers and coffee roasting optimization keywords.

Furthermore, understanding consumer perception and preferences is essential for producing coffee that meets market demands and the consumers are the focus on the third wave of coffee, based on a sophisticated coffee consumer, a "coffee lover" (Llobell et al., 2019; Samoggia & Riedel, 2018). This literature review aims to provide an overview of the state of the art in the optimization process of coffee roasting and explore consumer perception from the following scientific perspective points.

RQ1: Physical Analysis:

Green Coffee: The initial density, zero primary defects, homogeneous size, processing, fermentation and moisture content of green coffee beans affects the roasting process and subsequent flavor development. (Bustos-Vanegas et al., 2018; Edzuan et al., 2015; Pittia et al., 2011) investigated the influence of varietal, density, bean shape, processing, and moisture content on the formation of complex volatile and non-volatile compounds and found that genetics impact on the character of the beverage. Homogeneous density and shape allow to find the charge temperature point in profiling coffee. Intermediate moisture levels resulted in the highest levels of desirable aroma compounds. The water activity measures how much of that water is chemically available to react and is the precursor for the Maillard reactions. For example, a research gap on this topic may be a lack of understanding of the integration of collecting specialty coffee traceability information into a homogeneous dataset for further analysis.

RQ2: Roasting Process Optimization:

Roasting Temperature and Time: Researchers have investigated the effects of roasting temperature and time on the chemical and sensory characteristics of coffee. (Giacalone et al., 2019) demonstrated that higher roasting temperatures led to increased levels of desirable aroma compounds, while longer roasting times resulted in darker roasts with more bitter notes.

Roasting Profile: The roasting profile, which refers to the temperature-time curve during roasting, plays a crucial role in achieving desired flavor profiles. (Seninde & Chambers, 2020; Yang et al., 2016) conducted a study on different roasting profiles and found that a slower ramp-up phase followed by a shorter development time produced coffee with enhanced acidity and complexity including the low body non-volatile compounds. The challenge in this roasting stage is to achieve consistency in the roasting process, following a collection of time and temperature data, as well as the critical points of the roasting curve, on a standard data set format for its analysis.

RQ3: Consumer Perception:

Flavor and Aroma: Several studies have explored the relationship between coffee flavor and consumer perception (Gastón Ares, Dauber, et al., 2014; Bemfeito et al., 2021; Chambers IV et al., 2016; Llobell et al., 2019; Samoggia & Riedel, 2018; Sepúlveda et al., 2016) conducted sensory evaluations and found that consumers preferred coffee with balanced acidity, sweetness, and a pleasant aroma. Additionally, aroma was identified as a crucial factor influencing coffee quality perception by (Bhumiratana et al., 2011; Carvalho & Spence, 2018; Rune et al., 2022; Seninde & Chambers, 2020). In this item, the consumer preferences data is a subjective data, but can be structured by using sensorial and descriptive expensive methods. Also, can be introduced and validated methods like CATA (check-All-That-Apply) with CLUSCATA algorithms for study and optimizing the inclusion of the biological, psychological, and sociocultural dimensions, considering the intrinsic and extrinsic attributes of coffee that have not yet been systematically studied in Cauca coffee.

Specialty Coffee: The emergence of the specialty coffee market has heightened the importance of consumer perception (Poltronieri & Rossi, 2016; Velásquez et al., 2019). Specialty coffee is often associated with high-quality beans, unique flavor profiles, and ethical sourcing. (Giacalone et al., 2019; Llobell et al., 2019) investigated consumer preferences for specialty coffee attributes and found that factors such as origin, roast level, and taste complexity influenced consumer purchasing decisions. Specialty coffee is a sector of opportunity for Industry 4.0 technologies, thus making it possible to establish the state of the art, seek solutions to technological problems and identify trends, possible lines of research and technologies for free use. In Table 2.6, resume the relationship between raw coffee, roasting process, optimization approach and consumer perception data in the research coffee chart.

Table 2.6. Research coffee chart

Research Questions	**Criterion**	**Support tools**	**Authors**
RQ1: What techniques have been used to identify and classify coffee according to its origin, variety, benefit, value addition and sensory profile?	Conventional techniques	Seedling Planting Harvest Green coffee Traceability	(Barbosa et al., 2019; Bosselmann et al., 2009; Caporaso, Whitworth, Cui, et al., 2018; Casas et al., 2017; de Melo Pereira et al., 2019; P. R. A. B. De Toledo et al., 2016; Echeverri-Giraldo et al., 2020; Puerta Quintero, 2016; Sanz-Uribe et al., 2017; Selmar et al., 2006; Worku et al., 2018)
	Protocols	Q program – CQI - SCA Green coffee grading. Roasting standard for cupping. Brewing best practices. Experts	(Belchior et al., 2020; Chambers IV et al., 2016; Gutiérrez G. & Barrera B., 2016; Lingle & Menon, 2017; Osorio et al., 2021; L. S. Ribeiro et al., 2017; SCAA, 2009, 2015; Thomas et al., 2017; Velásquez et al., 2019; Vezzulli et al., 2021)
	Computational techniques	Statistical methods. Image processing. E-nose E-tonge	(Benitez & Campo-Ceballos, 2018; S Buratti et al., 2017; Susanna Buratti et al., 2015; Flambeau et al., 2017; Hernández et al., 2008; Kiani et al., 2016; Pittia et al., 2011; Radi et al., 2016; Rincon-Jimenez et al., 2021; Ruosi et al., 2012; Várvölgyi et al., 2014; Yuqin et al., 2015; Zajdenwerg et al., 2011; C. Zhang et al., 2018) (Caporaso, Whitworth, Grebby, et al., 2018; Chu et al., 2018; Kiani et al., 2016; Livio & Hodhod, 2018)
RQ2: What is the relationship and importance between the degree of roasting of coffee and the sensory attributes of fragrance, aroma, acidity, bitterness, body, and overall flavor?	Roasting curves. Chemistry of roasting. Cupping. Brewing	HTST: high temperature short time profiles. LTLT: low temperature long time profiles. RSM to experiments design for optimization. Roasting protocol for consistency. Roasting data capture.	(Amdoun et al., 2018; ARTISAN, 2022; Boot, 2005; Borém et al., 2013; J.-S. Cho et al., 2017; Chung et al., 2013; Cordoba et al., 2019; Fabbri, Cevoli, Alessandrini, et al., 2011; Khamitova et al., 2020; Ku Madihah et al., 2013; Mendes et al., 2001; Prakash Maran et al., 2013; W. Sunarharum et al., 2014; W. B. Sunarharum et al., 2019; Toci & Farah, 2008; Yang et al., 2016; Youn & Chung, 2012)
RQ3: What techniques have been used to identify the aroma and flavor components of roasted coffee?	Experts. Consumers.	Expert calibration. Sensors and systems. Consumers Objective and Subjective Measurement. Descriptive Analysis Check-All-That-Apply - CATA CLUSCATA algorithm Penalty analysis	(G. Ares & Jaeger, 2015; Gastón Ares et al., 2010; Gastón Ares, Dauber, et al., 2014; Bemfeito et al., 2021; Geel et al., 2005; Llobell et al., 2019; Meyners et al., 2013; Gloria Puerta, 2009)(Birwal P & BK, 2015; di Donfrancesco et al., 2019; Samoggia & Riedel, 2018; Sobreira et al., 2015)

The scientific challenges for coffee chain in industry 4.0 technologies are listed in table 2.7, which include electronic science tools such as sensors, the internet of things, communications, artificial intelligence, and the use of robots in some optimization tasks of the Colombian coffee roasting process.

Tabla 2.7. Colombian coffee challenges for electronics sciences in data capture and decision making (modified (Silva Rubio et al., 2022))

Beneficiaries	Small coffee producers	Coffee regional associations. Federación Nacional de Cafeteros	
Products	Coffee farmer support systems. Robots and machines	Systems for the tracking of coffee crops, harvest, transforming etc.	Smart systems for coffee: *Traceability. *Consistency.
Technologies	Instrumentation and electronic development systems.	Edge and/or cloud computing. Communication systems.	Data analytics and machine learning.
Research and development projects	Experts CQI system Sensors and actuators. Consumers perception tools.	Internet of things (IoT) systems for data acquisition	Data fusion from multiple coffee data sources

2.7. Research gap and hypothesis

Optimizing the coffee roasting process is essential for achieving desired flavor profiles and ensuring consumer satisfaction. The literature review highlighted the significance of green coffee free defects in the physical analysis, the temperature, time, and roasting profiles in determining coffee flavor and aroma. Furthermore, understanding consumer preferences, especially in the context of specialty coffee, is crucial for meeting market demands. Future research should focus on advanced roasting techniques, sensory analysis, and consumer perception studies to further enhance coffee quality and satisfaction. The conceptual framework and literature review allowing the understanding of the complexity and variety of aspects involved in coffee consumer perception in relation with the roasting process. However, there is a lack of integration between the roasting profile data and the data capture of perception of the coffee consumer in a systematic procedure. The methods to evaluate the quality of coffee beverages have been directed exclusively to experts. The actual gap in this research field is that there are not yet data analytic tools to integrate the perception data by not trained coffee consumers into the coffee roasting process; so that this information will be useful to close the gap between experts and consumers quality perceptions.

In this work the underlying hypothesis is that it is possible to find a correlation between the conditions of time and temperature in the roasting profile of the Castillo and Tabi varieties grown in the department of Cauca, with the attributes of acidity and body in cup acceptable to consumers of specialty coffee. Given the existence of such correlation, based on the studies reported in the literature, it is feasible to obtain a parametric mathematical model, such that its parameters, which define the time and temperature profile, could be adjusted by means of an optimization algorithm whose criteria should be established based on consumer acceptance.

CHAPTER 3

3. Materials and Methods

This chapter presents the implementation of the experimental scheme to approach the study of the variables of time and temperature in the consistency of the perception of acidity and body of the coffee beverage by consumers. Also presents the materials and methods that seek to clarify the relationship between the physical properties of green coffee, its roasting process and the attributes of acidity and body perceived by consumers of specialty coffee from Cauca, with the Castillo and Tabi varieties, and the study of the variables of time and temperature in the consistency of the perception of acidity and body of the coffee beverage due to consumers.

3.1. Selection of samples

The study was carried out with the following raw materials. Coffee cherries of Arabica Castillo Tambo harvested in May 2019 and Tabi harvested in April 2020. The crop is in Cajibío-Cauca, southwestern Colombia between the Western Mountain Range and Central Mountain Range (2.5864322371543524, -76.5534686799687), altitude 1,866 m.a.s.l, distinguished by its volcanic soils and highly diverse agricultural landscapes. The cherries sent through a pulper that removed the skin surrounding the inner seed. Fermentation was 12 hours following a washed coffee processing method, and the seeds put to dry on tarps in diffused sunlight until they reached 9 to 12% moisture. Grains density average: 750 g/L. Grain Size average: mesh 17-18/64 inches. Specialty grade coffee beans used have zero primary defects and only 0-3 full secondary defects.

For this study, coffee bean selection method was conducted using selected washed coffees of the Castillo and Tabi varieties from the TECNiCAFÉ production unit of the Los Naranjos farm, located in Venta de Cajibío in the department of Cauca. Approximate altitude between 1,800 and 1,900 meters above sea level.

Castillo coffee is a variety resistant to rust and Coffee berry disease (CBD), which allows for high planting densities and therefore high productivity. It is widespread in the department of Cauca and has good cupping properties (Alvarado-Alvarado et al., 2005; Rincon-Jimenez et al., 2021).

Tabi is also a variety resistant to rust, but with a tall growth habit, with low planting densities appreciated for special coffee batches (Farfán Valencia et al., 2000). These varieties were selected because we have all the agronomic and phenological monitoring of the micro batches for their study, taking into account the previous reference that the monitoring and traceability of the agroclimatic and post-harvest variables that affect the quality of coffee (Sanz-Uribe et al., 2017; Scheidig et al., 2019).

The classification methodology of the Coffee Quality Institute - CQI is adopted for cherry coffee, dry parchment, its processing, washing, and selection considering the amount of primary and secondary defects acceptable for specialty coffees. This process was carried out in the Parque Tecnológico de Innovación del Café, TECNiCAFÉ, Cajibio, Cauca and CESURCAFÉ, USCO, Neiva Huila.

3.1.1. Physical analysis of coffee beans

The interest behind the experimental development was to obtain sufficient information to generate the parameters of the optimization scheme of a roasting curve for the samples of specialty coffee, Castillo and Tabi varieties, taking into account the consistency in the perception of acidity and body obtained from the coffee consumers. This part of the procedure before the central composite design is aimed at ensuring homogeneity in the samples selected for the roasting process, in aspects such as size, humidity, etc. The purpose of this procedure is to ensure that the conclusions obtained from the study do not depend on these variables unrelated to the roasting process. In accordance with the traceability of the raw material, the characterization procedure of the Castillo and Tabi coffee samples was conducted. Figure 3.1, shows the experimental process for physical analysis of green coffee beans.

Figure 3.1. Assessment and physical selection of coffee samples.

For the physical assessment of the coffee, samples were initially received in dry parchment coffee (DPC). Samples of 250g of DPC were used as reference. The moisture percentage (%) of the DPC was measured with a KETT-SM-450 moisture meter, with which the bulk density was also measured by the gravimetric method. The sample was then threshed and weighed. With this procedure the threshing loss, Green Moisture (%) and defects (g) found were calculated and recorded by manual selection. The coffee sample was then passed through sizing screens to homogenize the samples. The meshes used were from 12 to 18 inches. However, only the samples that remained after passing the coffee through the meshes of 16, 17 and 18 inches were selected. Finally, the mass of the healthy kernel (g), the yield factor and the density in excelsior were calculated. Finally, samples of 250 g were taken to physical analysis according to SCA protocol. The samples that were prepared with this protocol were subjected to profiling tests, where the standard roasting curve was established, which was the input for the CCD-RSM experimental designs.

3.2. Roasting coffee samples

The response surface methodology (RSM) applying central composite design (CCD) was used to optimize the roasting profile based on time and temperature data with 13 runs. The roasting profiles for Castillo samples ranged from 177˚C to 195˚C for temperature and 420 s to 501 s for roasting time, and for Tabi samples ranged from

182˚C to 203˚C for roasting temperatures and 523 s to 637 s for roasting time, respectively. A quadratic model was used to find the optimal roasting conditions including the acidity and body consumer perception. Colorimeter measurements were included into experimental design to follow the visual develop of the color of the roasted beans in the SCA Agtron Roast Color Kit discs.

3.2.1. Roasting Samples

Coffee beans were roasted for 13 different combinations of time and temperature in the range of 175-195 °C and between 420 s and 501 s, for Castillo coffee beans and between 182˚C to 203˚C and 523 s to 637 s for Tabi coffee beans, using the central composite design CCD according to (Campo-Ceballos & Gaviria-López, 2019) with some modifications depending on the degree of roasting runs required (Benítez Urbano & Campo Ceballos, 2018; Poltronieri & Rossi, 2016; SCAA, 2015). Green coffee beans batches of 220 g, were roasted in a PROBAT sample roaster gas driven, with a precision accuracy of ±1 °C equipped with a time-temperature data logging and control system connected to the Artisan scope software (ARTISAN, 2022). The machine was first heated to 180˚C ± 1°C, and the batches were fed into the roasting cylinder. In this step 13 roasting samples were obtained. For each roasting run, the operating conditions were controlled with the preheating of the roaster cylinder and a sample-to-sample time of 300 s. After each roasting process, the roasted coffee beans were rapidly cooled to room temperature using a fan. This process was standard for all samples and took an average of 180 s. Quantik IR800 colorimeter was used to analyze the color of coffee beans to determine the degree of roasting in the 8-color disk of SCA - Agtron Roast Color Kit; 25=Very Dark, 35=Dark, 45=Moderately Dark, 55=Medium, 65=Light Medium, 75=Moderately Light, 85=Light, 95=Very Light. The coffee samples were packed in a sealed plastic bag and stored at room temperature.

3.2.2. Sensory data – intensity measures

The World Coffee Research Sensory Lexicon (World Coffee Research, 2017) was used to allow to this study be descriptive, replicable, and quantifiable, linking the intensity of acidity and body on a 15-point scale from consumers perceptions. This allowed to compare differences among coffees with a significantly higher degree of precision. The intensity score (0=none, 2=Barely detectable, 4=Identifiable, but not very intense, 6=Slightly intense, 8=Moderately intense, 10=Intense, 12=Very intense and 15=Extremely intense) allows consumers to compare the strength of the attribute in the sample against the strength in the reference.

In this experiment one hundred and four (104) pre-trained participants evaluated the acidity and body of the coffee brewing's. Coffee consumers were surveyed through the survey presented in Appendix G to data collect of acidity, body, and color perception. Categorical data were processed with central values as the median for acidity and body and the mode for the perception of color.

According with (N. Gutiérrez & Barrera, 2015) pre-trained protocol consider the eight (8) intensity scale with food grade citric acid solutions (0.25 to 2 g/L of 2-Hydroxy-1,2,3-propanetricarboxylic acid hydrate) as acid reference and eight (8) coffee solutions were prepared for body reference (1:10 to 1:18 French press commercial coffee:water ratio) to presented the 0-15-point scale to consumers.

Data collection was based on a direct face-to-face survey. The survey consists in each of the participants was faced with thirteen cups of coffee and prior to a training on acidity and body levels from prepared reference solutions, they identified according to their perception the levels of acidity and body in 15-point scale. The categorical data in 0-15 scale were processed with the statistical median for acidity and body and we use the statistical mode for the perception of Color. The median represents the mean value of the categorical data set defining acidity or body on the intensity scale 0-15. The median value divides the data set into two halves. Outliers and skewed data have less impact on the median. When we have a skewed distribution, as is common in consumer perceptions, the median is a better measure of central tendency than the mean. The mode represents the most frequent value in the data set. By including central tendency of color perception with the mode, a multimodal distribution can be analyzed, thus generating situations in which we have two or more color values that share the highest frequency. This is important since color is one of the most used indicators but where methods for its perception must be protocolized. In these case R1=acidity, R2=Body, and R3=Color were categorical variables. However, we need to transform these categorical variables to numbers such that the model can understand and extract valuable information. For acidity and body was used 0–15-point scale and for color the Agtron disc reference (25-95).

Fleiss kappa and Cronbach's alpha was calculated for strength of agreement between consumers and for intensity scale consistency study, respectively.

3.2.3. Brewing sample preparation - intensity

The beverages were prepared according to (SCAA, 2015) in the specialized coffee laboratory of TECNiCAFÉ considering the water quality in TDS of 125–175 ppm, water temperature of 93ºC, and a coarse grinding mill with a coffee grinder (Mahlkönig EK43 and Bunn G1) to obtain the ground coffee. Coffee cups were prepared with 18 g of roast coffee per 250 ml (coffee-to-water ratio of 1:14) in a french press at 93°C. It was left to rest for 4 min, after which time the crust was broken, the coffee was shaken, and the crust was removed and left to rest again for 5 more min. A French press was used because the coffee is immersed and completely saturated in a repeatable manner, which produces a homogeneous cup of coffee for consumers testing according with SCA protocols (SCAA, 2015). Because the water temperature can be easily changed, the French press allows greater control over the final thirteen brewing's samples, prepared with the 13 coffee samples obtained through the experimental setup.

3.3. Experimental design and statistical analysis for modeling acidity and body in coffee consumers perception.

Sensory data processing is an open research topic because of its specificity and ability to analyze large multivariate data sets. Data analytics is one of the fields that has begun to work to provide statistical support and adjustment, and its use will intensify and lead to more sensory evaluations with consumer data. Statistical techniques in comparison to other techniques represent the first step in the construction and processing of large sensory data sets through few experiments and is the most compelling advantage of RSM-CCD method for coffee industry. Thermal processing in food processing operations can be given as an example for a continuous problem (Erdogdu, 2008). This results in a continuous function indicating the optimal path as the solution to a continuous time dynamic problem. For this case, variation in process temperature can become one control variable, and maximization of acidity or body, for example, can be applied as an objective function. The constraints can be given as the lower and higher limits of the roasting profile as well as the temperature obtained at the end of the process where they might include differential equations and boundary conditions used in the solution of time temperature profiles to be described (Erdogdu, 2008). The continuous optimization problems are reported to be difficult to solve due to the possible nonlinear and distributed nature of the system dynamics and presence of explicit and implicit constraints on both control variable and objective function (Erdogdu, 2008).

RSM-CCD statistical modeling was used since it is necessary to understand how the data was collected including consumer preference data, as well as the statistical properties of the estimators, the distribution and segmentation of the consumers to show the consistency between the perception of acidity and body when the experiment is performed. In this case, it is necessary to know exactly what is being done and propose time and temperature parameters that provide predictive power. Design-Expert® software (Stat-Ease, 2022) for response surface methodology (RSM) and central composite design (CCD) was used for design, analysis, and post-analysis process. Lack of fit, Model Comparison Statistics, and ANOVA statistical analyses were used for data analysis. XLSTAT 2019 software (sensory data analysis package) was used for Fleiss kappa, Cronbach´s alpha, Shapiro-wilk normality test and the spearman correlation plots. Past 4.10 software was used for spearman correlation maps images (Hammer et al., 2001).

3.3.1. Response surface model: Central Composite Design (CCD-RSM) and mathematical modeling

The Response Surface Methodology (RSM) is a statistical and mathematical technique commonly used for optimizing processes, designing experiments, and analyzing complex systems like roasting coffee (Chung et al., 2013). It is often considered appropriate for addressing problems that involve the optimization of a response variable with respect to several input variables. The choice of the optimization methods for this study depends on various factors such as the problem's nature, available data, complexity, and specific objectives (Erdogdu, 2008). Taguchi, Genetic algorithms, and neural networks can be explored, but these methods may have been discarded for reasons such as the need for efficient optimization, cost-effectiveness, flexibility in handling variables, or the ability to perform response optimization, which are strengths of RSM.

For example, RSM allows for direct optimization of the response variable, whereas the Taguchi method focuses on reducing variability and improving robustness. RSM provides a more comprehensive approach when the goal is to optimize the response itself.

On the other hand, RSM is generally more interpretable than genetic algorithms GAs. The polynomial equations derived from RSM can provide insights into the relationship between input variables and the response. In contrast, GAs often provides optimal solutions without explicit information about the underlying relationships.

Finally, RSM typically requires fewer computational resources and less training data compared to neural networks ANN. RSM can work well with small to moderate-sized datasets, while neural networks often require large amounts of data for training. Additionally, RSM provides a mathematical equation that can be easily understood and analyzed, whereas neural networks are considered black-box models. Alternative methods that may be considered based on hybrid approach in future work (Aung et al., 2022).

The central composite design CCD is used in this work in RSM considering that a central point (time and temperature) can be taken that corresponds to the final stage of the roasting curve, as presented in Figure 2.15, the records of the data have shown that the coffee bean can be taken to the same point, but from different paths or profiles. In this instance important processes occur in the coffee bean that are the object of study of this work, where the intention is to extract mathematical models, involving the time and temperature of roasting, of the acidity and body attributes, with the intensity perception of the consumer.

The steps for the composite central design (CCD) are presented in Figure 3.2.

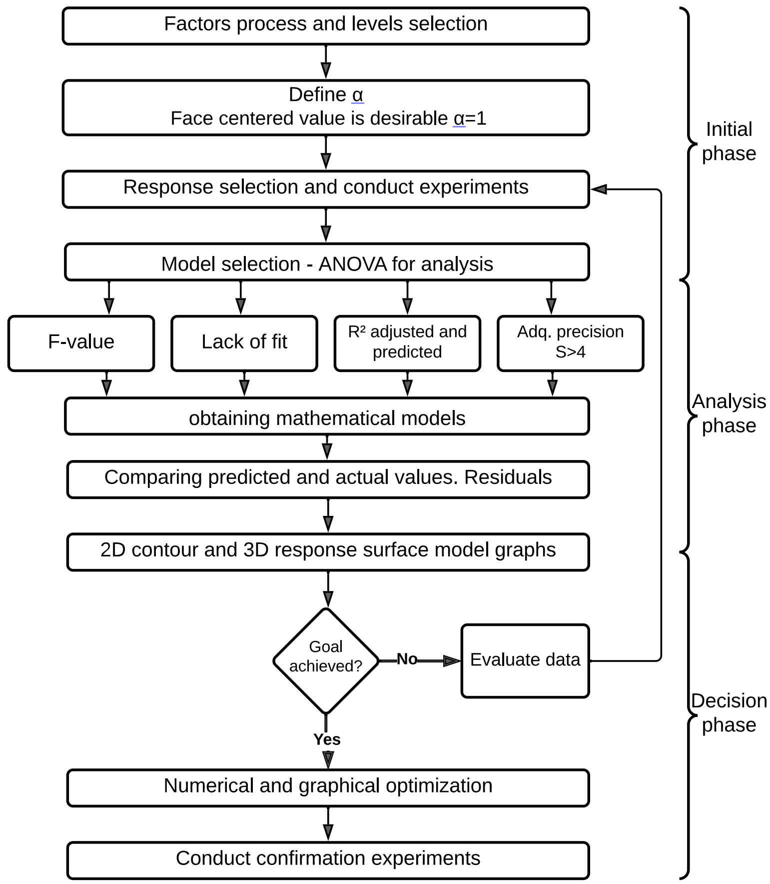


Figure 3.2. Flowchart of the detailed CCD design. (Asghar et al., 2014)

The optimal roasting profile depends on critical factors, including the quality of the raw material, the roaster, and its S-curve. The Parameters of the mathematical model that describe the acidity by consumers' perceptions in the roasting conditions were obtained following the flowchart of figure 3.2.

Mathematical modeling

CCD - Response surface models are used in this work as they can include not only the main effects and their interactions but can also have quadratic and possibly cubic terms to account for curvature. However, quadratic models are desired as they are very efficient and sufficient for industrial applications in the coffee industry. Quadratic regression is a way of modeling a relationship between two sets of variables(Yu et al., 2018). To assess the predictive confidence of the model, R squared indicates how much variation in the dependent variable (acidity, body, color) is explained by the independent variables of time and temperature. The range is 0 to 1, where 0 is

0% variation and 1 is 100% variation. It is used to analyze the extent to which differences in one variable can be explained by a difference in a second variable (Yu et al., 2018). Another element to analyze the model is the Adequate Precision that measures the signal to noise ratio. A ratio greater than 4 is desirable an adequate signal because the model has a strong enough signal to be used for optimization (Stat-Ease, 2019; Yu et al., 2018).

The central composite design CCD is performed to promote to calculate a math model that fit the effect of factors on a central environment. Considering factorial and axial points around this central point allows us to modulate and include variations of the coffee profiles around a critical point to obtain different possible consumer perceptions, and in this way relate the influence of the roasting profile on the perception (Anisa et al., 2017; Ku Madihah et al., 2013; Malaquias et al., 2018). The contour plot uses the predicted model to estimate the perceived acidity for a continuum of time and temperature variables near the center point. The utility of the model is to analyze the behavior of consumer perceived acidity and body in relation to roasting profiles, based on an estimated model.

The desired model has as input (predictor) variables the roasting time and temperature and as output (predictor) variables the perceptions of acidity, body, and color. The model allows to generate predictions for the expected value or for an individual value of the dependent variable. The model fit aims to explain the best relationship between roasting time and temperature and the perception of acidity, body and color perceived by consumers. The predictions arise from the experiments designed through the CCD, which allow knowing the conditions and estimating that, if repeated, the result will be the same, demonstrating that there is a mathematically predictable correlation. The mathematical models will contribute to study how a categorical central composite design can be used for the quality control of specialty coffee, generating strategies to unite concepts, expand knowledge and criteria between experts and consumers.

In view of the foregoing, for conduct the central composite design, it is important to calculate the alpha value as it could determine the location of the axial points in the experimental domain. Depending on the alpha value, the design is spherical, orthogonal, rotating or face-centered (Bozkurt Keser & Buruk Sahin, 2021). Practically, it lies between the centered and spherical face and is calculated as equation 3.1:

$$\propto = (2^{k})^{0.25} \tag{3.1}$$

The desirable value for alpha is 1 because it ensures the position of the axial point within the region of the factorial portion. It is called a face-centered design and provides three levels for the factors to be included in the experimental design matrix. The experimental results obtained are analyzed using the response surface regression procedure of the statistical analysis system. The correlation between the responses and the independent variables is obtained by including them in the second-order polynomial (Bozkurt Keser & Buruk Sahin, 2021; Youn & Chung, 2012) as shown in equation 3.3.

$$Y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \beta_{ii} x_{ii}^2 + \sum_{i=1}^{k} \sum_{i \neq j=1}^{k} \beta_{ij} x_i x_j + \varepsilon \tag{3.2}$$

Where, Y represents the responses, k is the total number of independent factors, $\beta 0$ is the intersection with the axis; βi, βii, and βij represent the coefficient values for linear, quadratic, and interaction effects, respectively, and xi and xj shows the coded levels for independent variables (Asghar et al., 2014). The convergence of the quadratic RSM algorithm is based on the property that the local quadratic model of the objective function provides a good approximation of the surface of the function in a neighborhood close to the local minimum. At each iteration of TIME and TEMPERATURE, the gradient and Hessian matrix of the objective function (ACIDITY OR BODY) at the current point are computed. The Hessian matrix provides information about how the function curves at that point, while the gradient indicates the direction of greatest growth. The system of linear equations H(x) Δx = -g(x) that is solved in the Gauss-Newton step seeks to determine a Δx that minimizes the local quadratic model. This step assumes that the quadratic model is a good approximation of the objective function in the near neighborhood (Erdogdu, 2008).

If the quadratic RSM algorithm converges, it means that the successive updates of the roasting profile variables get closer and closer to the local minimum of the objective function. This occurs because the quadratic model provides an accurate guide when looking for a local minimum in that neighborhood (Erdogdu, 2008). Based on the concepts of RSM technique, predictive models are evaluated with ANOVA using the F-value, Lack of fit, R^2 and Adequate precision statistics. When the model is accepted, numerical and graphical optimization is performed to obtain the key points or region for optimized samples. The Design-Expert software (Stat-Ease, 2019) by default performs regression computations using the coded scale where the low setting for each factor is set to -1 and the high set to +1 per the formula below.

$$Coded = 2 * \frac{Actual\ Setting - Average\ actual\ Setting}{Range\ between\ low\ and\ high\ actual\ settings} \tag{3.3}$$

The equation in terms of coded factors can be used to make predictions about the coffee acidity, body, and color perception for given levels of each factor (time-temperature profile). The coded equation is helpful for identifying the relative impact of factors by comparing factor coefficients.

3.3.2. Numerical optimization

Both responses (acidity and body) were concurrently optimized by multi-response analysis by using Derringer's desired function methodology (C. Buratti et al., 2017). The approach of desirability function is transforming each response into a dimensionless individual desirability function (di), ranging from lowest (0) to highest (1) desirability. According to (Amdoun et al., 2018; C. Buratti et al., 2017), researches applied a special function for the transformation of the Yi responses to the desirability $\mathrm{di(Yi)}$. So, two transformations are proposed. The one-sided transformation used to maximize or minimize Yi. The two-sided transformation described in equation 3.4 used to obtain the target value ti for Yi where li and ui are the lower and upper bounds on the studied response (for this case considering $li<ti<ui$).

$$di(Yi) = \begin{Bmatrix} 0, & if\ Yi < li \\ \left(\frac{Yi-li}{ti-li}\right)^{s}, & if\ li \le Yi \le ti \\ \left(\frac{Yi-ui}{ti-ui}\right)^{t}, & if\ ti \le Yi \le ui \\ 0, & if\ Yi > ui \end{Bmatrix} \tag{3.4}$$

The powers ***s*** and ***t*** correspond to the weighted factor. s and t are the parameters that determine the shape of $\mathrm{di(Yi)}$. For $\mathrm{s = t = 1}$, the desirability function increases linearly to ti. If $\mathrm{s} < 1$ and $\mathrm{t} < 1$, the function is concave and if $\mathrm{s}>1$ and $\mathrm{t}>1$, the shape is convex. The overall desirability function D is defined as the geometric average of the individual desirability functions of each response di, equation 3.5, and 3.6 (Amdoun et al., 2018). The desirable ranges are from 0 (least) to 1(most) desirable.

$$D = (d_1(Y_1) \cdot d_2(Y_2) \cdot \ldots \cdot d_n(Y_n))^{\frac{1}{n}} \tag{3.5}$$

$$D = \left(\prod_{i=1}^{n} di(Yi) \right)^{\frac{1}{n}} \tag{3.6}$$

Where n is the number of responses in the measure. If any of the responses or factors fall outside their desirability range, the overall function becomes zero. The optimal solutions are determined by maximizing D (Amdoun et al., 2018). The desired response of acidity and body was the maximum of the target goal.

3.3.3. Fleiss kappa statistics

The kappa is a coefficient for assessing the reliability of agreement among a panel of raters in assigning categorical ratings to a set of attributes. In this work is used If a fixed number of coffee consumers assign numerical ratings to several coffee samples, then kappa will give a measure of the consistency of those ratings. The kappa can be defined as equation 3.7. It also can be written in terms of common variables defined in equation 3.8.

$$\kappa = \frac{\text{Observed agreement} - \text{chance agreement}}{1 - \text{chance agreement}} \tag{3.7}$$

$$\kappa = \frac{Po - Pc}{1 - Pc} \tag{3.8}$$

where Po is the proportion of observed agreements and Pc is the proportion of agreements expected by chance. Kappa also can be adapted for more than one rating per coffee sample. This variant in called the Fleiss kappa. If the raters are in complete agreement, then $\kappa = 1$. If there is no agreement among the raters $\kappa \leq 0$. Table 3.1, shows Fleiss' kappa Strength of agreement. In these case null hypothesis

H0: Kappa value is not greater than 0 and the alternative hypothesis Ha: Kappa value is greater than 0 were used.

Table 3.1. Fleiss' kappa Strength of agreement

Value of Fleiss' kappa (κ)	**Strength of agreement**
< 0	Poor
0.01 - 0.20	Slight
0.21-0.40	Fair
0.41-0.60	Moderate
0.61-0.80	Substantial
0.81 - 1.00	Almost perfect

If the computed p-value is lower than the significance level alpha=0,05, one should reject the null hypothesis H0, and accept the alternative hypothesis, Ha.

Acidity and body data for both, Castillo, and Tabi, was analyzed using the Fleiss' kappa Strength of agreement in the same conditions of experimental setup. But, due to pandemic COVID-19, for bean color analysis, color testing of Tabi coffee beans was conducted using a 6,500 k - 38-watt LED lamp in an enclosed area.

3.3.4. Cronbach´s alpha statistics

Cronbach's alpha coefficient CA, measures the similarity in the assessment profiles of the panelists, indicating a scale to evaluate how consistent the assessments are within a group of evaluators (Pinto et al., 2014). Equation 3.9, gives the calculation of CA.

$$\text{Cronbach´s alpha(CA)} = \frac{Np * \overline{cov}}{\bar{v} + (Np - 1) * \overline{cov}} \tag{3.9}$$

where Np is the number of assessors (consumers), $\overline{cov}$ is the average covariance across the evaluations from all pairs of consumers, and $\bar{v}$ is the average variance of assessments from all consumers. Table 3.2, presents the Cronbach's Alpha Level of Reliability (Pinto et al., 2014). The CA output gives a consistency value for the panel of consumers assessing the coffee: the closer to one (1) the more consistent is the panel.

Table 3.2. Cronbach’s Alpha Level of Reliability.

Cronbach´s Alpha	Internal Consistency
$\alpha \geq 0.9$	Excellent
$0.9 > \alpha \geq 0.8$	Good
$0.8 > \alpha \geq 0.7$	Acceptable
$0.7 > \alpha \geq 0.6$	Questionable
$0.6 > \alpha \geq 0.5$	Poor
$0.5 > \alpha$	Unacceptable

3.4. CATA (Check-All-That-Apply) sensory characterization with consumers.

In this work, the CATA (Check-all-that-apply) technique was applied which includes consumer perception in the confirmation experiments of the optimization process obtained in the last step of Figure 3.2. In this process, a scheme is established to evaluate the samples from the acidity and body domain in terms of consumer-perceived flavor expression, including 18 common descriptors for untrained coffee consumers. Questionnaire-based methods or Check-all-that-apply (CATA) questions consist of a list of words or phrases from which respondents must select all the words they consider appropriate to describe the sample (G. Ares & Jaeger, 2015; Gastón Ares, Tárrega, et al., 2014). It is considered a practical approach to provide information, as a versatile and reliable option to assess consumers' sensory perceptions versus descriptive analysis, which is usually expensive and depends on expert people.

Both sensory and non-sensory attributes can be included in a list of terms to study the relationship between sensory characteristics of products and consumers' emotional or conceptual associations. In consumer research, CATA questions generally consist of 10 to 40 terms (Gastón Ares et al., 2010) suggest that there may be an optimal range for the number of terms in a CATA question. However, the use of short lists of terms may lead consumers to use all of them, which reduces their ability to discriminate between samples. On the other hand, long lists of terms may lead consumers to be biased towards choosing the first alternatives on the list, without thinking carefully about the sensory characteristics of the product (Gastón Ares et al., 2010).

The CATA technique extracts a matrix of binary data, 0-not there and 1-yes there, on consumer perception for all attributes listed. Similarly, the 1-9 hedonic scale allows to obtain an overall consumer perception of the sample (Barahona & Sanmiguel, 2016; Cotter et al., 2021). Statistical analysis of the data is performed based on the Q Cochran´s statistic, a non-parametric test to verify whether the analyzed treatments have identical effects (G. Ares & Jaeger, 2015; Giacalone et al., 2019).

3.4.1. Cochran's Q Test Statistic.

For binary responses, $Y_{i,j}$, in k matched groups from N subjects, subject i in category j (i = 1 to N, j = 1 to k), the Cochran's Q test statistic is computed as (Meyners et al., 2013; Sheskin, 2003). Equation 3.10, show the Cochran's Q mathematical expression.

$$Q = \frac{(k-1)[kC - T^2]}{kT - R} \tag{3.10}$$

Where,

$$C = \sum_{j=1}^{k}\left(\sum_{i=1}^{N} Y_{i,j}\right)^2 \quad , \quad T = \sum_{i=1}^{N}\left(\sum_{j=1}^{k} Y_{i,j}\right) \quad \text{, and} \quad R = \sum_{i=1}^{N}\left(\sum_{j=1}^{k} Y_{i,j}\right)^2 \tag{3.11}$$

For large samples, Q is distributed as chi-square with k − 1 degrees of freedom. The p-value for the test is computed as:

$$\mathrm{p-value} \; = \; \Pr\left(\mathrm{Q} > \chi^2{}_{1-\alpha,k-1}\right) \tag{3.12}$$

where $\chi^2{}_{1-\alpha,k-1}$, is the value of the (1 − α) quantile of the chi-square distribution with k − 1 degrees of freedom.

For a given attribute or descriptor, Cochran's Q test allows us to evaluate the effect of an explanatory variable (in this case the attributes of the Castillo and Tabi coffee samples) on whether consumers feel the attribute. A low p-value beyond a significant threshold indicates that the products differ significantly from each other. If the p-value is significant, is necessary to examine the multiple pairwise comparison.

3.4.2. Multiple Comparisons Sheskin

When the null hypothesis of success proportion equality is rejected by Cochran's Q test, you can proceed to determine which of the groups are different by computing multiple pairwise comparisons (Sheskin, 2003). Pairwise evaluates between groups "a" and "b" test the null hypothesis $H0$: πa = πb versus the alternative HA: πa ≠ πb

Sheskin method identifies the minimum required difference, MRD, needed to declare a pair of experimental conditions as significantly different (Sheskin, 2003). MRD in proportions for any pair of k experimental groups to be declared different is:

$$MRD = z_{adj}\sqrt{\left[\frac{kT - R}{N^2 k(k-1)}\right]} \qquad (3.13)$$

where N, T, and R, were defined as in Cochran's Q statistic. z_{adj} is the value of the (1 – α_{adj} / 2) quantile from the standard normal distribution (Sheskin, 2003).

Two groups are declared to be significantly different with protected overall alpha, α, if their absolute difference in proportions is greater than MRD, equation 6 show this (Sheskin, 2003).

$$|\pi a - \pi b| > MRD \qquad (3.14)$$

On the other hand, for each of the products, an attribute independence test is performed to determine if these attributes are not redundant. (G. Ares & Jaeger, 2015; Giacalone et al., 2019). This technique uses Correspondence Analysis (CA) and Principal Coordinates Analysis (PCoA) to indicate that the first two dimensions are sufficient to interpret the relationships between attributes, for consumer perceptions (Cotter et al., 2021; Oliver et al., 2018). However, product perceptions often differ among evaluators. Therefore, a cluster analysis of evaluators may be necessary, through the CLUSCATA technique (Llobell et al., 2019). The result is to verify the homogeneity of consumers and their consensus when evaluating different attributes in a cup of coffee.

3.4.3. CATA experimental setup in consumers' perception

Check-all-that-apply (CATA) is a rapid sensory profiling tool that can be applied by consumers, saving time and money in comparison to descriptive analysis (DA), and providing insight into the consumer (Oliver et al., 2018). According to (G. Ares & Jaeger, 2015; Gastón Ares et al., 2010), in this experimental setup for both Castillo and Tabi samples, 40 consumers had to select their overall liking using a nine-point hedonic scale and to answer a check-all-that- apply (CATA) question with 18 categorical attributes (Lime, Tangerine, Orange, Blueberries, Green banana, Grapes, Thin, Syrup, Buttery, Bitter, Panela, Pineapple, Green apple, Cinnamon, Scorched, Red fruits, and Chocolate) that the Geographical indications and the consumers preferences descriptors consider appropriate to describe the coffee brewing's prepare with the roasted coffee beans. The CATA data analysis tool of XLSTAT SOFTWARE has been used to automate the analysis of CATA data. Dataset consider have surveyed N assessors for P products (one of the products can be a virtual, often ideal, product) on K attributes, ((NXP) X (K) MATRIX). The CATA data for the K attributes are assumed to be recorded in a binary format (1 for checked, 0 for not checked). In section 3.4.6 (NXP) X (K) matrix are presented.

3.4.4. Acidity and body descriptors for CATA

Due to the complexity of coffee flavor, the author (W. Sunarharum et al., 2014) proposes a range of compounds for acidity and another for body. Acidity is not perceived alone, but rather is a relationship between acidity, saltiness and sweetness (W. Sunarharum et al., 2014). Coffee descriptors were assigned for consumers to draw on their sensory memory, with reference to familiar foods and beverages. The body is integrated into their analysis of beverage viscosity. Low, medium or heavy bodied beverages can be found, referring to the amount of soluble solids in the beverage, commonly reflected in its viscosity (W. Sunarharum et al., 2014). Considering the above in this work, a triangular scheme was proposed for both acidity and body from the consumer's perspective.

ACIDITY

Acidity is the flavor that gives coffee a certain vivacity or brightness. Without acidity, most coffees would be insipid and boring. The milder the coffee, the more acidic it is (W. Sunarharum et al., 2014). However, acidity can be represented in a triangle between acid, sweet and salty. Some commonly used descriptors for the coffee consumer are:

- Acid - salty: Lemon, Lime represented by citric acid with its sour acidity descriptor. Orange represented by citric acid with its bright acidity descriptor.
- Sour - sweet: Mandarin represented by citric acid and malic acid with its winey acidity descriptor. Blueberries represented by oxalic acid and malic acid with its honeyed acidity descriptor.
- Sweet - Salty: Grape or wine represented by the mixture of tartaric, malic, and citric acid, with its descriptor mild acidity. Green banana represented by malic acid with its neutral acidity descriptor.

When acidity has perceptions outside this triangle they can be considered as defects, since due to their strong intensity or presence of unusual flavors the authenticity of the raw material must be tested (Borràs et al., 2015). Common descriptors for these defects can be:

- Pineapple - citric acid, malic acid, oxalic acid.
- Green apples - strong - malic acid
- Cinnamon - linoleic acids, chlorogenic acids

BODY

The coffee body represents the amount of soluble solids and non-volatile organic components of coffee that give character to the coffee beverage (Cordoba et al., 2019). Figure 3.3 shows the scheme used for the triangular perception of acidity and the overall perception of the body of Cauca coffee beverages, respectively.

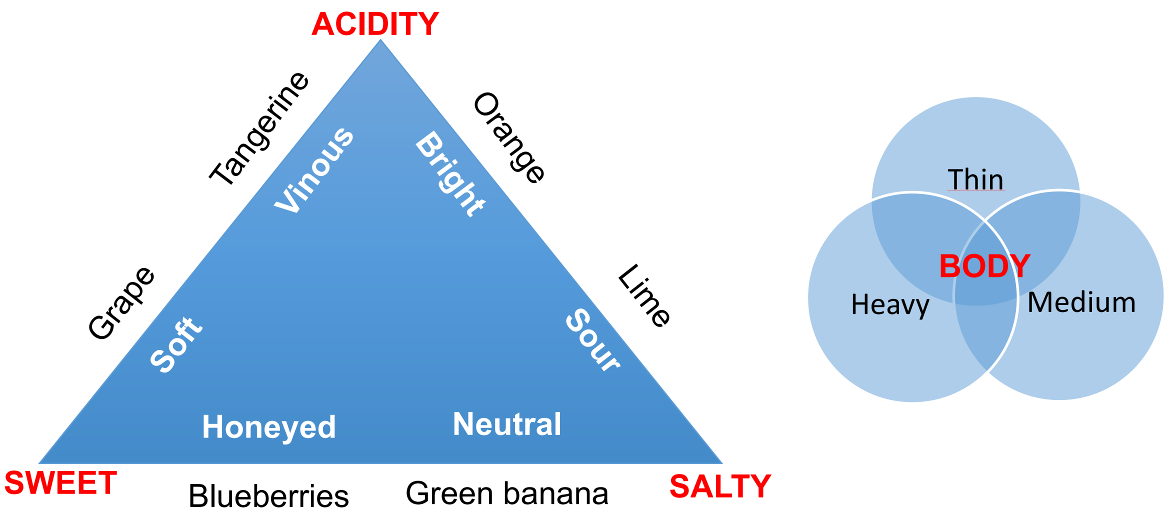


Figure 3.3. Acidity and body descriptors for consumers perception.

Some descriptors of the body used for the consumers can be. Water for light or thin body descriptor. Milk for medium-bodied descriptor. Honey for heavy-bodied descriptor. In practice, commercial coffee with different coffee/water ratio could be prepared to simulated the body perception scale (N. Gutiérrez & Barrera, 2015).

3.4.5. The hedonic scale.

Hedonic scales are proven tools for recording taste and preference data in consumer research (Everitt, 2009). The hedonic scale showed that longer scales, up to nine intervals, tended to be more discriminating than shorter scales (Barahona & Sanmiguel, 2016; Velásquez et al., 2019). Table 3.3 shows the hedonic scale and its score.

Table 3.3. Hedonic scale for consumer research taking into account acceptability test

Grade	Score
Like extremely	9
Like Very much	8
Like moderately	7
Like slightly	6
Neither like nor dislike	5

Dislike slightly	4
Dislike moderately	3
Dislike very much	2
Dislike extremely	1

This scale is used to describe overall consumer preference for a product. In this case it will be related to the consumer's preference in perceiving the acidity, the body, and their overall impression of the beverage.

3.4.6. CATA data analysis

This section presents the methods for the experiments related to consumer perception using the CATA - Check All that Apply methodology and the statistical analysis using the XLSTAT package with its SENSORY DATA ANALYSIS package and its embedded codes in R CATA, Clusblock and CATATIS. For more details on these packages, see Appendix G.

The experiments were conducted by preparing homogeneous beverages of roasted Castillo coffee (time of 473 s and temperature 192°C) and Tabi coffee (time of 540 s and temperature 195°C), in the range of optimized conditions following the optimization scheme of section 3.3.2. For that, 18 g of coffee in 250 ml of water (1:14 coffee-water ratio) at 93°C in a French press. It was left to stand for 4 minutes, after this time the crust was broken, the coffee was shaken, and the crust was removed and left to stand again for 5 more minutes.

At the end of this step the coffee beverages were given in triplicate (French press method no significant differences) to each participant (3 prepared with Castillo coffee: CASTILLO1, CASTILLO2, CASTILLO3 and 3 with Tabi coffee TABI1, TABI2, TABI3). An ideal coffee was required for each consumer, asked to check all the terms they considered appropriate to describe their ideal product, following that established in Figure 3.3, with the aim of testing the penalty technique. Finally, the CATA. surveys had the structure of Table 3.4.

According with (Gastón Ares, Tárrega, et al., 2014), 60 to 80 perception data of consumers can be regarded as a reasonable minimum compromise to get stable sample and descriptor configurations. In this experiment, each of the forty participants evaluated six cups of coffee of both, Castillo, and Tabi varieties obtaining overall 240 consumer perception data. All participants complete an introduction protocol for acidity and body descriptors. Each consumer data has 7 rows; 6 of assessment of coffees and 1 for ideal for proposed penalty technique analysis.

Table 3.4. CATA (Check-All-That-Apply) spanish questionarie with 18 attributes and the hedonic scale

TAZA ____	**¿Qué percibe en la taza de café? selección múltiple**		**GLOBAL Marque solo una opción**
	Lima	Naranja	Me gustó extremadamente
	Arándanos	Mandarina	Me gustó mucho
	Uvas	Plátano Verde	Me gustó moderadamente
	Bebida ligera/refrescante	Agua	Me gustó ligeramente
	Bebida pesada/viscosa	Bebida Jarabe	Ni me gustó ni me disgustó
	Amargo	Panela	Me disgustó levemente
	Piña	Manzanas verdes	Me disgustó moderadamente
	Canela	Quemado	No me gustó mucho
	Chocolate	Frutos rojos	Me disgustó en extremo

The dataset for analysis is present in Table 3.5. CATA data has (280x280)x(18) matrix shape. Liking and ideal data was used to penalty analysis.

Table 3.5. Dataset shape of first CATA data for analysis.

Consumer ID	**CODED Sample Coffee**	**DECODED sample coffee**	**LIKING DATA**	**CATA DATA Binary 0 – Unchecked | 1-Checked**																	
#	three-digit number	Sample	1-9 Hedonic scale	18 attributes list																	
1	IDEAL	IDEAL																			
1	828	TABI1	1-9																		
1	453	TABI2	1-9																		
1	691	TABI3	1-9																		
1	267	CASTILLO1	1-9																		
1	529	CASTILLO2	1-9																		
1	372	CASTILLO3	1-9																		

The samples must be coded with individual three-digit random numbers to avoid bias and presented at one time to the consumers. The serving orders was paired comparison test (TABI1-CASTILLO1), (TABI2-CASTILLO2) and (TABI3-CASTILLO3). The decoded sample coffee column in Table 3.5 was used in the CATA analysis algorithm.

3.4.7. CLUSCATA

The consumers involved in the CATA experiment are not trained. Therefore, they may differ in the interpretation of the attributes or may have different perceptions of the products. Thus, the segmentation of these subjects is of paramount interest. This issue has not sufficiently been addressed in the literature. However, since the CATA data are intrinsically binary the first idea that springs to mind is to use one of the proximity metrics used for such kind of data to assess the (dis)similarity between subjects. Thereafter, the clustering of the subject could be based on the (dis)similarity matrix thus obtained. The strategy of clustering the subjects called CLUSCATA. The objective of CLUSCATA is to constitute classes of assessors as homogeneous as possible, each class of assessors being represented by a latent table called consensus (Llobell et al., 2019). CLUSCATA consists of a hierarchical algorithm that can be consolidated by a partitioning algorithm (i.e., the partitioning algorithm is initialized by cutting the dendrogram). The rationale behind CLUSCATA is to find homogenous clusters of subjects in that sense that the datasets associated with the subjects in each cluster are as close as possible to a group average dataset to be determined. This latter dataset is computed by means of CATATIS and, thus, is a weighted average of the datasets in the cluster under consideration. In a second stage, the group average dataset within each cluster of subjects is submitted to correspondence analysis in order to depict the relationships between the products and the attributes (Llobell et al., 2019).

CLUSCATA starts with a hierarchical algorithm to determine the number of clusters, and then uses these cluster memberships to initialize a k-means algorithm that optimizes the solution. The solution is optimized using a k-means algorithm that permits many cluster memberships to be updated at each iteration until cluster memberships are finalized (Llobell et al., 2019). CLUSCATA is deterministic so only needs to be run once for a given data set. The reason is that for a given input (data set), the hierarchical cluster analysis always produces the same output (cluster memberships). This output then initializes the k-means algorithm, which also converges in a deterministic manner to produce the final cluster memberships. The k-means CLUSCATA algorithm also allows the possibility of a “noise cluster” for absorbing consumers who do not fit any cluster well (Llobell et al., 2019).

3.4.8. Penalty analysis

Penalty analysis is a method used in sensory data analysis to identify potential directions for the improvement of products, based on surveys performed on consumers or experts. The word penalty comes from the fact that we are looking for the characteristics which can penalize the consumer satisfaction for a given product (Addinsoft, 2019; Gastón Ares, Dauber, et al., 2014). When liking data is available, next results are related to the penalty analysis. In this case penalty analysis was applied to validated CATA dataset using hedonic scale, liking column in CATA dataset (Kemp et al., 2018). CLUSCATA algorithm and penalty analysis was fulfilled in sensory package XLSTAT 2022, in Microsoft excel 365.

3.5. Research approach

Figure 3.4 presents the research approach.

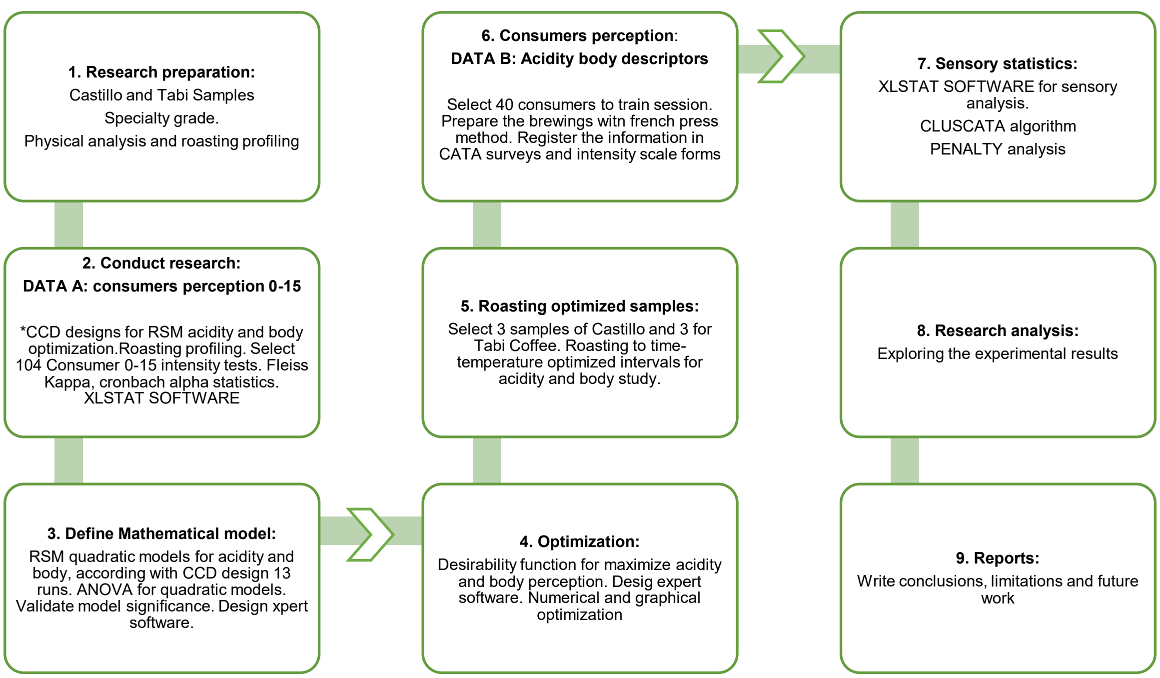


Figure 3.4. Sequence of research approach

CHAPTER 4

4. Results and Discussion

4.1. Physical properties of coffee samples

In this section the physical characteristics of coffee beans that make a sample to be analyzed acceptable for the study are reported. Appendix A, show the complete data set of physical analysis of coffee beans. In this first result the coffee samples presented an acceptable range of moisture, and it can be seen in Figure 4.1 that the humidity is stable in the range of 9 to 12%, despite the variability of the Castillo variety, in comparison with the Tabi variety.

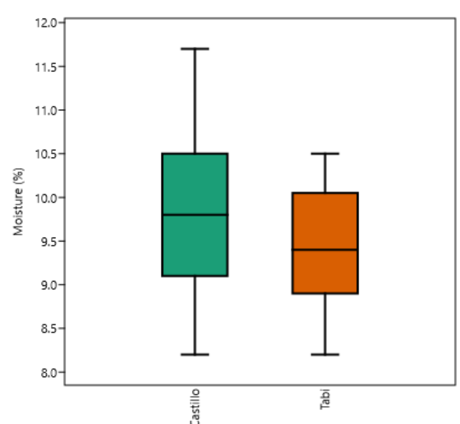


Figure 4.1. Castillo and Tabi coffee beans moisture content.

The coffee beans will retain this moisture until roasting as reported in the literature. The experiments in which the components of the Castillo and Tabi variety were selected were conducted below 1,800 m, for this reason there is no direct information at this altitude until now in Cauca. It is important to highlight that this range of humidity (9-12 %) is necessary to conserve the seed alive and fungi free, and that at the time of roasting the coffee the necessary amount of water is available to activate the aroma and flavor precursors through the heat transfer processes that occur in the roasting curve. This information is valuable because, according to moisture levels, the Castillo coffee samples should have greater control in the heat supply when roasting compared to the Tabi samples, to achieve consistency in the drying phase.

Another result from physical analysis was the quantification of green coffee defects percentage. Figure 4.2 presents the difference of both, Castillo, and Tabi raw coffee beans defects. As expected, Castillo coffee is considered to be more homogeneous and for a granulometry in which more than 83% of the beans are supreme coffee, and whose greater weight and density improves the levels of profitability in the industrialization processes, clarifying that for optimum results an integral agronomic management should be established (Federación nacional de Cafeteros, 2022) . Our results confirm the Castillo features in comparison with Tabi variety. Tabi Cauca variety defects are presented for first time and show a wide defects percentage from 2% to above 10%. When coffee defects are above 10%, we recommended the implementation of selection process of coffee beans and select a couple of mesh.

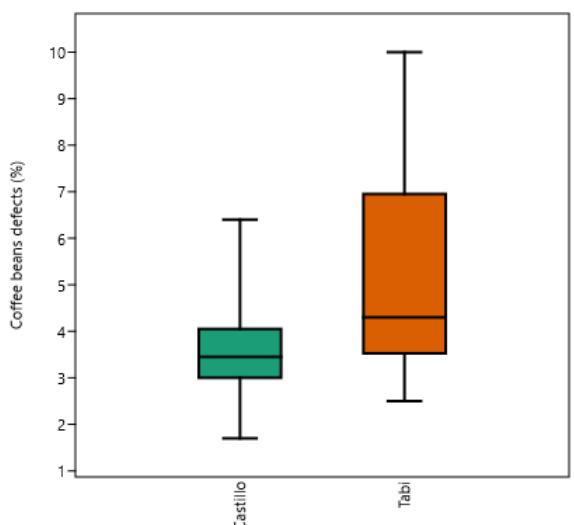


Figure 4.2. Defects percentage in Castillo and Tabi Green coffee samples for experimental study.

Other important result to achieve homogeneity of coffee samples are the size of coffee beans. The distribution of bean sizes is present in figure 4.3. The size of coffee beans should be evaluated to ensure uniformity, which allows specifying that the size for a given batch of coffee means that more than 85% of the beans should be in the same size range. For control and register purposes, the size and shape of coffee beans were evaluated by sieving. Sieve openings are round or oval with diameters ranging from 12 to 18 inches. It is evident that the sizes of the coffee beans are not homogeneous from batch to batch, with less variation in the Castillo coffee beans and a little more in the Tabi coffee beans, which due to its genetics is a little more oval, generating a more difficult classification by size. Coffee beans Size in mesh 16/64 were the samples with the highest percentage of occurrence.

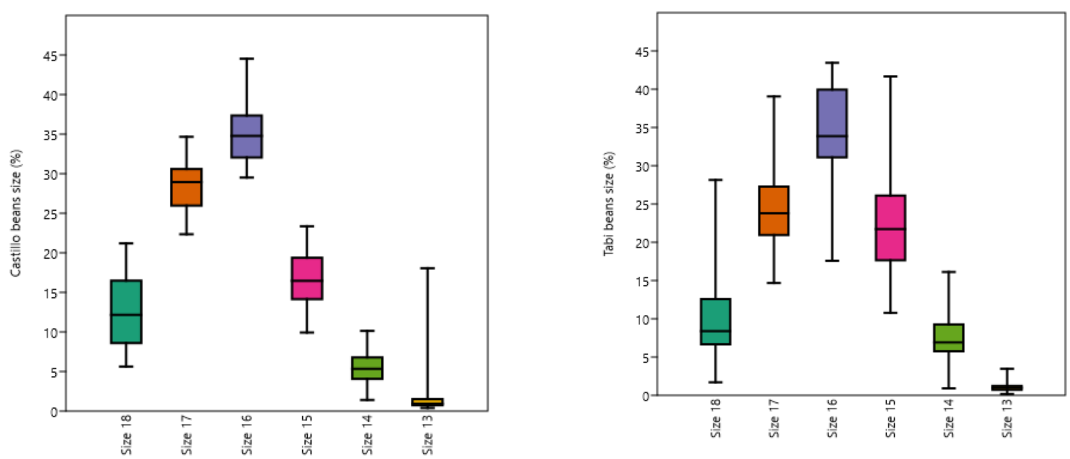


Figure 4.3. Castillo and Tabi coffee bean size characterization

On the other hand, bulk density measures were obtained from the selected 16 mesh coffee samples. All samples present high density >700 g/L, and the variation on the values means the variation in coffee sizes and shapes.

The shape of the coffee beans was not studied in this work, but it generates a wide field of possibilities to understand its relationship with the defects or potentialities of the selected coffee.

Figure 4.4 presents the bulk density comparison between Castillo and Tabi coffee beans in the physical analysis.

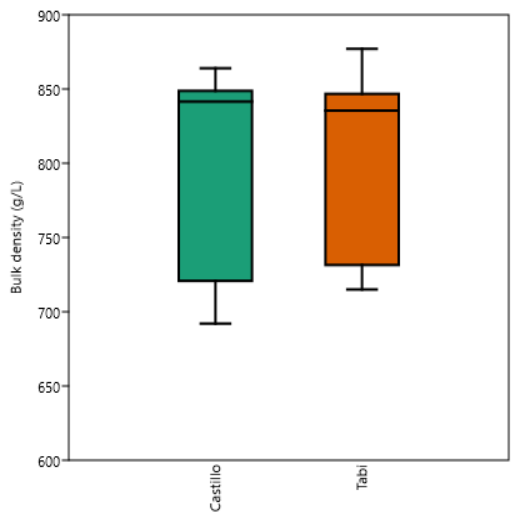


Figure 4.4. Bulk density of coffee beans in physical analysis.

The samples that were prepared with this protocol were subjected to profiling tests, where the standard roasting curve was established, which was the input for the central composite CCD designs. Bean size and shape affect roasting in critical ways. Therefore, careful selection of green coffee to ensure that the beans in each bath are identical, homogeneous, and controlled can help roasters obtain a more uniform result.

4.2. Roasting process and perception of acidity, body, and color for Castillo coffees

Response surface models generate the ability to reduce the number of experiments needed to provide enough information to obtain statistically robust results (Youn & Chung, 2012). To study the development region of the coffee bean, the Central Composite Design - CCD, was introduced. Table 4.1 shows the factors of the CCD design. One central point of 460.5 s for TIME and 186 degrees Celsius for TEMPERATURE, were defined according with coffee profiling protocol present in Appendix B. This point corresponds to a medium roast profile process. In the CCD design, there are three different points, the factor points, the center points, and the axial points. The factor points are the vertices of the n-dimensional cube that come from the full or fractional factorial design in which the factor levels are coded at -1, + 1. The central point is the point located at the center of the design space. The axial points are located on the axes of the coordinate system symmetrically with respect to the center point at a distance α from the center of the design.

Table 4.1 Factors for CCD design in Castillo coffee samples.

Factor	Name	Units	Type	Minimum	Maximum	Coded Low	Coded High	Mean	Std. Dev.
A	TIME	s	Numeric	403	517	-1 ↔ 420	+1 ↔ 501	460.5	33.07
B	TEMPERATURE	°C	Numeric	177	194	-1 ↔ 180	+1 ↔ 192	186	4.90

Using the Design expert software, the CCD design points shown in Figure 4.7 were obtained. Batches of 250 g coffee beans were prepared to obtain the thirteen roasting profiles.

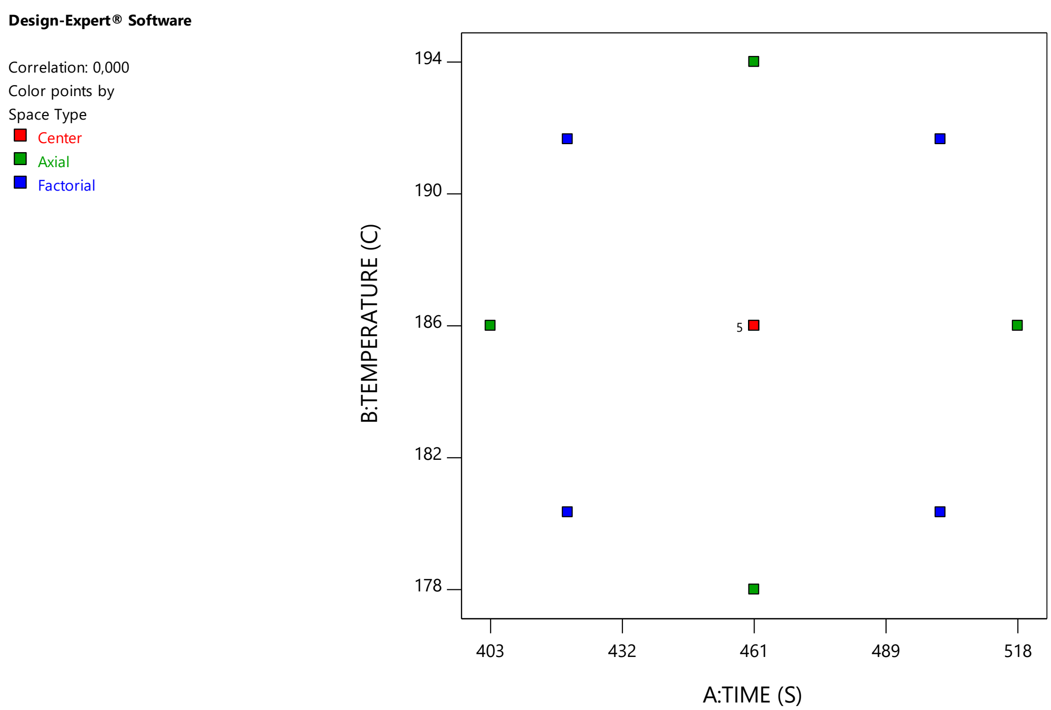


Figure 4.5. CCD design points for Castillo coffee samples. 4 factor points in the corner of cube. 4 axial points out of a cube and 5 central point in the center of design space. Colors means the type of point.

RUN in CCD corresponding to experiments or roasting curves to be performed. The midpoint of the CCD has five repetitions (run5, run8, run11, run4, run1). The outside points of domain (Factorial and axial) estimate the curvature of the response surface (run2, run3, run6, run7, run9, run10, run12 and run13) (El Hami & Pougnet, 2019). Table 4.2, presents the experimental data for the roasting samples of Castillo coffee from Response Surface Methodology with CCD.

Table 4.2. Experimental data from CCD design and the roasting profile points for Castillo coffees

CCD points				**Roasting profiles points**								
Std	Run	A: Time	B: Temp	Charge Temp	Turning Point		Dry or yellow		First Crack		Drop	
		s	°C	°C	t(s)	T(°C)	t(s)	T(°C)	t(s)	T(°C)	t(s)	T(°C)
13	1[c]	460	186	178	82	80	233	138	398	177	460	184
1	2[f]	420	180	179	81	82	230	139	393	177	418	180
5	3[a]	403	186	179	78	78	223	137	392	183	410	186
12	4[c]	460	186	180	73	76	229	138	423	182	455	185
9	5[c]	460	186	179	60	77	228	142	423	183	459	185
6	6[a]	517	186	178	70	77	224	136	424	179	517	186
3	7[f]	420	192	180	74	85	223	138	400	187	419	192
10	8[c]	460	186	179	78	83	206	135	437	185	459	186
8	9[a]	460	194	178	79	80	209	133	440	192	458	194
2	10[f]	501	180	181	71	84	222	141	440	177	500	180
11	11[c]	460	186	179	62	86	226	143	428	182	460	185
4	12[f]	501	192	177	66	83	241	139	471	187	500	192
7	13[a]	460	177	179	76	80	243	142	460	177	460	177
			Average	**180**	**73**	**81**	**226**	**139**	-	-	-	-

t: time, T: temperature. Std is the order of run execution. Run is each roasting curve. [c]CCD central points. [f]Factorial points. [a]Axial points. Charge Temp, Turning Point, Dry or yellow, First Crack and Drop are the experimental roasting profiles points.D

For all batches, the mean charge temperature was 180°C according with hardness bean from the bulk density category of physical analysis samples. Turning point was achieved on average for all roasting profiles in 73 s and at a temperature of 81°C. In the same way, it was observed that the yellow or drying stage was reached at an average of 226 s and 139 °C of temperature. On the other hand, the first crack has different points of occurrence, due to the experimental approach and the objective of each of the roasting curves, as expected according to the experimental knowledge on the behavior of roasted coffee. Finally, the discharge point was followed according to the experimental design, known as the final roasting point. The anatomy of roasting curves (Charge temperature, turning point, dry/yellow, first crack and drop) were the tool for the acidity, body, and color traceability of the coffee beans.

Figure 4.6 shows the experimental roasting curves to study how roasting affects the level of acidity, body and color that is perceived in coffee.

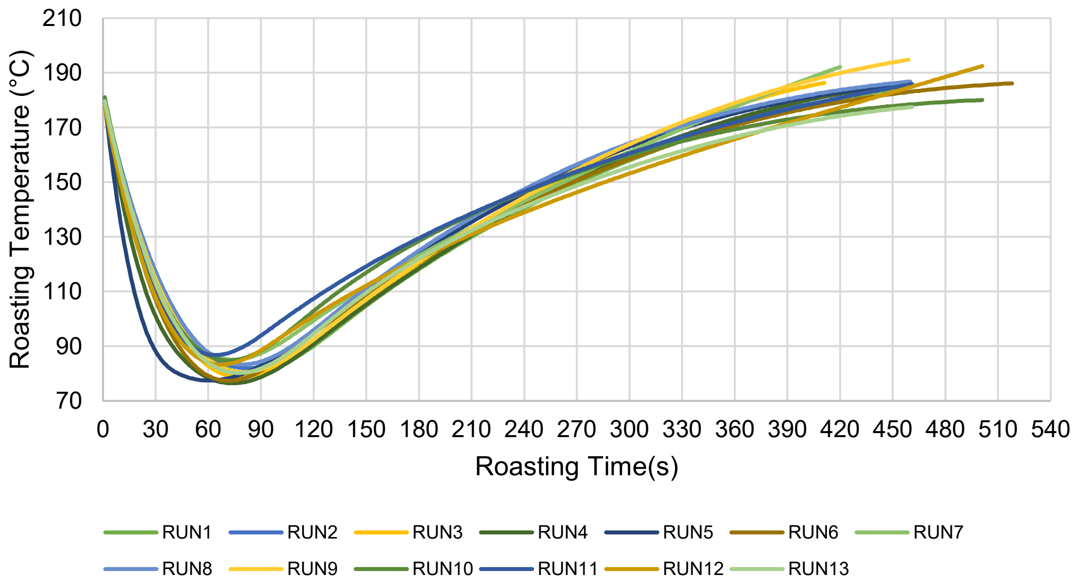


Figure 4.6. Roasting profiles for Castillo coffee samples. Run1 to Run 13 resulting in the 13 experiments from CCD design

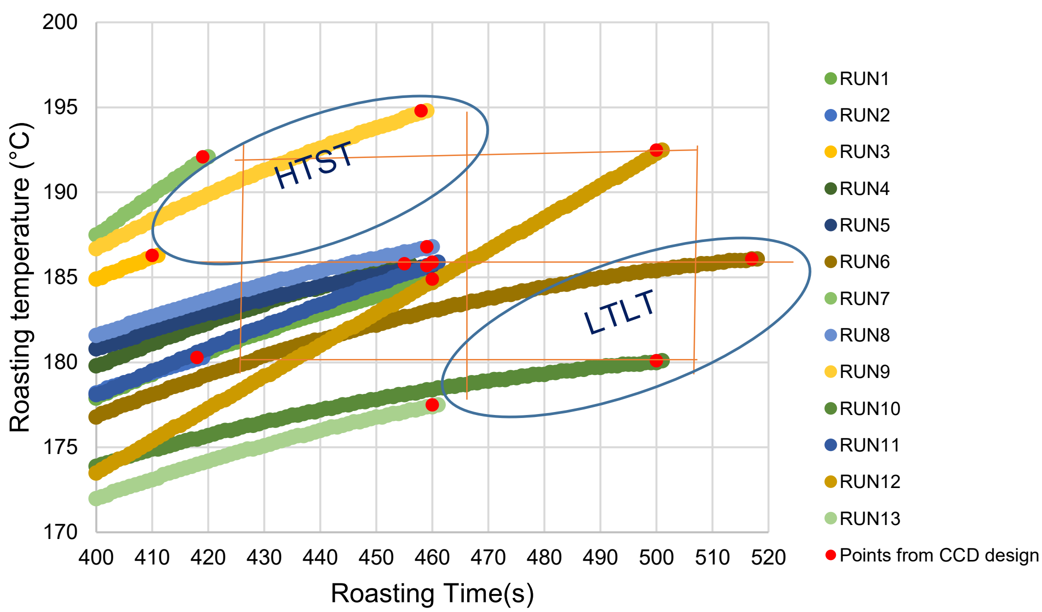


Figure 4.7. Region of interest (ROI) in the experimental Castillo coffee roasting profiles, highlighting the red dots from CCD points.

Roasting profiles (time-temperature data) were obtained from *alog files register in the ARTISAN software scope. A MATLAB script was created to export the roasting profile data *.alog to Excel to plot the 13 roasting curves (view Appendix E). High

Temperature Short Time (HTST) profiles aims to accentuate the acidity and the Low Temperature Long Time (LTLT) accentuate the body (J. S. Cho et al., 2017; Giacalone et al., 2019). This data supports the experimental design to propose the relationship between acidity and body from consumer perceptions. Figure 4.7 present the region of interest (ROI) in more detail (400-520 s). Red points indicate the drop time and drop temperature for each of 13 samples from CCD design. Due to the thermal inertia of the roasters, sometimes it was not possible to drop the coffee at the desired time-temperature, so it must be repeated until the designed CCD point was achieved.

Roasting Coffee process modeling and optimization have been performed by focusing on the effect of changes in one parameter on a response and holding all other factors constant due complex (Malaquias et al., 2018). The main limitation of this approach is that it does not consider the interactive effects between variables and lacks an explanation of the full effect of the factors on the response or an overview of the behavior of the variables within the entire experimental space(Bozkurt Keser & Buruk Sahin, 2021). To address this limitation in coffee, the central composite design - CCD is outstanding for optimization studies by applying procedures such as response surface methodology (RSM), in which multiple factors are considered at once. CCD has proven to be an effective method for modeling and optimization of food products, and in this work RSM scope allows formulating a sampling scheme systematically to achieve differences in perception of acidity and body by coffee consumers from modulating the roasting curves obtained from different paths as reported in section 2.3.3., Figure 2.15. In Coffea arabica, for example, optimization studies are reported that show mathematical models that obtain linear coefficients for time and temperature and the interaction between these variables as significant at a probability level of 5% in the determination of antioxidant activity (Chung et al., 2013). In Ethiopia, an optimization study was conducted for specialty coffee from the Hararghe region, where for the first time the effect of optimizing roasting conditions on consumer perception of coffee-based beverages from that region is reported. The results of the study indicated that the color, bulk density, and true density of roasted coffee beans were significantly affected at a 5% probability level by a non-trivial interaction model between roasting time, temperature, while weight loss, susceptibility to breakage and breaking strength were significantly affected by a linear relationship of roasting time and temperature (Anisa et al., 2017). In Brazil, the Empresa Brasileira de Pesquisa Agropecuária Embrapa, Brazil, reported a study of Arabica coffee grown under controlled water stress to optimize time and temperature conditions and to determine the potential use of this coffee in the instant coffee industry due to its high soluble solids content (Malaquias et al., 2018). A mathematical model was found that relates the development of coffee color in the roasting process and the content of soluble solids consistent with the optimized roasting profile, showing the potential of this coffee for the freeze-dried coffee industry (Malaquias et al., 2018). Optimizations based on perceptions of acidity and body due to untrained coffee consumers have not been reported so far, and we report for the first time this scheme using CCD as new knowledge for quality control of coffee.

4.2.1. Correlation analysis between roasting profiles and the perception of acidity and body of Castillo coffee

Tabla 4.3. Contingency table from consumers' perception of Castillo coffee.

	CONSUMER PERCEPTION		
RUN	**R1** Acidity 0-15 scale	**R2** Body 0-15 scale	**R3** Color SCA disc
1[c]	Moderately intense	Slightly intense	Light
2[f]	Very intense	Barely detectable	Very Light
3[a]	Very intense	Barely detectable	Light
4[c]	Very intense	Barely detectable	Light
5[c]	Very intense	Barely detectable	Light
6[a]	Moderately intense	Moderately intense	Light
7[f]	Intense	Barely detectable	Light
8[c]	Intense	Identifiable, but not very intense	Light
9[a]	Intense	Slightly intense	Moderately Light
10[f]	Moderately intense	Slightly intense	Very Light
11[c]	Very intense	Barely detectable	Light
12[f]	Slightly intense	Intense	Moderately Light
13[a]	Extremely intense	Barely detectable	Very Light

[c] CCD central points. [f] Factorial point. [a] Axial points. R1,R2,R3 median values from 104 consumers perception (0-15 scale) categorical values. Intensity 0-15 scale, 0=none, 2=Barely detectable, 4=Identifiable, but not very intense, 6=Slightly intense, 8=Moderately intense, 10=Intense, 12=Very intense and 15=Extremely intense. Bean Color; 25=Very Dark, 35=Dark, 45=Moderately Dark, 55=Medium, 65=Light Medium, 75=Moderately Light, 85=Light, 95=Very Light.

According to 3.2.2 section, 104 coffee consumers participated in the experiment, rating their perception on the intensity scale (0-15) for acidity, body, and color (25-95 SCA color disc reference) in 13 coffee beverages. R1, R2 and R3 were the responses from consumer perceptions. Data collected results in 1,372 data. Table 4.3 presents the contingency table after data pre-processing measure of central tendency for the thirteen experimental runs.

The applied Shapiro wilk normality tests to the dataset of the response variables revealed that their distribution is non-normal. According to normality test, nonparametric Spearman correlation tests were performed. Figure 4.8 shows the spearman correlation matrix for Time, temperature, acidity, body, and color correlations.

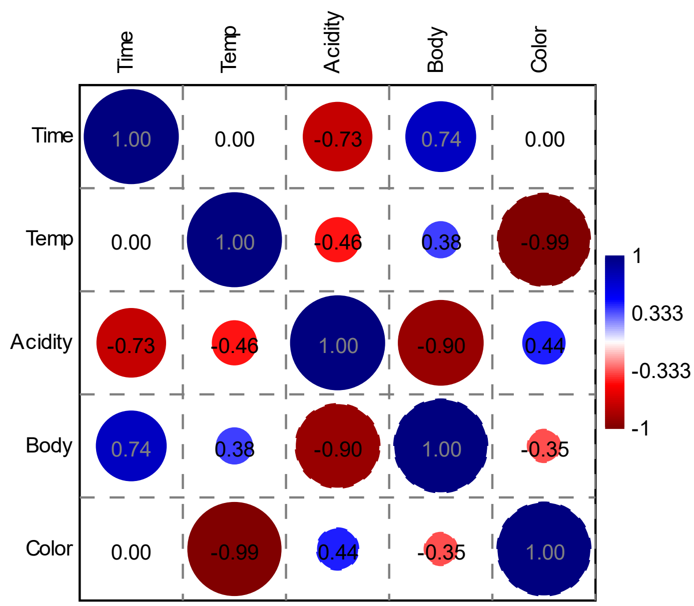
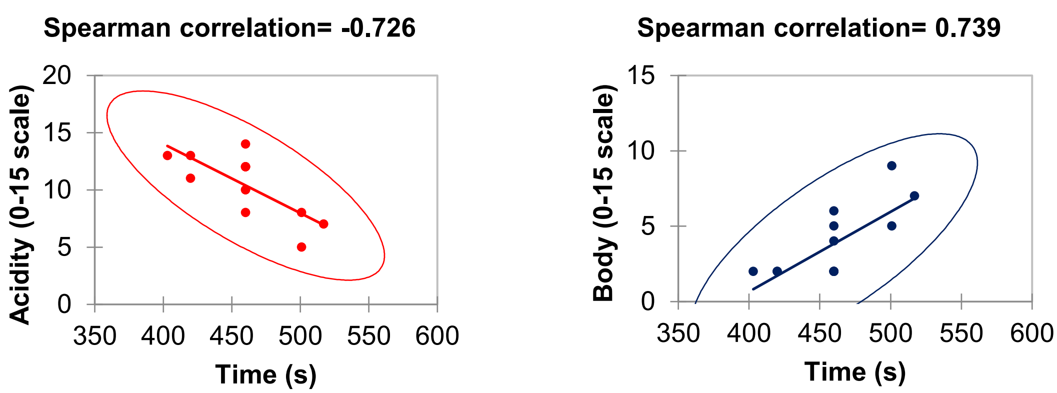


Figure 4.8. Spearman correlation for the Castillo samples.

Results confirms, there is little correlation between color-acidity (0.44) and color-body (-0.35). The results agree with what was found by (Barbosa et al., 2019; Osorio & Pabón, 2022), who affirm that color alone is not an indicator of a correct roasting process, that is why it must be accompanied by its respective roasting curve, and because it does not guarantee the presence of all the sensory attributes of the coffee beverage, these depend on the chemical compounds of the variety and their interaction during the process. In addition, the definition of the color of the coffee bean includes the difficulty that an untrained person has physical and knowledge limitations by the simple visual inspection of these characteristics.

The perception of acidity shows a negative correlation with the body (-0.90), which suggests the two variables are inversely associated, which can be studied in the course of the roasting process. The acidity shows that its intensity decreases as the degree of roasting increases, this result is consistent with that reported by (Barbosa et al., 2019), and is also in agreement with that found by (Giacalone et al., 2019), where the decrease in acidity is related to the variation in the concentration of organic acids such as acetic acid, butanoic acid and hexanoic acid due to pyrolysis and the body is highly and significantly ($p<0.01$) affected by the interaction effect of coffee beans by roasting time, which is in agreement with (Osorio & Pabón, 2022)

Likewise, a moderate and negative relationship between the perception of acidity and roasting time (-0.73) and the positive relationship between the perception of body and roasting time (0.74) can be evidenced. In this sense, the results show that the perception of acidity and body can be affected by the time and temperature profiles, keeping a point-to-point record in the roasting profile. Also, it is observed that while body has a positive relationship of 0.38 with temperature, acidity shows a negative relationship of -0.46 with the same variable. Although these values are expected, it was not yet clear how they relate to each other, including consumers perception. As strong correlations were found between roasting time and acidity and body, Figure 4.9, show the correlation of perception between acidity and body against the roasting time of the Castillo coffee.



(a) *(b)*

Figure 4.9. Correlation of roasting time and (a) acidity and (b) body Castillo coffee

In both cases, the marked dependence of both acidity and the body is reported from consumers perception. Figure 4.9a presents a behavior when the time increases. Negative correlation (above -0.726) indicates a decreasing slope of the perception of acidity in consumers. In contrast, in Figure 4.9b, the positive correlation (above 0.739) between body and the roasting time shows the increasing of body perception when increasing roasting temperature.

Finally, the relation between acidity and body progress in the roasting process was found. The correlation between acidity and body is shown in Figure 4.10. The correlation (above -0.9) represents a very strong inverse relationship in the perception of acidity and body due to the roasting profiles of the coffee. This is another result that is known from the literature, however an inverse relationship between acidity and body has been reported from chemometric data (Belchior et al., 2020; De Luca et al., 2016; Giacalone et al., 2019; W. Sunarharum et al., 2014; Zakidou et al., 2021). In this case we report the inverse behavior between acidity and body but from consumer perception following our experimental approach confirming this relationships. These correlations are indicative of associations among the attributes but at this moment do not reveal cause and effect relationships, however, it is evident that it is possible to affect the consumer's perception of body and acidity through the proposed roasting profiles. Therefore, obtaining a mathematical model for both acidity and body attributes through RSM includes the possibility of optimizing these relationships by taking into account consumer perception.

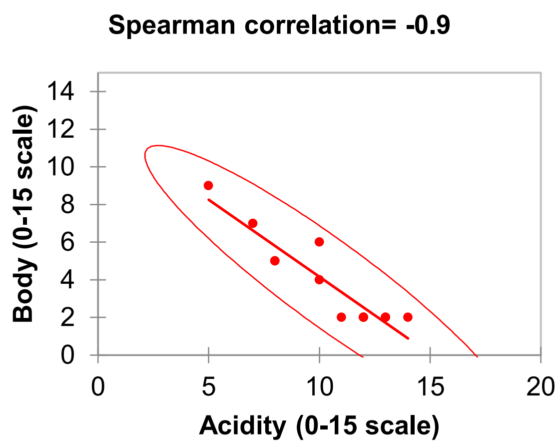


Figure 4.10. Acidity – Body spearman correlation for Castillo samples.

4.2.2. The Fleiss kappa (κ) analysis from Castillo coffee data

For the contingency data matrix presented in table 4.3, reliability analysis was performed using the Fleiss kappa statistic as inter-rater agreement measure for evaluating the level of agreement between two or more consumers, for acidity, body, and color of coffee samples. Because that the perceptions of coffee consumers are opposed or even lacking in rigor, it is necessary to evaluate the strength of agreement among consumers. Table 4.4, Table 4.5, and Table 4.6 present the Fleiss kappa calculations for consumers' perception of acidity, body, and color, according to section 3.3.3.

Table 4.4. Castillo acidity perception agreement between consumers.

Acidity Response	Fleiss' kappa	Standard error	Z	p-value
15=Extremely intense	0.353	0.004	93.139	< 0.0001
4=Identifiable, but not very intense	0.369	0.004	97.427	< 0.0001
10=Intense	0.336	0.004	88.576	< 0.0001
8=Moderately intense	0.467	0.004	123.273	< 0.0001
6=Slightly intense	0.425	0.004	112.272	< 0.0001
12=Very intense	0.496	0.004	130.889	< 0.0001
Overall	**0.425**	**0.002**	**216.088**	**< 0.0001**

The agreement and consistency among consumers in relation to acidity is considered moderate strength of agreement (overall (κ)=0.425), considering that these are non-experts, who were only pre-trained on a scale of intensities (0-15) to perceive the acidity attributes. Values between (κ)=0.496 (Very intense) and (κ)=0.467 (Moderately intense) may be taken to represent moderate agreement beyond chance. On the other hand, Table 4.5, show the body perception between consumers - Fleiss' kappa. Moderate strength of agreement assessment of the perception of the body was obtained for the Castillo coffee.

Table 4.5. Castillo Body perception agreement between consumers.

Body Response	Fleiss' kappa	Standard error	Z	p-value
2=Barely detectable	0.644	0.004	169.805	< 0.0001
4=Identifiable, but not very intense	0.563	0.004	148.681	< 0.0001
10=Intense	0.504	0.004	133.017	< 0.0001
8=Moderately intense	0.427	0.004	112.695	< 0.0001
0=None	0.227	0.004	59.875	< 0.0001
6=Slightly intense	0.332	0.004	87.553	< 0.0001
Overall	**0.481**	**0.002**	**247.992**	**< 0.0001**

Using the classification presented in Table 3.1, since Fleiss' kappa (κ)=0.481, this represents a moderate strength of agreement. However, the value of kappa for Body Barely detectable was (κ)=0.644, that represents substantial strength of agreement. Other body response as Identifiable, but not very intense (κ)=0.563, Intense (κ)=0.504 and moderately intense (κ)=0.427, may be taken to represent moderate agreement beyond chance.

To this point, from a total of 104*13 dataset for each acidity and body perceptions, Fleiss kappa statistics value of (κ)=0.425 for acidity and (κ)=0.481 for body, is considered a moderate strength of agreement among consumers of Castillo coffee. This result is especially important as a tool to evaluate our experimental protocol to perform the data collect protocol, considering the pre-train step for consumers.

The results of the moderate level of agreement are related to the process that consumers were faced with in order for them to know the basic information about the intensity levels for acidity with the citric acid solutions, for body with the commercial coffee beverages in different concentrations, as well as for color with the SCA disc kit for present the information about the type of roast (light, medium and dark), favoring the acceptance of specialty coffees. Therefore, the disclosure of the different characteristics present in specialty coffees can be used as a strategy to optimize the sensory experience of consumers with the beverage.

These results are consistent with (Bemfeito et al., 2021) since, at a general level, experts' assessments of coffee quality do not correspond with consumers' preferences. However, the gap between coffee experts and consumers, which is still under investigation, can be reduced when consumers perceive sensory differences when they learn information about coffee quality or are stimulated to motivate sensory exploration of coffee as reported by (Carvalho & Spence, 2018; Spence & Carvalho, 2019). In this case, our results are intended to promote the ability of a consumer panel to detect differences in the acidity intensity and body of specialty coffee samples prepared using the adopted methods, with a moderate level of agreement, as would be perceived by a single coffee expert. When the attributes of coffee are better defined, whether expert or consumer, it is easier for researchers and roasters to define and measure quality objectives. The degree of agreement related to the quality of coffee samples that unites consumers, experts and roasters helps to align methodologies and vocabulary and defines quality outcomes in an optimization scheme.

On the other hand, the reliability test for color perception is shown in Table 4.5. In this case the overall (κ)=0.226 represents fair agreement beyond chance. This result could be associated with variations in light conditions for each consumer. It could also be attributed to the reduced color scale of Agtron discs observe and measure naked eye. However, Light Medium (κ)=0.465, and Very Light (κ)=0,443 values may be taken to represent moderate agreement beyond chance.

Table 4.6. Roasting bean color perception agreement between consumers.

Color Response	Fleiss' kappa	Standard error	Z	p-value
85=Light	0.088	0.004	23.129	< 0.0001
65=Light Medium	0.465	0.004	122.770	< 0.0001
75=Moderately light	0.210	0.004	55.438	< 0.0001
95=Very Light	0.443	0.004	116.948	< 0.0001
Overall	**0.226**	**0.003**	**86.521**	**< 0.0001**

Overall results for roasting bean color perception agreement between consumers - Fleiss' kappa, had a (κ)=0.226 representing fair agreement beyond chance. This result could be associated with variations in light conditions for each consumer. In addition, the visual analysis of the color of roasted coffee beans would require more rigorous training or the use of specialized equipment. As a contribution of this work, we developed a colorimetric device called PICAFÉ, with which we correlated measurements of near infrared spectroscopy-NIR, hyperspectral images and industrial colorimetry in the CIE Lab color space. This device helps both consumers and experts to relate a color measurement with spectral bands that characterize and evaluate the quality of coffee, as proposed in Appendix B. The color of the roasted coffee should be accompanied by its respective roasting curve, for the purposes of transparency of the process. Although coffee research has contributed to generate different routes for the assessment of color, its relationship with its organoleptic properties continues to be a matter of research.

4.2.3. The Cronbach´s alpha from Castillo coffee data

Table 4.7 show the Cronbach's alpha statistics for acidity and body consistency in Castillo roasting samples.

Table 4.7. Cronbach's alpha statistics for acidity and body consistency.

Cronbach's Alpha - CA	Number of data 13*208 matrix
0.806	2,704

Cronbach's alpha index (CA) measures internal consistency, which is, how closely related a set of items are. Cronbach´s alpha is a measure of the internal consistency of a 0-15 intensity scale and used to verify consumers training efficiency. According to Table 4.7, the value of Cronbach's alpha value means the consumers present good consistency when evaluating attributes of acidity and body in 0–15-point scale, meaning that attribute descriptions were understood homogeneously by panelists, pointing to good training. We can confirm what was reported by (Pinto et al., 2014), where sensory analysis of coffee requires human perception, and all senses are used to generate an individual (expert) or collective (consumers) ability to detect differences. The repeatability in the assessments and the agreement between panelists (or reproducibility), are the valuable data to estimate or not the consistency of the panel. Cronbach's alpha coefficient allows the identification of acidity and coffee attributes better understood by consumers and it's reported for first time. However, it should be noted that acceptable Cronbach's alpha values range from 0.70 to 0.95, according to various publications. If the alpha is excessively high, it could indicate that some items are redundant, since they are in evaluating the same attribute in different ways (Pinto et al., 2014). Cronbach's alpha coefficient for Acidity and Body Castillo coffee in this study showing correspondence with acceptable levels to trust the consistency of consumers' panel perceptions, therefore, intensities scales (0-15) to capture the information for this work were deemed reliable and capable of performing consistently. This supports the strength of our experimental protocol, highlighting the possibility of linking the concepts among the participants of a consumer panel, providing consistency in the data obtained. Likewise, value is given to the pre-training process reported by (N. Gutiérrez & Barrera, 2015), which rigorously generated an understanding of the acidity intensity scale (with the citric acid solutions) and a global panorama for the definition of the coffee body by modulating the brewing coffee-water ratio to obtain the different intensities

4.2.4. Mathematical modeling for acidity from RSM in Castillo coffee samples.

According to section 3.3.1, Mathematical model for the factors of time, temperature, and acidity, it is proposed to study the quadratic model (R^2=0.8). These statistics indicate that 80% of the date variability related to the response variable could be explained by the fitted model. However, is a good value to represent for first time this relationship, according with our optimization protocol. Previous studies have reported on the optimization of roasting time and temperature using CCD-RSM models, for the determination of physical characteristics and mostly chemical elements of coffee such as acrylamide, ochratoxin, antioxidant activity with chlorogenic acid, caffeine, total sugar, phenolic compounds, and pH. This work extends the findings into coffee consumers' perception acidity. Adequate Precision for Castillo coffee acidity model was of 6.97 indicates an adequate signal. Then the model has a strong enough signal to be used for optimization. Analysis of variance ANOVA was performed for the proposed quadratic model. This result can be seen in Table 4.8.

Table 4.8**.** ANOVA from quadratic model in Castillo coffee acidity perception

Source	Sum of Squares	DF	Mean Square	F-value	p-value	
Model	67.31	5	13.46	4.77	0.0324	significant
A-TIME	47.46	1	47.46	16.80	0.0046	
B-TEMPERATURE	14.20	1	14.20	5.03	0.0599	
AB	0.2500	1	0.2500	0.0885	0.7747	
A^2	4.88	1	4.88	1.73	0.2301	
B^2	0.1837	1	0.1837	0.0650	0.8060	
Residual	19.77	7	2.82			
Lack of Fit	6.97	3	2.32	0.7260	0.5874	not significant
Pure Error	12.80	4	3.20			
Cor Total	87.08	12				

The model F-value of 4.77 implies that the model is significant. There is only a 3.24% chance that such a large F-value could occur due to noise. The F-value of unadjusted 0.73 implies that the lack of adjustment is insignificant for the pure error. There is a 58.74% chance of a considerable lack of fitness due to noise. The significant lack of fit is good; the model was required to fit the behavior of the acidity data. Finally, the estimated coefficients of the quadratic model can be obtained, extracting the terms (AB, A^2, B^2) that allow to explain or predict the perception of acidity from consumers through the time-temperature profiles. Table 4.9 presents these calculations.

Table 4.9. Coefficients in terms of coded factors for Castillo coffee acidity perception model

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	10.80	1	0.7516	9.02	12.58	
A-TIME	-2.44	1	0.5942	-3.84	-1.03	1.0000
B-TEMPERATURE	-1.33	1	0.5942	-2.74	0.0729	1.0000
AB	-0.2500	1	0.8403	-2.24	1.74	1.0000
A^2	-0.8375	1	0.6372	-2.34	0.6692	1.02
B^2	0.1625	1	0.6372	-1.34	1.67	1.02

DF: degree of freedom. CI: confidence Interval. VIF: variance inflation factor

The coefficient estimate represents the expected change in response per unit change in factor value when all remaining factors remain constant. A-TIME (-2.44), B-TEMPERATURE (-1.33), and A^2 (-0.86) indicating inversely proportional relationship with acidity perception in a high relative impact.

The regression coefficients indicate how the response changes in relation to the intercept. The intercept is the overall average response of all careers. The intercept in coded values is at the center of the design. In real values, the intercept can be, and usually is, far from the design space.

The units of measurement are normalized (eliminated) by coding. Coefficients are adjustments around that average based on the configuration of the factor. When the factors are orthogonal, the VIFs are 1; VIFs greater than 1 indicate multi-collinearity. The higher the VIF occurs with A^2 and B^2, however it is only just 0.02 above 1. Also 95% CI-confidence interval is presented for each factor value.

The model in terms of real factors presented in Table 4.10, can be used in practical applications (time-temperature profiles).

Table 4.10. Final equation for acidity model in terms of actual factors

ACIDITY (Castillo)	=
+39.55534	
+0.601474	TIME
-1.42742	TEMPERATURE
-0.001029	TIME * TEMPERATURE
-0.000511	TIME^2
+0.004514	TEMPERATURE^2

Here, the levels must be specified in the original units for each factor. Seconds for Time and Celsius degrees for temperature. The study of the residuals and the predicted values were presented in Figure 4.11.

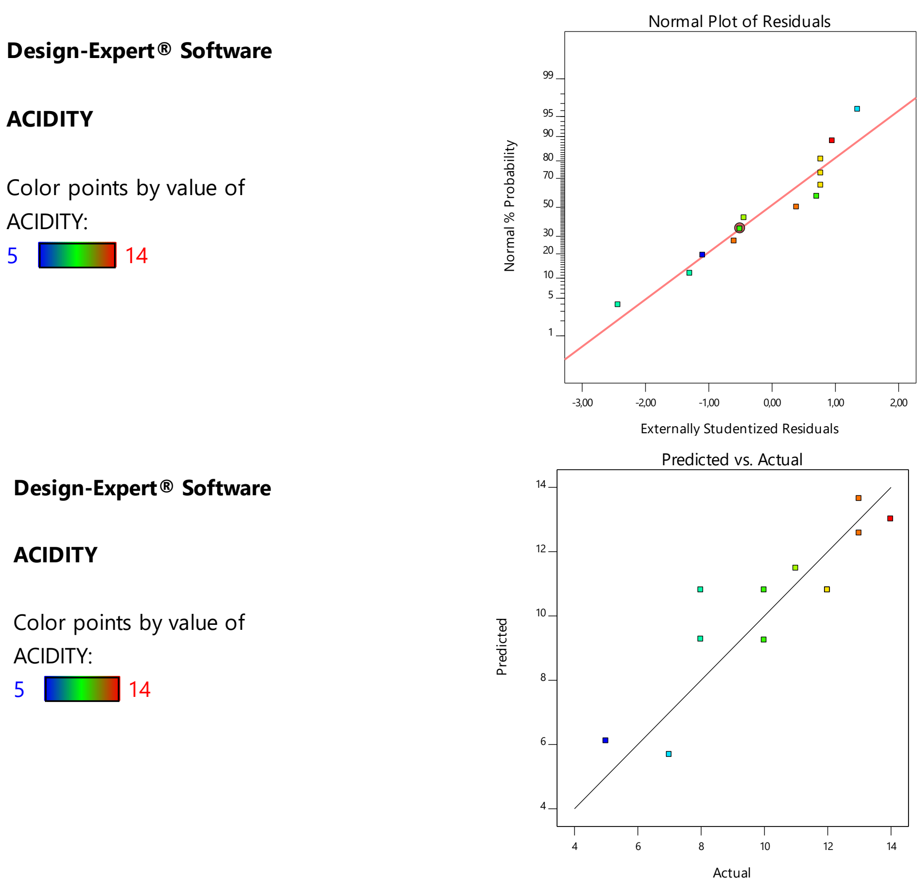


Figure 4.11. Residuals and predicted vs Actual plots from the Castillo coffee acidity perception model.

The normal probability plot indicates whether the residuals follow a normal distribution, thus follow the straight line. Predicted vs. Actual is a graph of the predicted response values versus the actual response values. In this case, the roasted coffee samples roasted with run 3, run 6 and run 9 were detected with an acidity that is not easily predicted by the model because it is the furthest point from the straight line. Even so, the model responds significantly to the consumers' description of the attribute. The contour diagram and response surface of the acidity perceived by consumers in the designed experiment are presented in Figure 4.12.

The contour plot is a two-dimensional (2D) representation of the response plotted against combinations of numeric factors. It can show the relationship between the responses of acidity consumers perception. The design points are present in the figure with red circle and allows to analyze the predicted perception of acidity from consumers related with the roasting profiles. The contours plot on the left, close to the high temperature and short duration (HTST) roasting profiles, have a curvature that leads to a perception of high acidity(contour 13.7 to 11.6). The central contours (Contours 11.1; 10; 9; 8.1 and 7.1) show a homogeneous trend and relate the roasting profiles run9 and run10, obtaining a predicted acidity in the range of contours 10 – 9 (green region lines) on the 15-point scale used in this work. This result shows that there is a region where consistent acidity can be achieved as a function of mathematical models with time and temperature parameters.

On the other hand, the predicted perception of acidity for low temperature and long time (LTLT) roasting profiles shows low acidity values(contour 5 and 2.9), that include the run 6 and run12 roasting profiles and show lower values of acidity perceived from consumers in the range of 7-5 (blue region) on the 0-15 point scale. Consumer perception of acidity can be affected in a controlled manner by taking into account the appropriate roasting profiles to accentuate or not this attribute. Although this fact has been reported from chemometric data, this is the first time that the perception of acidity in coffee and its relationship to roast profile has been reported from a consumer data perspective.

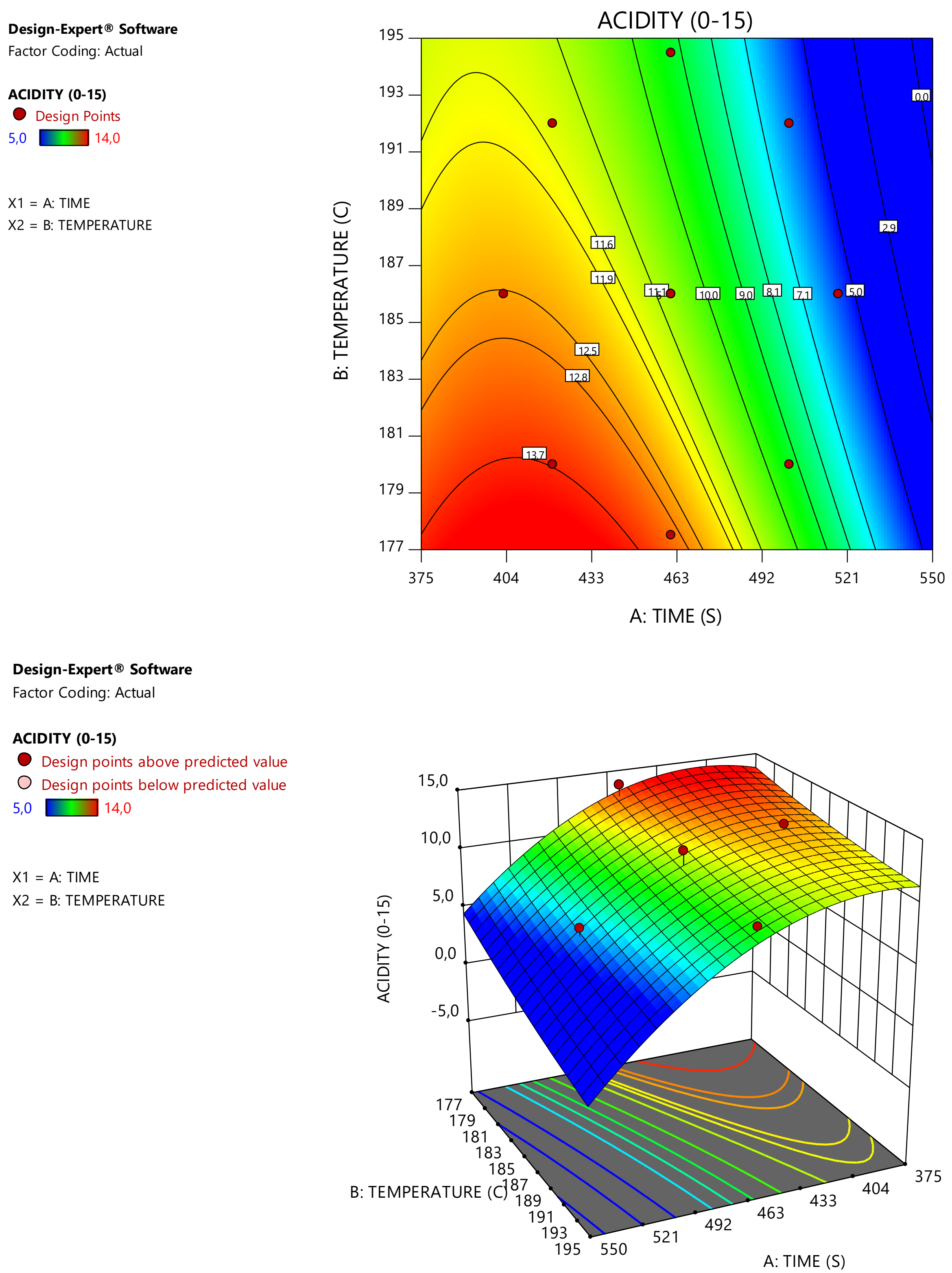


Figure 4.12. Contour plot and response surface for Castillo coffee acidity perception

In several studies it has been observed that consumers do not differentiate between acidity. While coffee professionals value acidity in coffee and often roast to accommodate this flavor, consumers often do not appreciate this acidity, as they do not have the tools to differentiate acidity from bitterness, which in general, diminishes the pleasantness of all coffees. This being the first study that involves the perception of consumers on the acidity of specialty coffees from Cauca, our results are the new findings of those reported in the literature. Although there are several limitations that should be recognized and addressed in future research on the subject, we can explain this fact in our study, because it is most likely that our panelists would have adapted to the acidity of the beverages, and still perceived the differences between the general intensity perception and a true expression of acidity in coffees prepared on the 0 to 15 intensity scale. Also, it should be said that although these methods could be used to distinguish samples of characteristic quantities, the chemical differences between samples can hardly be explained directly without the guidance of professionals.

Our findings agree on the need to close gaps between experts and consumers by distinguishing key attributes of specialty coffee markets where quality has increased and is noticed by experts through tasting notes, certifications, or publications, while the growing number of new consumers start with limited tasting discernment skills.

4.2.5. Mathematical modeling for body from RSM in Castillo coffee samples

Likewise, the result for the body consumers' perceptions of the coffee samples was obtained. R^2=0.9, and F-value of 10.15 implies that the model is significant. There is only a 0.41% chance that such a large F-value could occur due to noise. The lack of Fit F-value of 0.30 implies that the lack of adjustment is not significant in relation to the pure error. There is an 82.20% chance that such a large F-value lack of adjustment will occur due to noise. Adequate precision for Castillo coffee body model was of 9.8 indicates an adequate signal. Table 4.11 presents the ANOVA results for the quadratic model.

Table 4.11. ANOVA for quadratic model in Castillo coffee body perception

Source	Sum of Squares	DF	Mean Square	F-value	p-value	
Model	71.25	5	14.25	10.15	0.0041	significant
A-TIME	47.46	1	47.46	33.81	0.0007	
B-TEMPERATURE	18.21	1	18.21	12.97	0.0087	
AB	2.25	1	2.25	1.60	0.2460	
A²	2.72	1	2.72	1.94	0.2067	
B²	0.9783	1	0.9783	0.6969	0.4314	
Residual	9.83	7	1.40			
Lack of Fit	1.83	3	0.6089	0.3044	0.8220	not significant
Pure Error	8.00	4	2.00			
Cor Total	81.08	12				

On the other hand, Table 4.12 shows the coefficients of the model in terms of coded factors. The equation in terms of coded factors can be used to make predictions about the coffee body perceptions for given levels of each factor (time-temperature profiles). The coded equation is helpful for identifying the relative impact of the factors by comparing the factor coefficients. In all factors it is positive, indicating that high relative impact is in A-TIME (2.44), B-Temperature (1.51), and AB factor (0.75).

Table 4.12. Coefficients in terms of coded factors for Castillo body perception model

Factor	Coefficient Estimate	DF	Standard Error	95% CI Low	95% CI High	VIF
Intercept	3.00	1	0.5299	1.75	4.25	
A-TIME	2.44	1	0.4189	1.45	3.43	1.0000
B-TEMPERATURE	1.51	1	0.4189	0.5183	2.50	1.0000
AB	0.7500	1	0.5924	-0.6508	2.15	1.0000
A²	0.6250	1	0.4492	-0.4372	1.69	1.02
B²	0.3750	1	0.4492	-0.6872	1.44	1.02

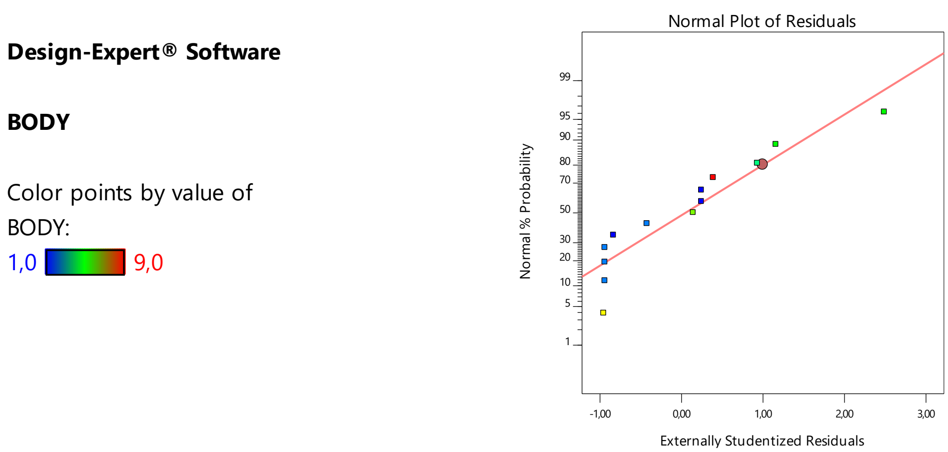
DF: degree of freedom. CI: confidence Interval. VIF: variance inflation factor

The coefficient estimate represents the expected change in response per unit change in factor value when all remaining factors are held constant. The intercept is the overall average response of all careers. The intercept in coded values is at the center of the design. Coefficients measure half the change from -1 to +1 for all factors. When the factors are orthogonal, the VIFs are 1; VIFs greater than 1 indicate multi-collinearity. The higher the VIF occurs with A^2 and B^2, however it is only just 0,02 above 1. Also 95% CI-confidence interval is presented for each factor value. The mathematical model from body-Time-Temperature relationship is presented in Table 4.13 shows the final equation in terms of actual factors. The actual factor model can be used in practical applications (real time-temperature profiles). Here, the levels should be specified in the original units for each factor. Seconds for TIME and Celsius degrees for TEMPERATURE.

Table 4.13. Final equation for Castillo coffee body perception in terms of actual factors

BODY (Castillo)	=
+634.06969	
-0.864872	TIME
-5.04482	TEMPERATURE
+0.003086	TIME * TEMPERATURE
+0.000381	$TIME^2$
+0.010417	$TEMPERATURE^2$

In Figure 4.13, the study of residuals and predicted values for coffee body perception is presented. The normal probability plot indicates whether the residuals follow a normal distribution. The relationship is approximately linear except for a few data points. Roasting profiles run6 present the greatest distance from the normality line. This event is probably due to difficult to tunning the roaster machine for this roasting sample and the perception.



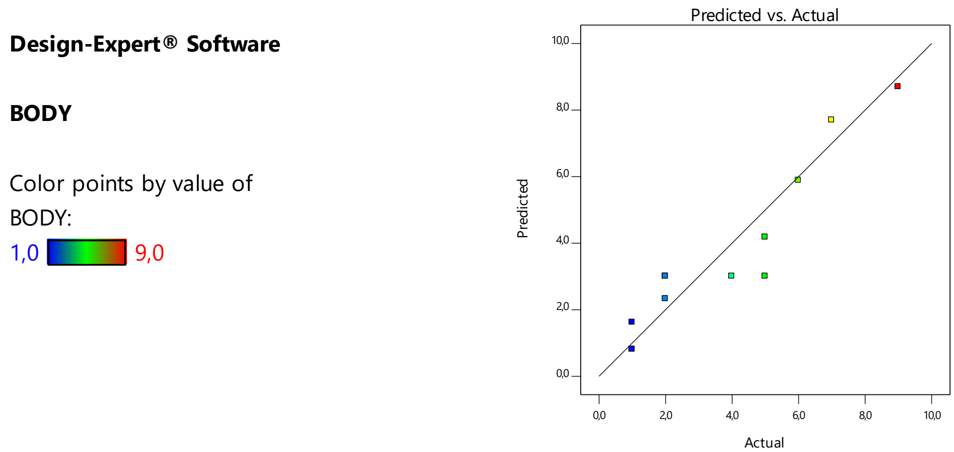


Figure 4.13. Residuals and predicted vs Actual plots from the Castillo coffee Body perception model.

The predicted vs actual plot indicates that the roasted coffee samples obtained with run 1 and run6, have coffee body perception values that is not easily predicted by the model because it is the furthest point from the straight line. This is related possibility to the first batch being affected by the thermal inertia of the roaster when starting the experiments from room to the charge temperature. So, this thermal phenomenon occurs due to the technology of the roasters and their construction materials as previously section mentioned. On the other hand, the body's perception could be biased because the coffee preparations for training saturated the consumers in the first instance. Even so, the model responds significantly to the consumers' description of the attribute. The response surface and contour plots of the coffee body perceived by consumers in the designed experiment are presented in Figure 4.14. The prediction of the coffee body perception value is restricted to the width of the homogeneous contour regions to be found. In this case, only regions that encompass the roasting profiles mentioned above can be seen and can largely predict this perception for high body perception. Contours between 0.8 and 2.9 presents a complex relationship for run2, run3 and run13 to predict a body perception value.

Our results report for first time one of the characteristics of Café de Cauca from consumers perception is its medium body. The values in the range of contour lines 4.2 to 5.9 on the scale of 0-15 points, show the profiles run10 and run9 coffee samples, respectively, to obtain these organoleptic properties. Although this result was expected, it has not been reported to date from a consumer perspective.

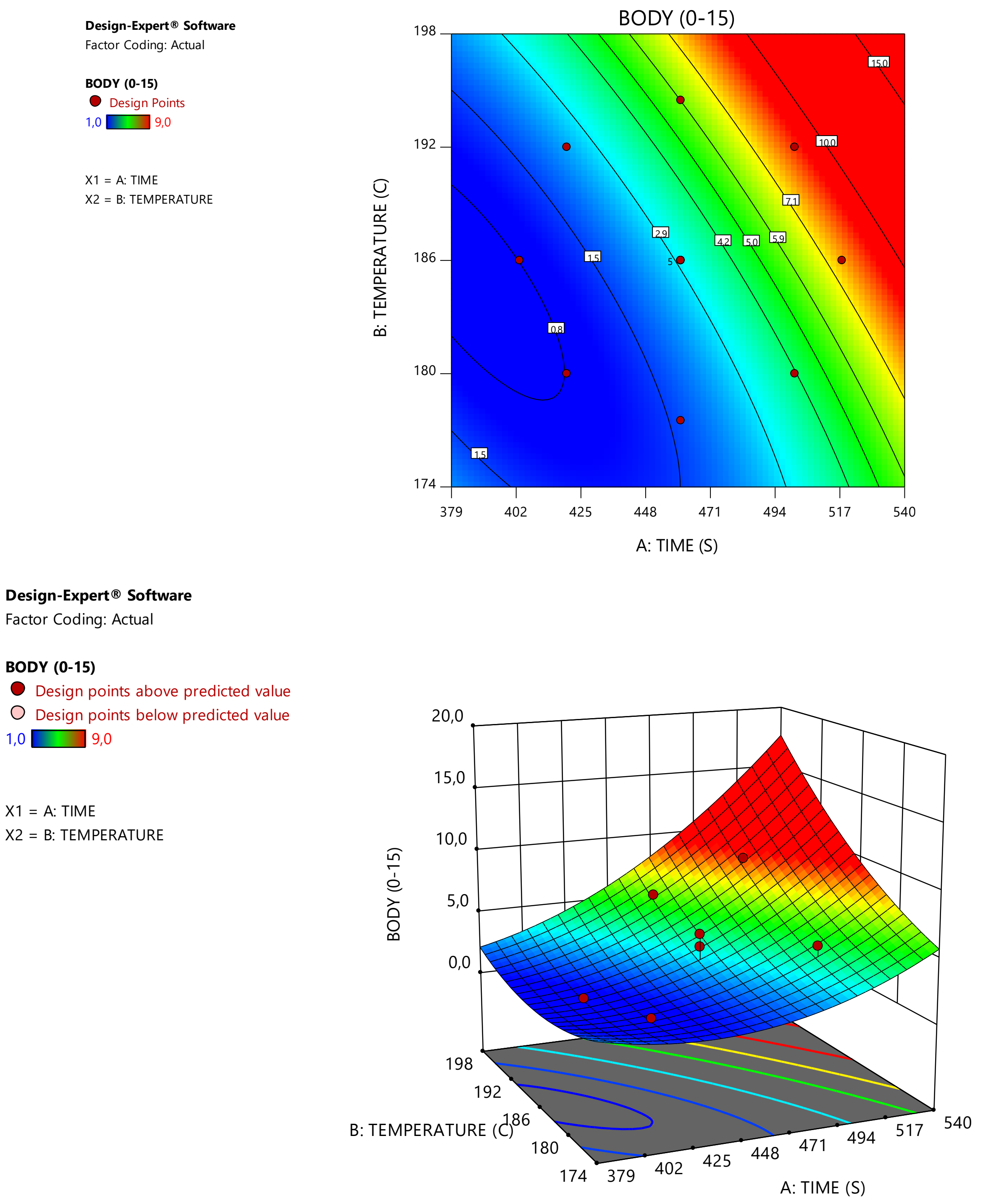


Figure 4.14. Contour plot and response surface for Castillo body perception.

However, our results confirm the effect of moving from an HTST region (curved lines) to an LTLT region where homogeneity of body (straight lines) is appreciated. These results suggest that higher temperatures and longer roasting times should be used in roasting coffee to achieve full-bodied beverages. According to the literature the definition of body is used to indicate the structure of the beverage and corresponds to a certain consistency of coffee that is felt on the mouth (Giacalone et al., 2019; W. Sunarharum et al., 2014). We can explain this affirmation because to the variations in the origin of a coffee, the body of the coffee is mainly affected by the method of elaboration and, at some point, by the degree of roasting. With our results we contribute to report the effect that the modulation of roasting curves has on the perception of coffee body. The French press method, used in the preparation protocol of the beverages of the experiment, contribute to a great extent to generate a frame of reference for consumers to differentiate between the samples and what the body component in Castillo coffee means.

4.2.6. Numerical optimization for Castillo Coffee

The optimal roasting temperature and time were obtained by superimposing the contour plots of the responses. According to section 3.3.2.

The optimization criteria were the maximization of the desirability function D in equation (3.4), for both, acidity, and body perception. Table 4.14 shows the lower (*li*) and upper(ui) for acidity, body, and color perceptions. By default, thresholds will be set at the observed response range.

Table 4.14. Desirability function parameters for Castillo coffee

Attribute	Lower bound (*li*)	Upper bound(*ui*)	Target (*ti*)
Acidity	5 =Slightly intense	9= Intense	maximum
Body	4= slightly intense	8=Moderately intense	maximum
Color	75=Moderately Light	85=Light	NA

li, ui, ti, are the parameters for desirability function.

The lower limit is the lowest acceptable outcome. The upper limit is desired best result. In this case for acidity the selected range was 5 to 9, to validate upper limit close to 10=Intense, and for body from 4 = slightly intense to 8 = moderately intense. These values result, taking into account that it was found that the acidity perceived by the consumer has an inverse relationship with the perception of body (see Figure 4.10), and the fact that the greatest challenge in the roasting process is the balance between the attributes, it is now desired to find an optimum point where, through an optimized roasting curve, the coffee samples are taken to get the best of both, acidity and body, taking into account the mathematical models calculated.

The numerical optimization from desirability function in Castillo samples is presented in Figure 4.15.

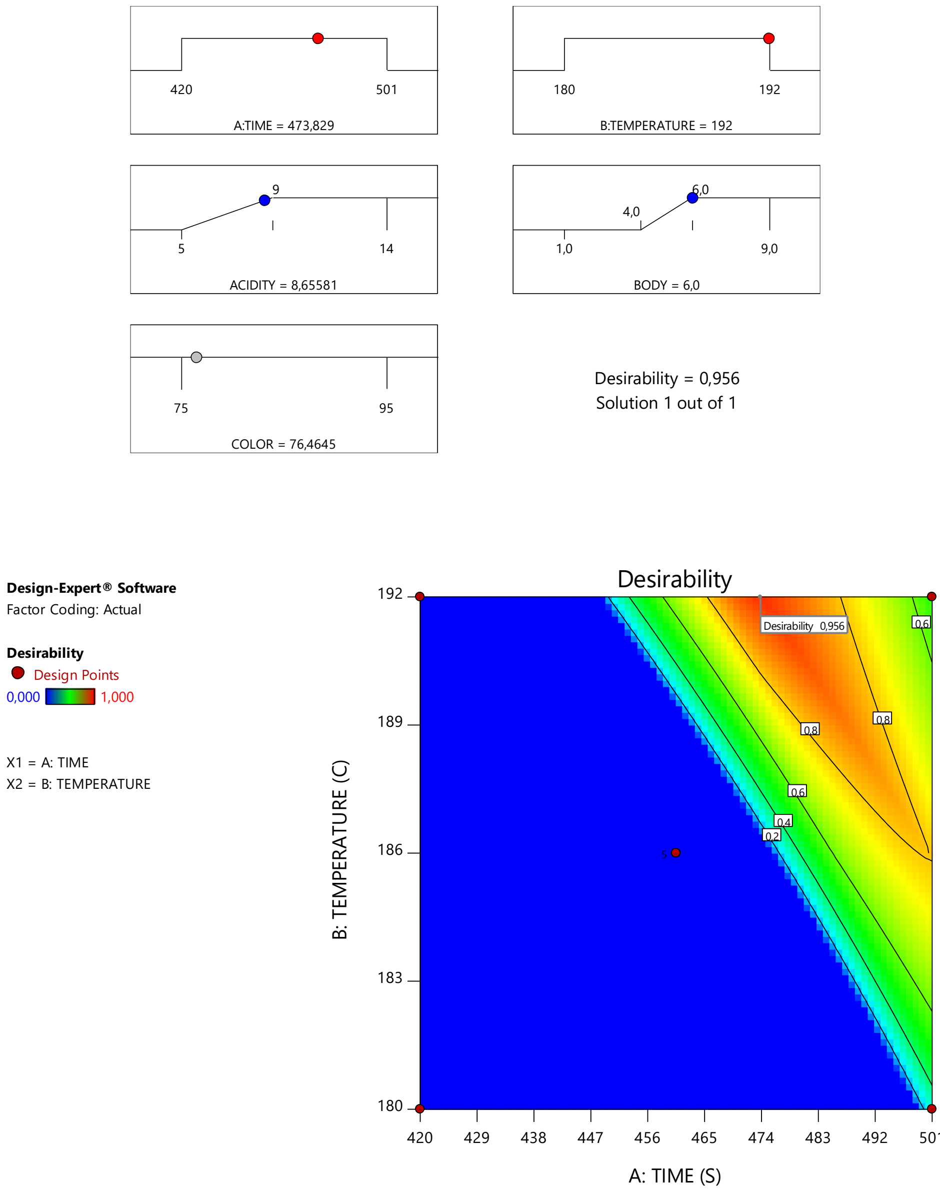


Figure 4.15. Numerical optimization from desirability function for acidity, body and color in Castillo coffee samples.

Previous studies on the optimization of the coffee roasting process were based on the assessment of the chemistry point of view. In this case employing the Derringer's desirability function methodology, the optimum level of the independent variables was obtained focused on consumers perception; in particular, the maximum desirability is predicted to be 95.6% at the roasting time (473 s) and temperature (192°C) optimized conditions, predict an acidity (8.65-moderately intense) and Body (6=Slightly intense) for consumer's perceptions. The color index above 76, can be related with the 75-Moderately light. Color is a measure of the transparency and traceability to compare the coffee bean at optimum roasting stage.

The advantage of the numerical optimization results considering the consumer's perception is to provide a systematic tool to the roaster to avoid the common, trial and error experiments when seeking to obtain the same coffee characteristics, with the desired profile. Numerical optimization linking consumers perception math models, allows to know the roasting time and temperature points, generates a competitive advantage for the roaster to concentrate on a specific point of roasting, which is generally after the first crack, and to achieve a balance between acidity and body.

4.2.7. Graphical optimization for Castillo coffee

The numerical optimization criteria were carried over and then the Design expert software automatically initializes the graphical optimization criteria. Figure 4.16 present the graphical optimization. A region of optimization points was generated to achieve the maximum of acidity and body perceptions with the roasting profiles associated to mathematical models used in this experiment. The contours are plotted at the limits specified by the criteria. One color (bright yellow) defines the acceptable factor settings. Another color (grey) defines the unacceptable factor settings. The numerical optimization solutions (flags) are carried over and displayed in the yellow region of the design points.

The focus of this study was to understand how acidity and body intensity perceived by consumers were integrated with the proposed optimization scheme, in relation to roasting time and temperature modulations. According with (Rao, 2019), one of the common practices of roasters is to look for a late first crack and extend the Maillard phase. By example, the production of melanoidins during the Maillard reaction affects bean color, but also contributes to mouthfeel and body. Therefore, lengthening this phase can contribute to a heavier body without losing the more nuanced flavors of the origin. However, it is not reported how long this process should take or at what range of temperatures.

Our graphical optimization results report that there is no single optimization point where acidity and body are perceived consistently by consumers, but rather a whole yellow region has been found in Figure 4.16.

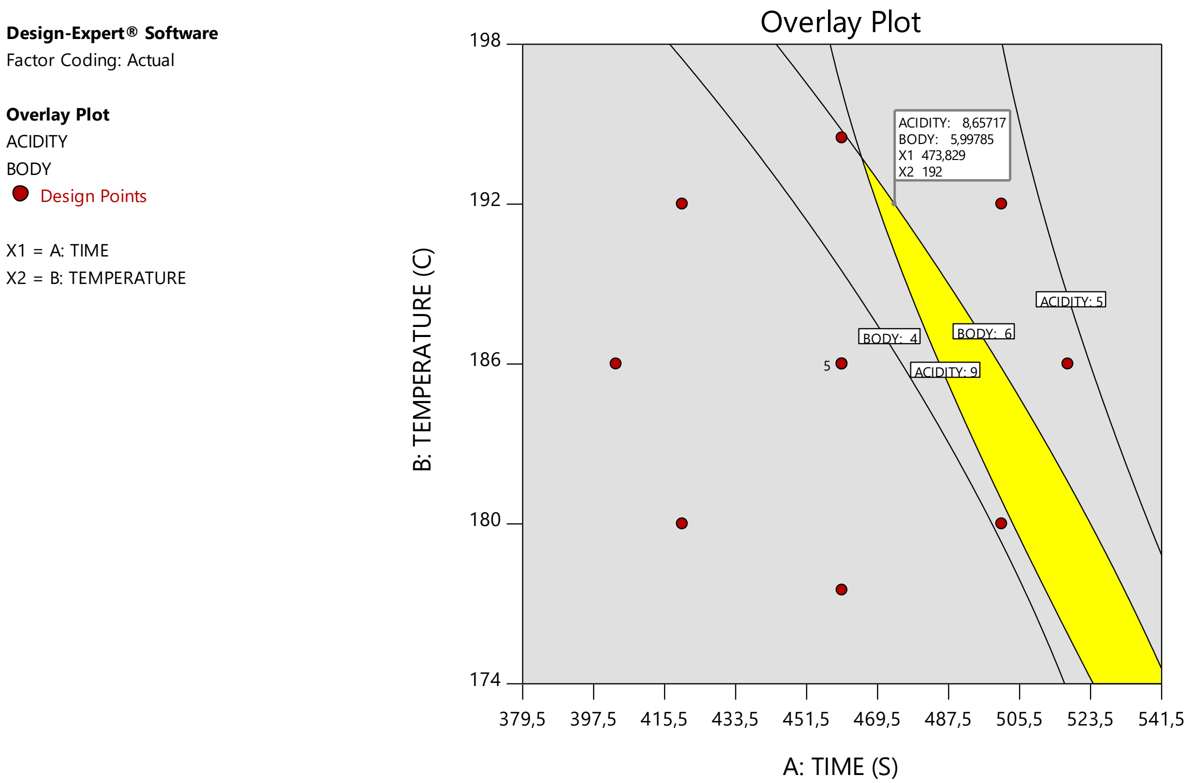


Figure 4.16. Graphical optimization from desirability function for acidity and body in Castillo coffee

This information can be used by roasters to conduct experiments focusing on the optimum roasting region for roasting coffee products with an acidity/body consistency with the desired quality properties of Cauca coffees, especially for the Castillo variety.

Expert SCA scores for Castillo variety samples used in this work are reported in Table A2 of appendix A (36 random Castillo coffee samples were assessment by experts, labeled from c1 to c36 in the dataset) for coffee quality assurance. Although the information contained in this table is not used for comparison purposes, since the experts have a calibrated sensitivity to evaluate the quality of the coffee and the consumers do not (this work introduce only intensity scale), important data can be extracted. One of them is that the coffees evaluated by experts obtained scores >80 points, that means zero primary defects (full black, full sour, dried cherry, fungus damage, foreign matter, and severe insect damage) and less than five secondary defects (partial black, partial sour, parchment, floater, immature or unripe cherries, withered cherries, broken, chipped, or cut beans, and slight insect damage)(SCAA, 2015).This supports the results obtained focused mostly on the modulations of the roasting curves to study the relationship between the perception of acidity and body of the consumers. On the other hand, in terms of acidity and body, we can propose a contribution in that the expert can bring consumers closer to knowing the quality of coffee on the SCA scale and the experts can use the information on intensities from a panel of consumers to complement their mutual awareness.

4.3. Roasting process and perception of acidity, body and color for Tabi coffees

CCD central composite design was adopted to roast the coffee samples considering the same steps following in section 4.2. To study the development region of the coffee bean around central point, the experimental CCD time-temperature points scheme is presented in Figure 4.17. Each point represents the time and final temperature to which the roasted coffee should be taken. The experiments were carried out following section 3.3, using the Tabi variety coffee. The factors detail for CCD design can be seen in Table 4.14.

Table 4.15. Factors for CCD design in Tabi coffee samples

Factor	Name	Units	Type	Minimum	Maximum	Coded Low	Coded High	Mean	Std. Dev.
A	TIME	s	Numeric	523	636	-1 ↔ 540	+1 ↔ 620	580	32.66
B	TEMPERATURE	°C	Numeric	181	203	-1 ↔ 185	+1 ↔ 200	192	6.12

According to roasting experimental setup, batches of 250 g of Tabi Specialty coffee beans were used for conducting the 13 experiments following the experimental design. In this case turning Point was achieved on average for all roasting profiles in 151 s and at a temperature of 76°C. Drying / yellow stage was reached at an average of 289 s and 115 °C of temperature. The first crack has different points of occurrence, due to the CCD experimental approach, as expected. The drop point was achieved according to the experimental design. All coffee samples drop from the roasting drum to be cooled to room temperature in a maximum time of 120 s.

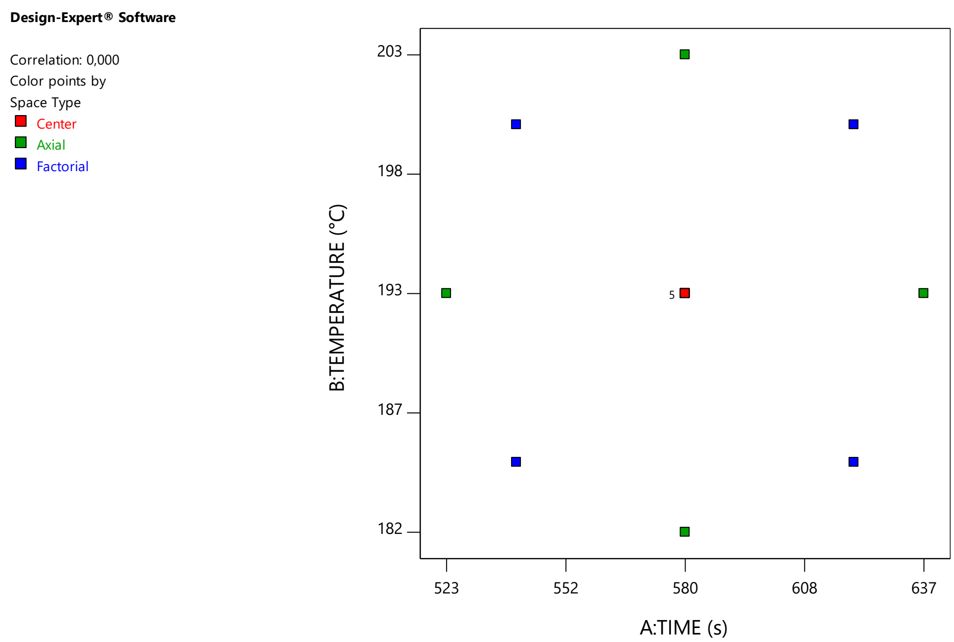


Figure 4.17. CCD design points for Tabi coffee samples. 4 factor points in the corner of cube. 4 axial points out of a cube and 5 central point in the center of design space. Colors means the type of point.

Table 4.16, presents the experimental data for Tabi coffee samples.

Table 4.16. Experimental data from CCD design and the roasting profile points for tabi coffee

Std	Run	Time A: Time s	Temp B: Temp °C	Roasting Profiles Points: Charge Temp °C	Turning Point t(s)	Turning Point T(°C)	Drying or yellow t(s)	Drying or yellow T(°C)	First Crack t(s)	First Crack T(°C)	Drop t(s)	Drop T(°C)
1	1[f]	540	185	178	162	76	305	112	501	172	539	181
5	2[a]	523	193	179	145	76	288	120	474	180	522	191
3	3[f]	540	200	181	143	74	266	109	458	177	539	199
4	4[f]	620	200	181	144	75	279	115	496	178	619	201
9	5[c]	580	193	182	151	77	289	115	477	171	579	192
12	6[c]	580	193	178	159	73	304	113	485	170	582	193
11	7[c]	580	193	182	152	75	280	108	487	171	578	193
8	8[a]	580	203	179	148	72	279	109	493	182	580	203
6	9[a]	637	193	179	151	73	305	119	489	172	636	192
13	10[c]	580	193	181	148	77	274	121	480	174	579	193
7	11[a]	580	182	179	155	78	288	110	473	160	581	181
10	12[c]	580	193	182	161	80	299	114	480	170	578	193
2	13[f]	620	185	179	148	85	298	126	501	173	618	184
			Average	**180**	**151**	**76**	**289**	**115**	-	-	-	-

t: time, T: temperature. Std is the order of run execution. Run is each roasting curve. [c]CCD central points. [f]Factorial points. [a]Axial points. Charge Temp, Turning Point, Dry or yellow, First Crack and Drop are the experimental roasting profiles points.

Temperature Short Time (HTST) profiles are in agreement with (J. S. Cho et al., 2017; Giacalone et al., 2019) and aims to accentuate the acidity and the Low Temperature Long Time (LTLT) for accentuate the body. This data supports the experimental design to propose the relationship between acidity and body from consumer perceptions. Roasting profile curves fulfill the experimental design and propose a relationship between acidity and body from consumer perceptions. Figure 4.18 shows the experimental roasting coffee curves. Figure 4.19 expand the region of interest (ROI) in more detail (400-520 s) for CCD points comparison with experimental points. Here, five points are center points, and 8 points are the star points to estimate curvature in the response surface. Red points indicate the drop time and drop temperature for each of 13 samples from CCD design. Due to the thermal inertia of the roasters, sometimes it was not possible to drop the coffee at the desired time-temperature, so it was necessary to repeated until the designed CCD point was achieved.

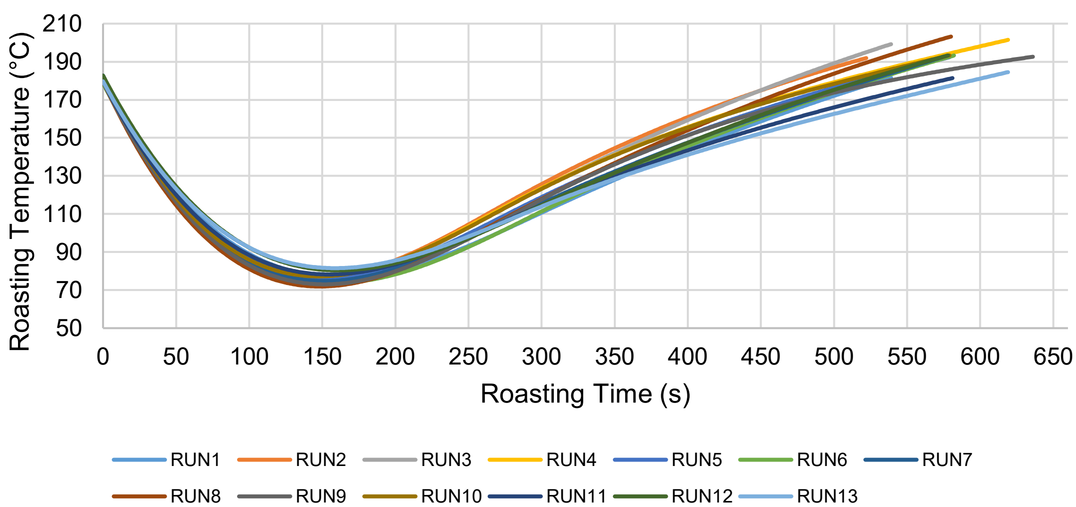


Figure 4.18. Experimental curves from roasting process of Tabi coffee samples.

As mentioned in section 4.2, the results of this CCD-RSM curves are in agreement with (Giacalone et al., 2019; Yu et al., 2018) for arabica coffees, however, the contribution made is also to obtain information on Tabi variety coffees using the consumers' perception of acidity and body as a source of information. Optimizations curves based on perceptions of acidity and body due to untrained coffee consumers have not been reported so far in Tabi Cauca coffee variety, and we report for the first time this scheme using CCD as new tool for quality control of coffee.

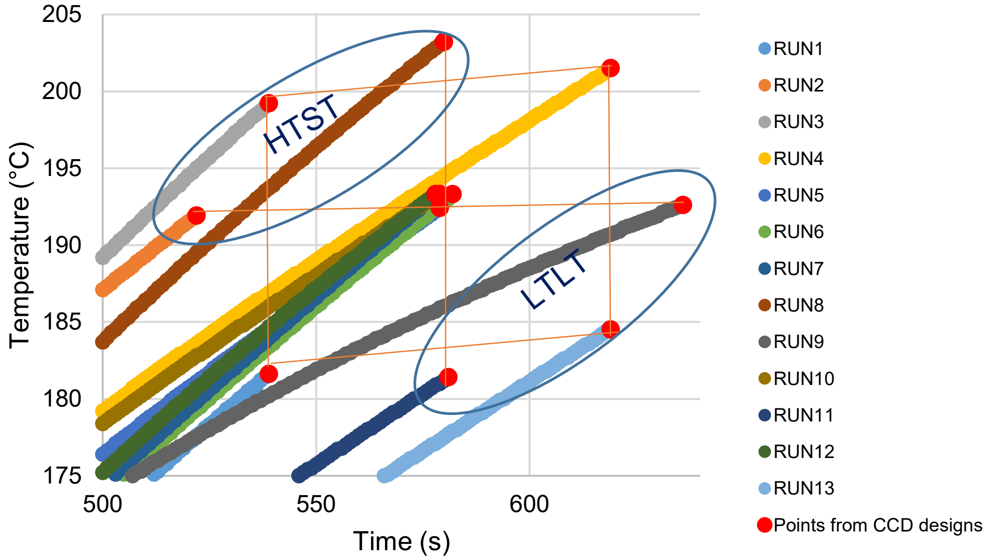


Figure 4.19. Region of interest (ROI) in the experimental Tabi roasting profiles, highlighting the red dots from CCD points.

4.3.1. Correlation analysis between roasting profiles and the perception of acidity and body of Tabi Coffee.

According to 3.2.2 section, 104 coffee consumers participated in the experiment, rating their perception on the intensity scale (0-15) for acidity, body, and color (25-95 SCA color disc reference) in 13 coffee beverages. R1, R2 and R3 were the responses from consumer perceptions. Data collected results in 1372 data. Table 4.16 presents the contingency table after data pre-processing measure of central tendency for the thirteen experimental runs.

Tabla 4.17. Contingency table from consumers' perception of Tabi coffee.

	CONSUMERS PERCEPTION		
RUN	**R1 Acidity 0-15 scale**	**R2 Acidity 0-15 scale**	**R3 Acidity SCA Disc**
1[f]	Intense	Barely detectable	Moderately Light
2[a]	Very intense	Identifiable, but not very intense	Light Medium
3[f]	Intense	Identifiable, but not very intense	Medium
4[f]	Slightly intense	Moderately intense	Medium

5[c]	Intense	Slightly intense	Light Medium
6[c]	Intense	Identifiable, but not very intense	Light Medium
7[c]	Moderately intense	Slightly intense	Light Medium
8[a]	Moderately intense	Slightly intense	Medium
9[a]	Slightly intense	Intense	Light Medium
10[c]	Moderately intense	Slightly intense	Light Medium
11[a]	Intense	Identifiable, but not very intense	Moderately Light
12[c]	Moderately intense	Slightly intense	Light Medium
13[f]	Slightly intense	Slightly intense	Moderately Light

[c] CCD central points. [f] Factorial point. [a] Axial points. R1,R2,R3 median values from 104 consumers perception (0-15 scale) categorical values. Intensity 0-15 scale, 0=none, 2=Barely detectable, 4=Identifiable, but not very intense, 6=Slightly intense, 8=Moderately intense, 10=Intense, 12=Very intense and 15=Extremely intense. Bean Color; 25=Very Dark, 35=Dark, 45=Moderately Dark, 55=Medium, 65=Light Medium, 75=Moderately Light, 85=Light, 95=Very Light

The applied Shapiro wilk normality tests (alpha=0.05) to the data of the response variables revealed that their distribution is non-normal. According to normality test analysis, nonparametric Spearman correlation tests were performed. Figure 4.20 shows the spearman correlation matrix for Time, temperature, acidity, body, and color for Tabi coffee samples.

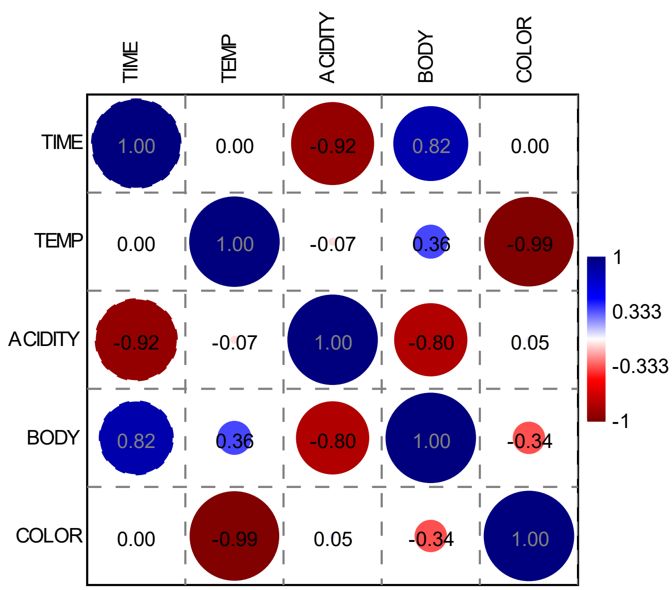
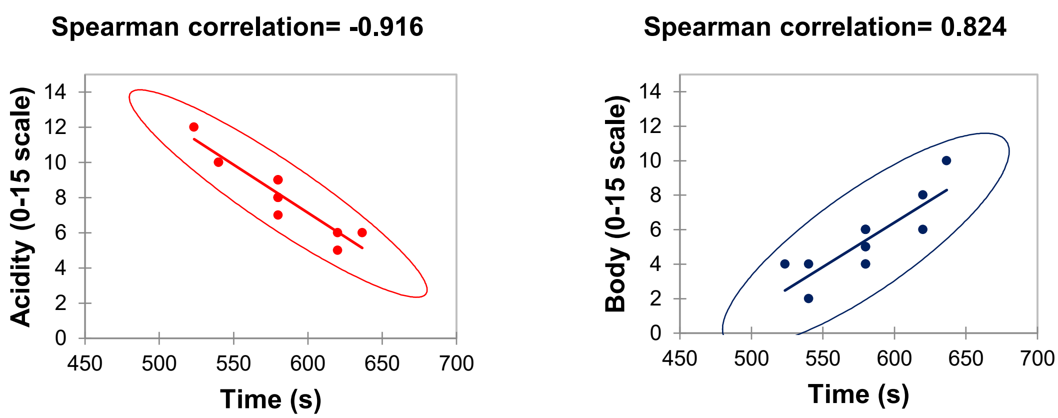


Figure 4.20. Spearman correlation for Tabi roasting profiles.

Results are in agreement with (Barbosa et al., 2019; Osorio & Pabón, 2022), finding that there is low correlation between color-acidity (0.05) and color-body (-0.34) in this samples. These results confirm that, so far, no clear relationship can be found in this experiment. The definition of the color of the coffee bean includes the difficulty that an untrained person has physical and knowledge limitations by the simple visual inspection of these characteristics.

This analysis shows again that the perception of acidity and body can be mainly affected by roasting time. Negative relationship between the perception of acidity and roasting time (-0.92) and the positive relationship between the perception of body and roasting time (0.82) was found. These findings are in agreemente with (Barbosa et al., 2019; W. Sunarharum et al., 2014). The importance of this results are reported in Figure 4.21a. The correlation of perception between acidity and body against the roasting time of the coffee sample has a negative value (above -0.929) indicates a decreasing behavour of the perception of acidity in consumers. In contrast, in Figure 4.21b, the positive correlation (above 0.832) between body and the roasting time shows the increasing of body perception when increasing roasting temperature. This is reported based on consumers perceptions. Although these values are expected, it was not yet clear how they relate to each other, including consumers perception. As strong correlations were found between roasting time and acidity and body, Figure 4.21, present the correlation of perception between acidity and body against the roasting time of the Tabi coffee. These correlations between acidity and body have been reported in tecnhical papers by baristas and professional brewers, but their intensity and shape based on consumer perception have not been shown. Here we demonstrate that from a consumer panel this information can be extracted and used as a basis for decision making by both roasters and experts who want to bring their product closer to consumer preferences and close the knowledge gap in specialty coffees, especially in coffees such as Tabi.



(a) *(b)*

Figure 4.21. Spearman correlation of Tabi coffee roasting time and (a) acidity and (b) body.

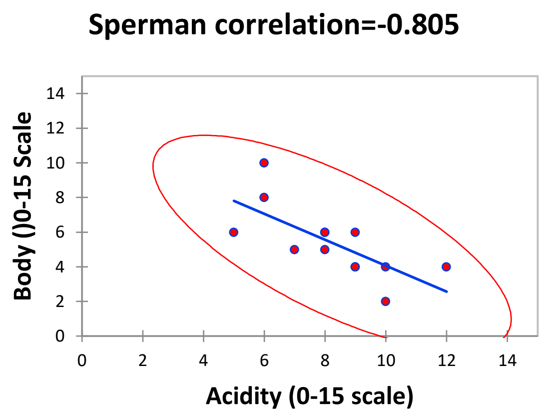


Figure 4.22. Acidity – body spearman correlation from Tabi coffee data

With the aim of representing relationship between acidity and body the Figure 4.24 shows the value and shape the correlation (-0.805). This value represents a link due to the roasting profiles of the acidity-body of Tabi coffee samples, perceived from consumers. In opposite with (Thomas et al., 2017), what has been stated by coffee experts consumers may have the capacity to discriminate cups of tabi coffee, showing that the intensity of acidity is inversely proportional to what they perceive of their body in the cup, in terms of their preference. In evaluating these methods, bridging the gap between the sensory experiences of experts and those of consumers are considered as a new tool.

4.3.2. The Fleiss kappa (κ) from Tabi coffee data

For the contingency data matrix presented in table 4.16, reliability analysis was performed using the Fleiss kappa statistic as inter-rater agreement measure for evaluating the level of agreement between two or more consumers, for acidity, body, and color of coffee samples. Because that the perceptions of coffee consumers are opposed or even lacking in rigor, it is necessary to evaluate the strength of agreement among consumers. Table 4.18, Table 4.19, and Table 4.18, presents the statistical measure for assessing the reliability of agreement between consumers through Fleiss' kappa for acidity, body, and color in Tabi coffee samples.

Table 4.18. Tabi acidity perception between consumers.

Acidity Response	Fleiss' kappa	Standard error	Z	p-value
4=Identifiable, But Not Very Intense	0.671	0.004	177.158	< 0.0001
10=Intense	0.498	0.004	131.410	< 0.0001
8=Moderately Intense	0.406	0.004	107.168	< 0.0001
6=Slightly Intense	0.475	0.004	125.265	< 0.0001
12=Very Intense	0.814	0.004	214.899	< 0.0001
Overall	**0.521**	**0.002**	**248.129**	**< 0.0001**

The agreement and consistency among consumers in relation to acidity is considered moderate (overall (κ)=0.521), considering that these are non-experts, who were only pre-trained on a scale of intensities (0-15) to perceive the acidity attributes. Very Intense acidity was a (κ)=0.814 (Almost perfect agreement Fleiss kappa strength) and for Identifiable, But Not Very Intense acidity perception the (κ)=0.671 (Substantial agreement) may be taken to represent moderate agreement beyond chance.

On the other hand, the reliability assessment of the perception of the body was obtained for the Tabi coffee. Table 4.19 presents the Fleiss kappa to body perception between consumers.

Table 4.19. Tabi Body perception between consumers.

Body Response	Fleiss' kappa	Standard error	Z	p-value
2=Barely Detectable	0.580	0.004	152.954	< 0.0001
4=Identifiable, But Not Very Intense	0.559	0.004	147.456	< 0.0001
10=Intense	0.810	0.004	213.701	< 0.0001
8=Moderately Intense	0.501	0.004	132.076	< 0.0001
6=Slightly Intense	0.519	0.004	136.837	< 0.0001
Overall	**0.564**	**0.002**	**252.489**	**< 0.0001**

According to strength of agreement scale, overall Fleiss' kappa (κ)=0.564, represents a moderate strength of agreement. However, the value of kappa for Intense was (κ)=0.81 that represents substantial strength of agreement. Other body response as Barely Detectable (κ)=0.580, and Identifiable, But Not Very Intense (κ)=0.559, Slightly Intense (κ)=0.519 and Moderately Intense (κ)=0.501, may be considered to represent moderate agreement beyond chance. To this point, from a total of 104*13 dataset for each acidity and body perceptions, Fleiss kappa statistics value for body, is considered a moderate strength of agreement among consumers of Tabi coffee. This result is very important as a tool to evaluate our experimental protocol to perform the data collect protocol, considering the pre-train step for consumers, which offers value to the mathematical model that resulted from the application of CCCD-RSM.

Finally, the reliability test for color perception is shown in Table 4.20. In this case the overall (κ)=0.596 represents moderate agreement beyond chance. This can be shown since controlled lighting conditions were used for color assessment by coffee consumers due to pandemic COVID-19 situation, an illumination control and computer screen presentation of SCA color disc results in Light Medium (κ)=0.497, has moderate agreement between consumers and Medium (κ)=0,640 and moderately Light (κ)=0.686 color values achieve a substantial agreement in the Fleiss kappa. This result is in agreement with the (Bemfeito et al., 2021), when consumers know the information about the type of roasting, by example, they begin to perceive attributes that differentiate special coffees from non-special coffees, and the type of roasting (light or dark), favoring the acceptance of special coffees.

Table 4.20. Tabi beans color perception between consumers - Fleiss' kappa.

Color Response	Fleiss' kappa	Standard error	Z	p-value
65=Light Medium	0.497	0.004	131.201	< 0.0001
55=Medium	0.640	0.004	168.852	< 0.0001
75=Moderately Light	0.686	0.004	181.110	< 0.0001
Overall	**0.596**	**0.003**	**217.343**	**< 0.0001**

As a contribution of this work, we developed a colorimetric device called PICAFÉ, with which we correlated measurements of near infrared spectroscopy -NIR, hyperspectral images and industrial colorimetry in the CIE Lab color space. This device helps both consumers and experts to relate a color measurement with spectral bands that characterize and evaluate the quality of coffee, as proposed in Appendix B.

4.3.3. The Cronbach´s alpha from Tabi coffee data

Table 4.21 shows the Cronbach's alpha statistics for acidity and body consistency in Tabi roasting samples.

Table 4.21. Cronbach's alpha statistics for Tabi acidity and body consistency

Cronbach's alpha	Number of data 13*208 matrix
0.967	2,704

According to Table 4.21, the consumers present CA=0.967 excellent internal consistency when evaluating attributes of acidity and body in 0–15-point scale, meaning that attribute descriptions were homogeneously understood by panelists, pointing to good training. Consumers present adequate CA values on all remaining attributes. We can confirm what was reported by (Pinto et al., 2014), where sensory analysis of coffee requires human perception, and all senses are used to generate an individual (expert) or collective (consumers) ability to detect differences.

4.3.4. Mathematical modeling for acidity from RSM in Tabi coffee samples

According to section 3.3.1, Mathematical model for the factors of time, temperature, and acidity, it is proposed to study the quadratic model (R^2=0.87). These statistics indicate that 87% of the date variability related to the response variable could be explained by the fitted model. This value is a good value to represent for first time this relationship, according with our optimization protocol. Previous studies have reported on the optimization of roasting time and temperature using CCD-RSM models, for the determination of physical characteristics and mostly chemical elements of coffee such as acrylamide, ochratoxin, antioxidant activity with chlorogenic acid, caffeine, total sugar, phenolic compounds, pH, etc. This work extends the findings into consumers' perception acidity for Tabi variety. Adequate Precision for Tabi coffee acidity model was of 10.209 indicates an adequate signal. Then the model has a strong enough signal to be used for optimization. Analysis of variance ANOVA was performed for the proposed quadratic model. This result can be seen in Table 4.22.

Table 4.22**.** ANOVA for ACIDITY Quadratic model -Tabi coffee samples

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	38.75	5	7.75	9.75	0.0047	significant
A-TIME	38.22	1	38.22	48.10	0.0002	
B-TEMPERATURE	0.0214	1	0.0214	0.0270	0.8741	
AB	0.2500	1	0.2500	0.3147	0.5923	
A^2	0.1565	1	0.1565	0.1970	0.6705	
B^2	0.0696	1	0.0696	0.0876	0.7759	
Residual	5.56	7	0.7945			
Lack of Fit	2.76	3	0.9206	1.32	0.3859	not significant
Pure Error	2.80	4	0.7000			
Cor Total	44.31	12				

The model F-value of 9.75 implies that the model is significant. There is only a 0.47% chance that such a large F-value could occur due to noise. The Lack of Fit F-value of 1.32 implies that the lack of Fit is insignificant for the pure error. There is a 38.59% chance a Lack of Fit F-value this large could occur due to noise. The significant lack of fit is good; the model was required to fit the behavior of the acidity data perception. Finally, the estimated coefficients of the quadratic model can be obtained, extracting the terms (AB, A^2, B^2) that allow to explain or predict the perception of acidity from consumers through the time- temperature profiles. Table 4.23 presents these calculations.

Table 4.23. Coefficients in Terms of Coded Factors for coffee acidity perception model

Factor	Coefficient Estimate	df	Standard Error	95% CI Low	95% CI High	VIF
Intercept	8.20	1	0.3986	7.26	9.14	
A-TIME	-2.19	1	0.3151	-2.93	-1.44	1.0000
B-TEMPERATURE	-0.0518	1	0.3151	-0.7970	0.6934	1.0000
AB	0.2500	1	0.4457	-0.8039	1.30	1.0000
A^2	0.1500	1	0.3380	-0.6491	0.9491	1.02
B^2	-0.1000	1	0.3380	-0.8991	0.6991	1.02

DF: degree of freedom. CI: confidence Interval. VIF: variance inflation factor

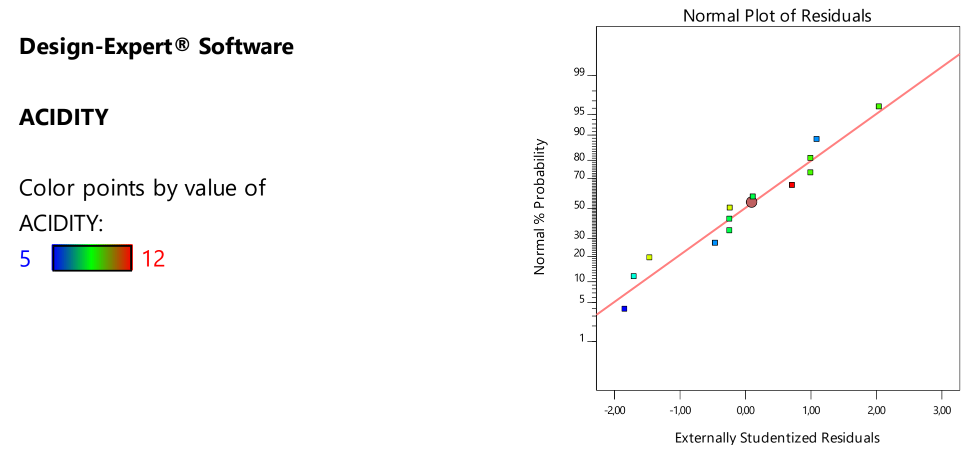
The coefficient estimate represents the expected change in response per unit change in factor value when all remaining factors remain constant. The A-TIME, B-TEMPERATURE, and B^2 is negative, indicating that the probability of acidity perception of coffee increases as time or temperature roasting profile decreases. The intercept in an orthogonal design is the overall average response of all careers. The intercept in coded values is at the center of the design. In real values, the intercept can be, and usually is, far from the design space. When the factors are orthogonal, the VIFs are 1; VIFs greater than 1 indicate multi-collinearity. The higher the VIF occurs with A^2 and B^2, however it is only just 0.02 above 1. Also 95% CI-confidence interval is presented for each factor value.

The equation in terms of coded factors can be used to make predictions about the coffee acidity perception for given levels of each factor (time-temperature profile). By default, high levels of factors are coded as +1, and low levels are coded as -1. The coded equation identifies the relative impact of factors by comparing factor coefficients. On the other hand, the model in terms of real factors is presented in Table 4.24. It can be used to make predictions about the coffee acidity perception for given levels of each factor (time-temperature profiles). Here, the levels must be specified in the original units for each factor: Seconds for TIME factor and Celsius degrees for TEMPERATURE factor. The model in terms of real factors presented in Table 4.23, can be used in practical applications (time-temperature profiles).

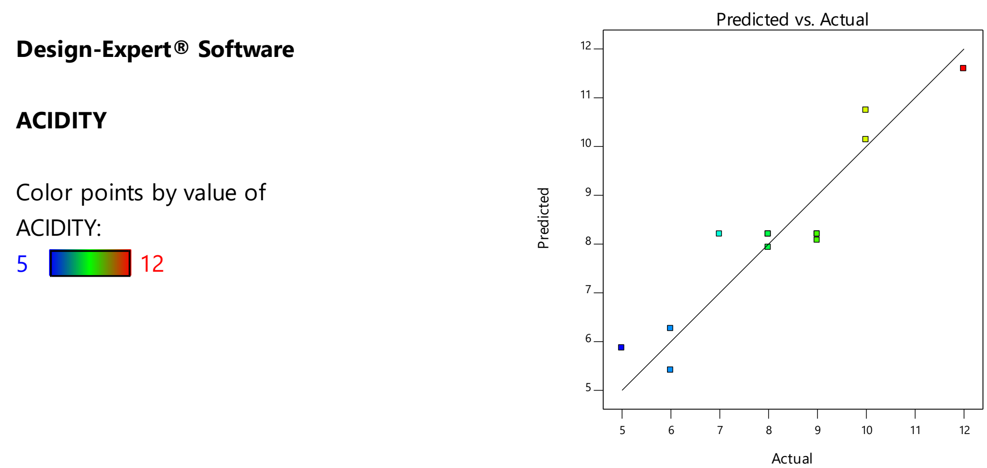
Table 4.24. Final equation for acidity model in terms of actual factors

ACIDITY (Tabi)	=
+99.92240	
-0.323808	TIME
+0.194208	TEMPERATURE
+0.000833	TIME * TEMPERATURE
+0.000094	TIME^2
-0.001778	TEMPERATURE^2

Finally, the study of the residuals and the predicted values were presented in Figure 4.23. The normal probability plot indicates whether the residuals follow a normal distribution, thus follow the straight line. Expect some scatter even with normal data. Predicted vs. Actual is a graph of the predicted response values versus the actual response values. The purpose is to detect a value, or group of values, that are not easily predicted by the model. Experimentally it can be verified that some points are outside the straight line. The furthest away were the coffee samples with the curve run5, run11, run12 and run13. Although the significance level of the model can predict the acidity values in an acceptable range for the experimental conditions.



(a)



(b)

Figure 4.23. (a) Normal plot of residuals and (a) predicted vs. actual plot for acidity model of Tabi samples.

The contour diagram and response surface of the acidity perceived by consumers in the designed experiment are presented in Figure 4.24. Design points are present in the figure with red circle and allows to analyze the predicted perception of acidity from consumers related with the roasting profiles. Contours 10 to 6 can be identified in the design space for predict intensity of acidity from consumers' perception. Contour (12 and 11) are in a curvature in the design space. This result shows that there is a region where consistent acidity and can be achieved as a function of identified time and temperature profiles. Consumer perception of acidity may be affected in a controlled manner by considering the appropriate roasting profiles to accentuate or not this attribute.

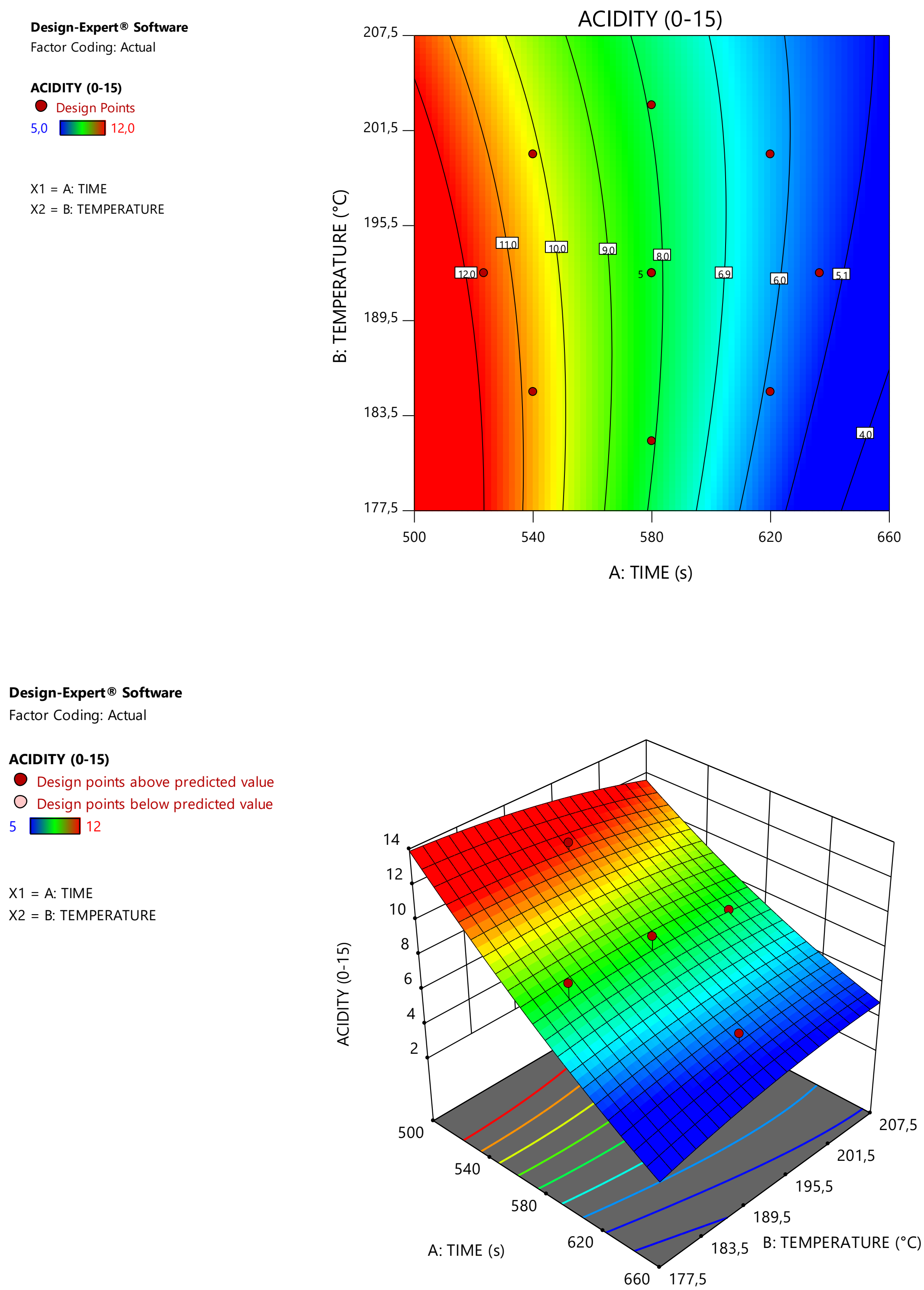


Figure 4.24. Contour plot and response surface for acidity perception in Tabi coffee samples.

This being the first study that involves the perception of consumers on the acidity of specialty coffees from Cauca, our results are the new findings of those reported in the literature, considering both Tabi varieties in the study and consumers perception data. It should be noted that the Tabi variety is planted in some regions of Cauca with special climatic conditions, such as prolonged summers, inadequate rainfall distribution, high sunshine, and where coffee growing is practiced with little technology, characterized by the planting of varieties of this tall size, low planting densities, use of shade or semi-shade, and low fertilizer applications. Perceiving high acidity in this variety represents an interesting finding, because this was not expected, but it is related to an interaction between altitude and shade positively affects the acidity of coffee reported by (Worku et al., 2018). According to contour plot acidity in tabi samples is Soft. It could be said that the acidity of these samples is not as complex as that of the Castillo coffee.

4.3.5. Mathematical modeling for body from RSM in Tabi coffee samples

Likewise, the result for the body consumers' perceptions of the coffee samples was obtained. R^2=0.89, and F-value of 12.34 implies that the model is significant. There is only a 0.23% chance that such a large F-value could occur due to noise. The lack of Fit F-value of 1.05 implies that the lack of adjustment is not significant in relation to the pure error. Table 4.25 presents the ANOVA for Quadratic model in Tabi Coffee body perception.

Table 4.25. ANOVA for Quadratic model in Tabi Coffee body perception

Source	Sum of Squares	df	Mean Square	F-value	p-value	
Model	44.08	5	8.82	12.34	0.0023	significant
A-TIME	33.97	1	33.97	47.55	0.0002	
B-TEMPERATURE	5.83	1	5.83	8.16	0.0245	
AB	0.0000	1	0.0000	0.0000	1.0000	not significant
A^2	2.94	1	2.94	4.11	0.0821	
B^2	0.8522	1	0.8522	1.19	0.3109	
Residual	5.00	7	0.7144			
Lack of Fit	2.20	3	0.7337	1.05	0.4628	not significant
Pure Error	2.80	4	0.7000			
Cor Total	49.08	12				

There is an 46.28% chance that such a large F-value lack of adjustment will occur due to noise. AB factor shows no contribution (0) to model explain. This results in not expected and for this case, coffee body model works as a reduced quadratic model. The coefficient estimate represents the expected change in response per unit change in factor value when all remaining factors are held constant. In all factors it is positive, indicating that the probability that the perception of body in the coffee increases as the TEMPERATURE and TIME of roasting increases. The intercept in an orthogonal design is all the runs' overall average response. The coefficients are adjustments around that average based on the factor settings. When the factors are orthogonal, the VIFs are 1; VIFs greater than 1 indicate multi-collinearity. The higher the VIF occurs with A^2 and B^2, however it is only just 0.02 above 1. Also 95% CI-confidence interval is presented for each factor value.

Table 4.26. Coefficients in terms of coded factors for Tabi coffee body perception model.

Factor	Coefficient Estimate	df	Standard Error	95% CI Low	95% CI High	VIF
Intercept	5.20	1	0.3780	4.31	6.09	
A-TIME	2.06	1	0.2988	1.35	2.77	1.0000
B-TEMPERATURE	0.8536	1	0.2988	0.1469	1.56	1.0000
A^2	0.6500	1	0.3205	-0.1078	1.41	1.02
B^2	-0.3500	1	0.3205	-1.11	0.4078	1.02

The equation in terms of coded factors can be used to make predictions about the coffee body perceptions for given levels of each factor (time-temperature profiles). By default, the high levels of the factors are coded as +1, and the low levels are coded as -1. The coded equation is helpful for identifying the relative impact of the factors by comparing the factor coefficients. The mathematical model from body-Time-Temperature relationship is presented in Table 4.27

Table 4.27. Final equation for coffee body perception in terms of actual factors

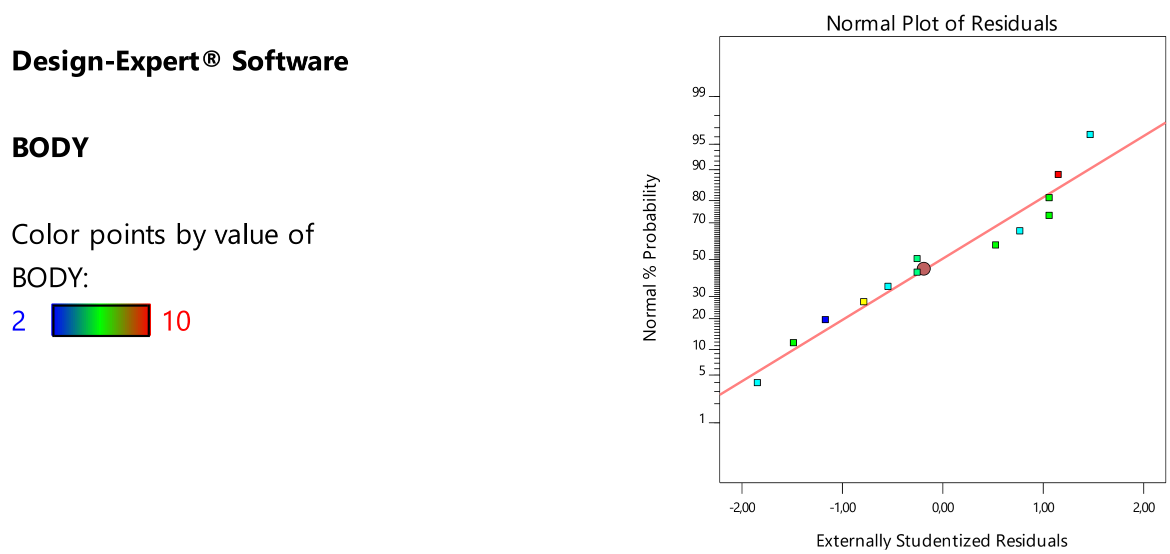
BODY (Tabi)	=
-140.49717	
-0.419733	TIME
+2.50936	TEMPERATURE
+0.000406	$TIME^2$
-0.006222	$TEMPERATURE^2$

Here, body present the final equation in terms of actual factors.

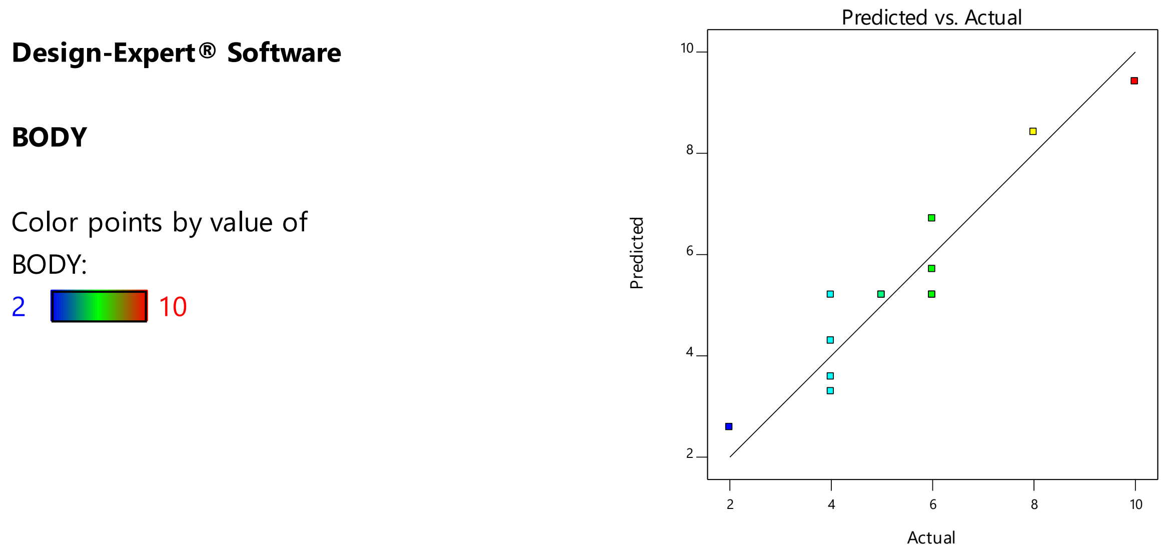
The actual factor model can be used in practical applications (real time-temperature profiles). Here, the levels should be specified in the original units for each factor. Seconds for TIME and Celsius degrees for TEMPERATURE.

In Figure 4.25, the study of residuals and predicted values for coffee body perception is presented. The normal probability plot indicates whether the residuals follow a normal distribution. The relationship is approximately linear except for a few data points.

Roasting profile 11 (run 11) presents the greatest distance from the normality line. The predicted vs actual plot indicates that the roasted coffee samples obtained with run 6 and run 11, have coffee body perception values that is not easily predicted by the model because it is the furthest point from the straight line. Even so, the model is significant and can be used to show the relationship between the body of the coffee, its roasting curve and the consumer's perception.



(a)



(b)

Figure 4.25. (a) Normal plot of residuals and (a) predicted vs. actual plot for body model of Tabi samples.

The response surface and contour plots of the coffee body perceived by consumers in the designed experiment are presented in Figure 4.26. The design points are present in the figure with red points and allows to analyze the predicted perception of body from consumers related with the roasting profiles.

One of the characteristics of Cauca coffee is its medium-low body, thus, from the Figure 4.26. The values in the range of 4 - 6 on the scale of 0-15 points, show the profiles 10 and 9 (design points) respectively, to obtain these organoleptic properties. The prediction of the coffee body perception value is restricted to the width of the homogeneous contour regions to be found. In this case, only regions that encompass the roasting profiles mentioned above can be seen and can largely predict this perception. Contour lines between 6 to 8 show a confidence area in the design space to predict body perception. Contours 2 and 4 present a complex behavior sensible to time-temperature changes.

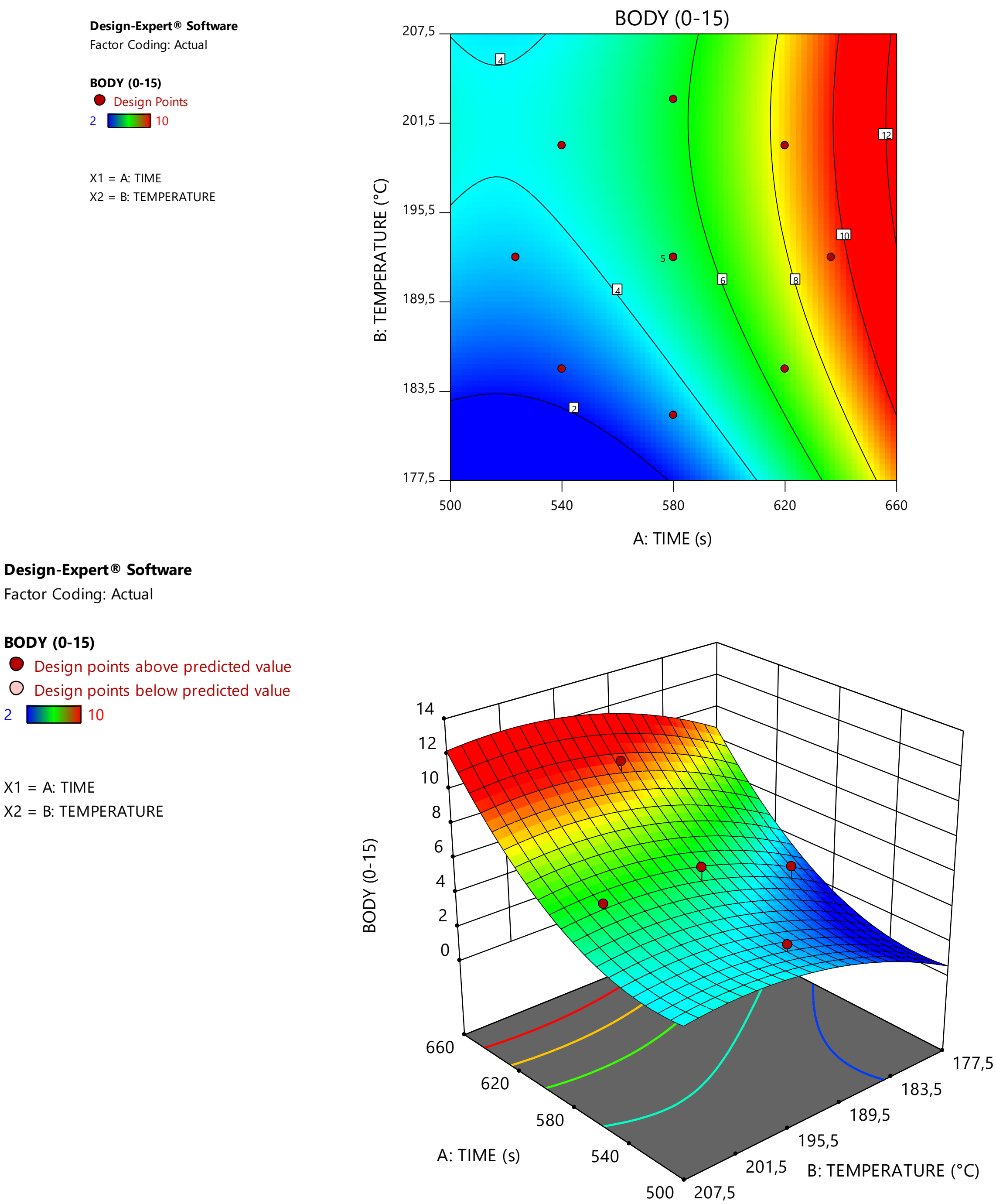


Figure 4.26. Contour plot and response surface for Tabi coffee body perception.

4.3.6. Numerical optimization for Tabi coffee

The numerical optimization from desirability function for acidity and body perception of Tabi coffee Samples was performed. The optimization criteria were the maximize desirability function D, for both, acidity, and body perception. Selecting the maximize from the results as present in Figure 4.27.

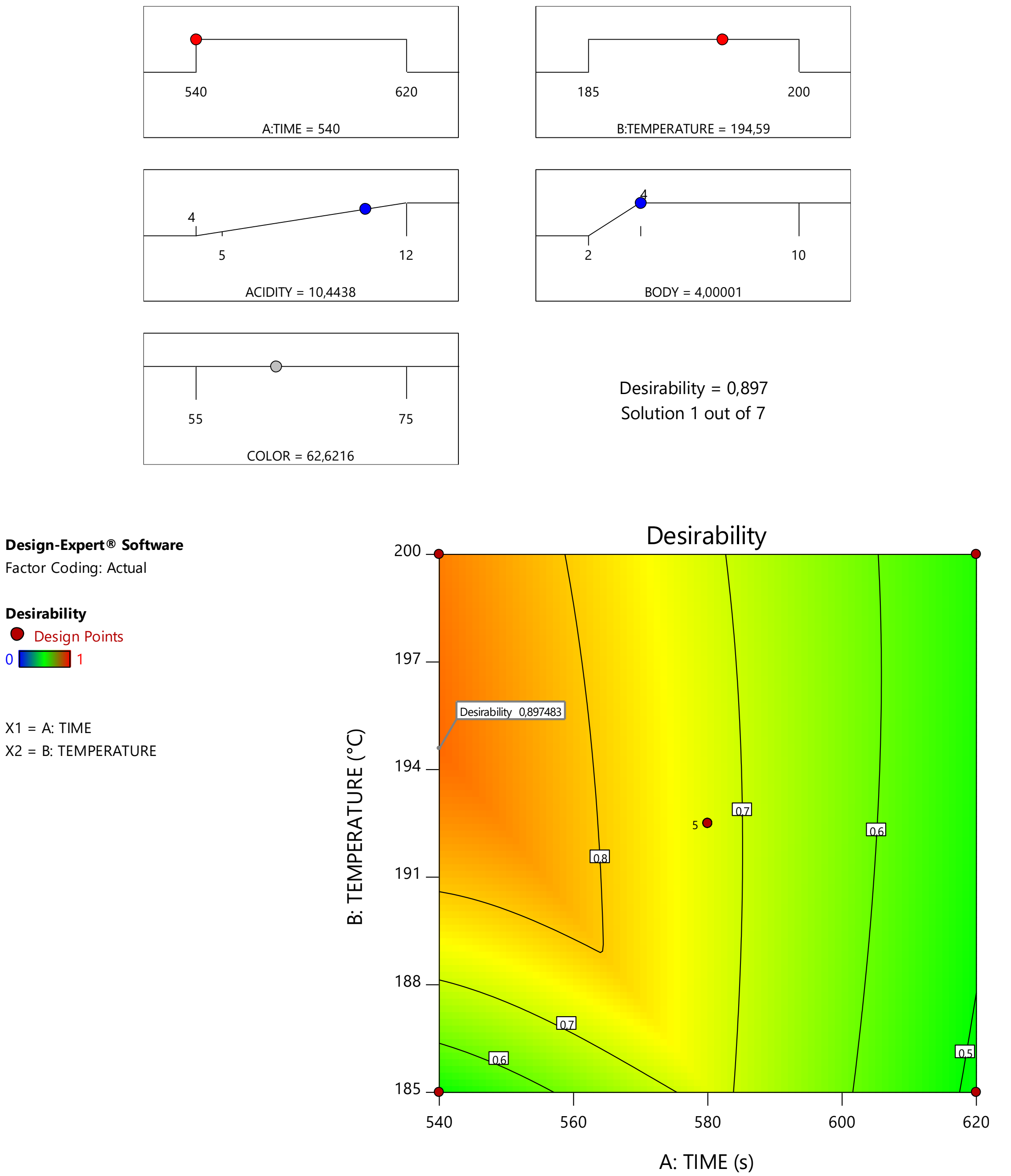


Figure 4.27. Numerical optimization from desirability function for acidity, body, and color in Tabi coffee samples.

Table 4.28 shows the lower (*li*) and upper(ui) for acidity, body, and color perceptions. By default, thresholds will be set at the observed response range.

Table 4.28. Desirability function parameters for Tabi coffee

Attribute	Lower bound (*li*)	Upper bound(*ui*)	Target (*ti*)
Acidity	4=identifiable, but not very intense	12=very intense	maximum
Body	2=Barely detectable	4=identifiable, but not very intense	maximum
Color	55=Medium	75=Moderately Light	NA

li, ui, ti, are the parameters for desirability function.

The lower limit is the lowest acceptable outcome. The upper limit is desired best result. In these results, the roasting time (540 s) and temperature(195°C) optimized conditions, predict an acidity (10-intense) and Body (4= Identifiable but not very intense) for consumers' perceptions. The color index of 62-Light Medium is a measure of the transparency and traceability for the roasting process. we report optimization results for the first time and will be the basis for roasters with the Tabi variety, which in practical work is difficult to enhance because of the related agronomic relationships and possible benefits to be made to the bean, such as fermentation.

Modulated acidity could be a very interesting topic in coffees of this type, and according to (L W Lee et al., 2015) as they could be more appreciated by consumers who see high acidity as a defect or prefer their beverage to be smooth without bright expressions such as those presented here.

4.3.7. Graphical optimization for Tabi Coffee

Figure 4.28 shows the graphical optimization. A region of optimization points was generated to achieve the maximum of acidity and body perceptions with the roasting profiles associated to mathematical models used in this experiment. The contours are plotted at the limits specified by the criteria.

One color (bright yellow) defines the acceptable factor settings. Another color (grey) defines the unacceptable factor settings. The numerical optimization solutions (flags) are carried over and displayed in the yellow region of the design points. run1, run2 and run11, are in the yellow optimization area.

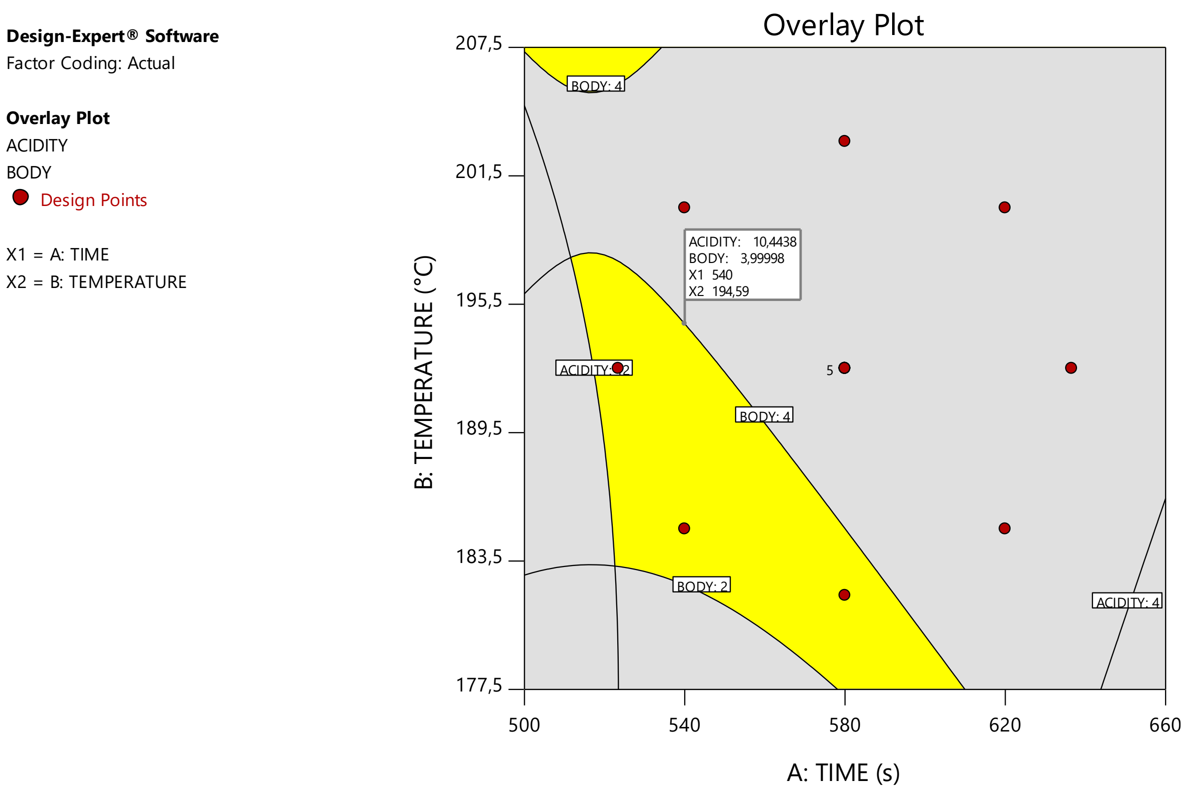


Figure 4.28. Graphical optimization from numerical criteria for tabi coffee samples

Unexpectedly, the region of optimization for the tabi variety is in the region of low roasting time and temperature profiles. This result could be related to the modulation in both acidity and body, in the optimization scheme, perhaps showing its complexity for the acceptance of consumers, being an exotic coffee as reported in (Echeverri-Giraldo et al., 2020; Osorio & Pabón, 2022), confirm that the interaction of the initial roasting temperature and the variety had an effect on the total process time, while the sensory attributes fragrance/aroma, flavor, and total score have an effect only due to the variety.

Variety effects could be confirmed according to the expert SCA scores for Tabi variety samples used in this work are reported in Table A2 of appendix A (36 random Tabi coffee samples were assessment by experts, labeled from T1 to T36 in the dataset) for coffee quality assurance. A score >80 is detailed on the SCA specialty coffee scale, the same as in the Castillo variety, however the production characteristics of this variety are traditional and it stands out because its fruits are full of sugars that are reflected in the final beverage (Echeverri-Giraldo et al., 2020; Farfán Valencia et al., 2000; Osorio & Pabón, 2022). If we compare the maximum score obtained by this Tabi variety, it was 88.8 (sample t27) describing notes of caramel and hazelnut, compared to the Castillo variety, whose sample with the highest score was 87.3 in the SCA protocol (sample c14), with notes of chocolate, red fruits, hazelnut. This information may be related to optimization region of Figure 4.28, since the tabi variety, as it contains a greater number of sugars. The optimized roasting curve configures its best performance at low roasting times and temperatures, since the Sugars in the Maillard reaction process are more likely to scorched in LTLT profiles, and both, the consumer and expert can perceive this defect.

4.4. Sensory characterization with consumers

According to section 3.4, CATA (check-all-that-apply) method provides information about confirm experiments both, Castillo and Tabi coffee brews preparing with optimized conditions from section 4.2.7 and 4.3.7, evaluating specific attributes such coffee acidity (acidity, sweet and salty) and, body (light, medium, heavy), using descriptors and grouping the information to facilitate analysis through the CLUSCATA algorithm, and penalty analysis.

4.4.1. CATA data validation

Once the consumer assessment data are available, the first step of the automated analysis is the creation of a contingency table. A contingency table displays frequencies for the categorical variables. Check or not-checked descriptor in CATA surveys. Table 4.29 presents the contingency table built from CATA data.

Table 4.29. Contingency table built from CATA data.

Dimensions /Products	CASTILLO1	CASTILLO2	CASTILLO3	IDEAL	TABI1	TABI2	TABI3
Lime	30	26	27	21	4	2	1
Tangerine	11	28	5	24	32	35	30
Orange	26	34	23	22	8	30	22
Blueberries	3	3	9	0	28	16	22
Green banana	**0**	**0**	**0**	**0**	**0**	**0**	**0**
Grapes	**0**	**0**	**0**	**0**	**0**	**0**	**0**
Thin	8	7	9	0	34	34	30

Syrup	32	33	30	39	6	6	10
Buttery	1	4	3	1	0	0	0
Bitter	17	21	16	0	14	18	17
Panela	13	14	18	31	18	18	22
Pineapple	**0**	**0**	**0**	**0**	**0**	**0**	**0**
Green apple	**0**	**0**	**0**	**0**	**0**	**0**	**0**
Cinnamon	2	0	0	22	4	16	12
Scorched	2	2	4	0	2	3	0
Red fruits	0	0	0	5	2	3	2
Chocolate	1	0	0	14	15	11	11

Optimized samples of Castillo coffee: CASTILLO1, CASTILLO2, CASTILLO3. Optimized samples of Tabi coffee TABI1, TABI2, TABI3. IDEAL asked to check all the terms they considered appropriate to describe their ideal product.

According to Table 4.29, green banana, grapes, pineapple, and green banana attributes were not selected by any assessor, therefore it can be said that it was not perceived by consumers. For all the other attributes, independence between the rows and columns was evaluated. As the p-value ($p<0.0001$) is lower than the significance level (0.05) the conclusion is that it is highly likely that real differences exist between the products in terms of their sensory profiles. Considering test of independent results, validation of CATA data through lower and upper bounds explores the percentage of checked attributes (Coffee acidity and body descriptors) for each assessor. Figure 4.29 presents these results. All the results were in the acceptable bounds, and the CATA analysis can be performed with the (240x240)x(18) dataset.

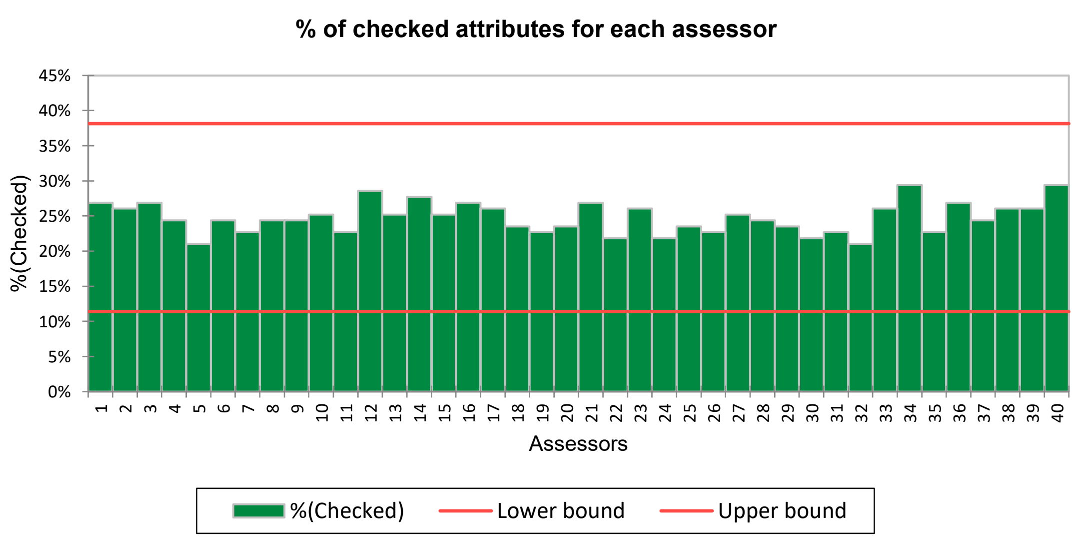


Figure 4.29. CATA validate data - % of checked attributes for each assessor.

In the same way, CATA data validation shows the lower and upper bounds to accept the CATA dataset for attributes (the coffee acidity and body descriptors). Figure 4.30, presents the percentage of checked for each attribute.

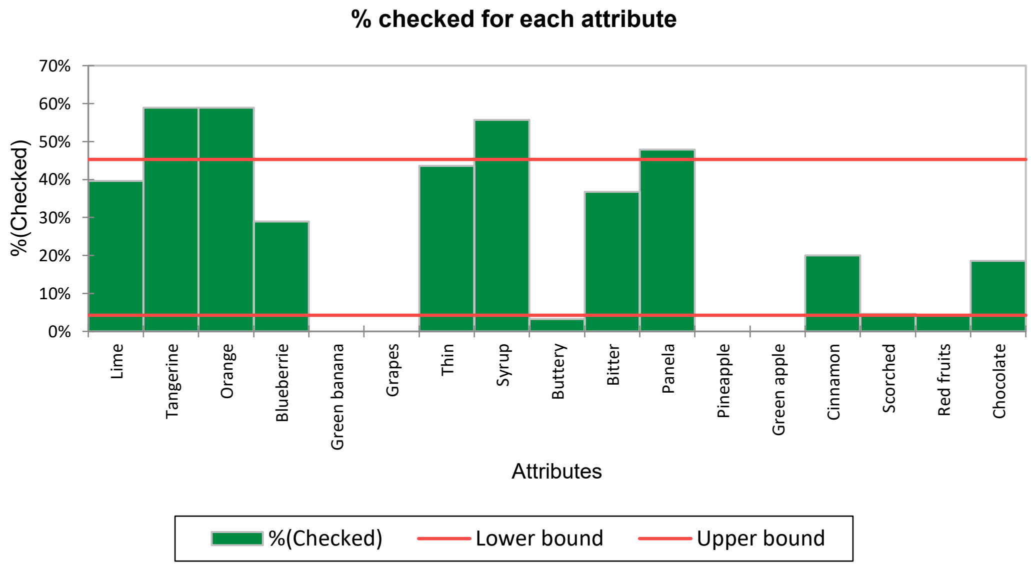


Figure 4.30. CATA validate data - % of checked for each attribute.

All attributes between the bounds are acceptable for the CATA analysis. Buttery is an out of lower bound attribute and Scorched and Red fruits attributes were in the limit of acceptable attributes.

Finally, one interesting graphical tool is the percentage of checked for each assessor and each attribute. In Figure 4.31, the consolidated information is displayed through colored segments in groups of 0-20, 20-40, 40-50, 50-60, 60-80, and 80-100%. This figure can be used for qualitative analysis, in fact, to define the proposal IDEAL coffee sample that should have the most checked attributes to perform the penalty analysis. According with (Llobell et al., 2019), this strategy encompasses the assessment of the agreement among the respondents at a global level and for each attribute considered separately.

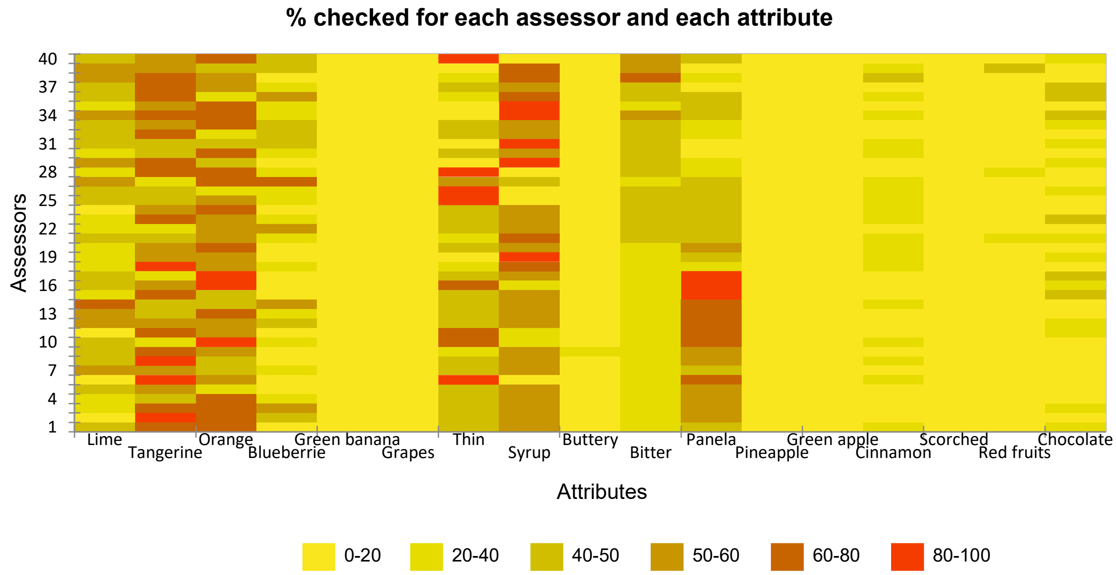


Figure 4.31. CATA validate data. % checked for each assessor and each attribute.

In this work, a set of acidity and body descriptors were included for the first time to expand the knowledge of the optimized configurations achieved for the Castillo and Tabi varieties.

4.4.2. Cochran's Q test

After validating the data, Cochran's Q non-parametric test was performed on the data associated to each attribute to assess whether these attributes were discriminant. Significant differences ($p < 0.05$) in the frequency of terms of the CATA question were used to describe the Coffee samples, suggesting that consumers perceived differences in the sensory characteristics of the evaluated coffee brewing's.

All the attributes that turned out to be discriminant have p-values<0.0001. Other attributes (p-values>=1) can be considered to remove (Green banana, grapes, pineapple, and green apple). Even though buttery, bitter, panela, and scorched were 0.0001<p-values<0.787 were include in CATA ANALYSIS. Table 4.30 presents the Cochran's Q test.

Table 4.30. Cochran's Q test for each attribute in sensory characterization of optimized samples of Castillo and Tabi

Attributes	p-values
Lime	<0.0001
Tangerine	<0.0001
Orange	<0.0001
Blueberries	<0.0001
Green banana	**1.000**
Grapes	**1.000**
Thin	<0.0001
Syrup	<0.0001
Buttery	0.042
Bitter	0.787
Panela	0.364
Pineapple	**1.000**
Green apple	**1.000**
Cinnamon	<0.0001
Scorched	0.538
Red fruits	0.155
Chocolate	<0.0001

Considering the significant attributes, the next step was examining multiple pairwise comparisons using the critical difference (Sheskin) procedure. Table 4.31, shows the calculations, represented by small letters inside table cells. Two products sharing the same letter(s) don´t differ significantly. Two products having no letter in common differ significantly.

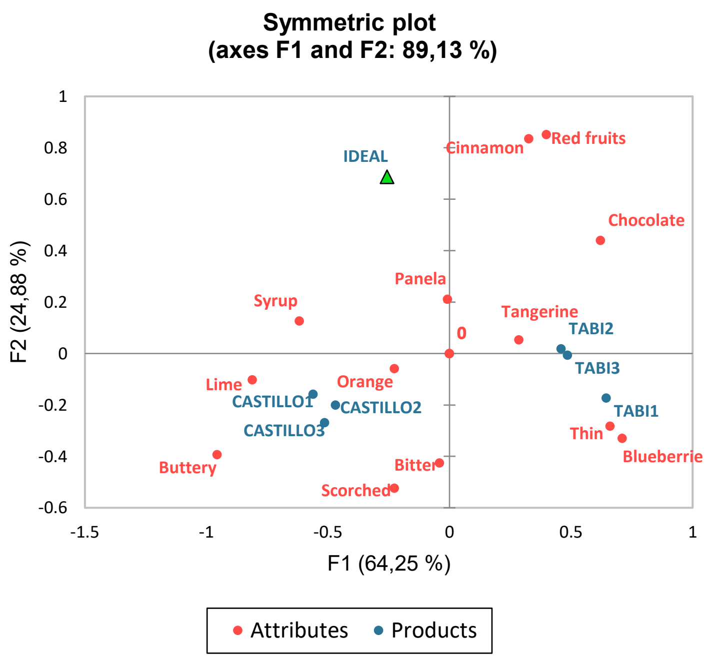
Table 4.31. Multiple pairwise comparisons from critical difference (Sheskin)

Attributes	CASTILLO1	CASTILLO2	CASTILLO3	TABI1	TABI2	TABI3
Lime	0.750 (b)	0.650 (b)	0.675 (b)	0.100 (a)	0.050 (a)	0.025 (a)
Tangerine	0.275 (a)	0.700 (b)	0.125 (a)	0.800 (b)	0.875 (b)	0.750 (b)
Orange	0.650 (b)	0.850 (b)	0.575 (b)	0.200 (a)	0.750 (b)	0.550 (b)
Blueberries	0.075 (a)	0.075 (a)	0.225 (ab)	0.700 (c)	0.400 (bc)	0.550 (c)
Thin	0.200 (a)	0.175 (a)	0.225 (a)	0.850 (b)	0.850 (b)	0.750 (b)
Syrup	0.800 (b)	0.825 (b)	0.750 (b)	0.150 (a)	0.150 (a)	0.250 (a)
Buttery	0.025 (a)	0.100 (a)	0.075 (a)	0 (a)	0 (a)	0 (a)

Bitter	0.425 (a)	0.525 (a)	0.400 (a)	0.350 (a)	0.450 (a)	0.425 (a)
Panela	0.325 (a)	0.350 (a)	0.450 (a)	0.450 (a)	0.450 (a)	0.550 (a)
Cinnamon	0.050 (a)	0 (a)	0 (a)	0.100 (ab)	0.400 (c)	0.300 (bc)
Scorched	0.050 (a)	0.050 (a)	0.100 (a)	0.050 (a)	0.075 (a)	0 (a)
Red fruits	0 (a)	0 (a)	0 (a)	0.050 (a)	0.075 (a)	0.050 (a)
Chocolate	0.025 (a)	0 (a)	0 (a)	0.375 (b)	0.275 (b)	0.275 (b)

From Table 4.31, both CASTILLO and TABI samples differs significantly with the orange and tangerine acidity attributes. It means the assessors could not differentiate the coffees from each other using these descriptors but were able to differentiate the Tabi and Castillo coffees with the attributes of lime, Blueberries for acidity descriptor and with thin and syrup for body descriptors. Buttery, Bitter, Panela Scorched and red fruits although cannot differentiate between samples, were a transversal checked attributes in Castillo and Tabi consumers' perception. Cinnamon and chocolate descriptor may be used to discriminate coffees and to provide the differentiating character of the beverage. Considering the contingency table, the Symmetric plot shows the correspondence analysis (CA) for coffee samples and the descriptors validated for the consumers. Figure 4.32, presents the symmetric plot for CATA data.

It may be observed that consumers have been able to discriminate between the attributes of Tabi coffees versus Castillo coffees. Tabi coffee is framed in the right plane of Figure 4.32, where the attributes of tangerine and blueberries for acidity descriptor, and the attribute of light body (Thin) were present. Also, Chocolate descriptor was present in Tabi area. On the other hand, Castillo coffees, was found on the left side of the symmetric plot, together with the attributes orange and lime, acidity descriptors, and the attribute of medium body (syrup). Panela and bitter attributes were in both, Tabi, and Castillo coffees. Scorched attribute was more associated with Castillo samples. IDEAL product is close to cinnamon and red fruits descriptor. Test of independence of the attributes, run for each product shows CASTILLO1, CASTILLO2 and TABI2 with a strong link according to consumers.



Test of independence of the attributes, run for each product:

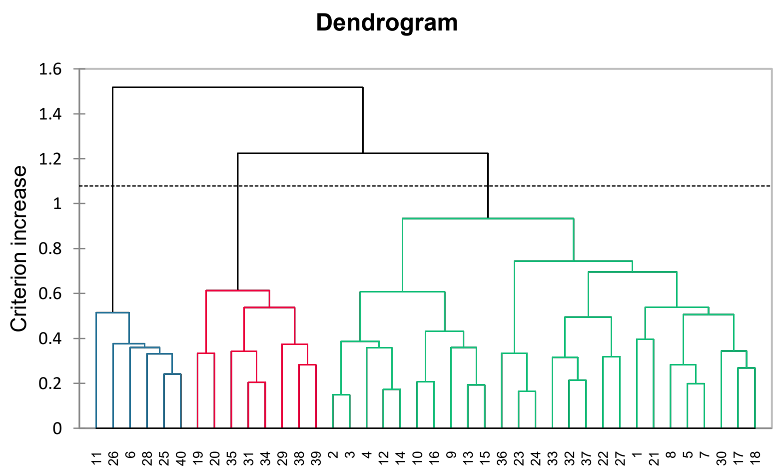
Products	p-values
CASTILLO1	**1.000**
CASTILLO2	<0.0001
CASTILLO3	**1.000**
IDEAL	<0.0001
TABI1	<0.0001
TABI2	**1.000**
TABI3	<0.0001

Figure 4.32. Symetric plot for CATA data in CASTILLO and TABI optimized confirmation experiments

4.4.3. CLUSCATA

For assessment purposes, CLUSCATA analysis was conducted based on the product space created by correspondence analysis (CA) of the CATA attributes selected by the consumers that varied significantly among the coffees, determined by Cochran's Q Test. This result is in agreement with (Bemfeito et al., 2021), in the CATA test, when consumers receive information about coffees, in terms of acidity and body descriptors, they evaluated these products more closely, demonstrating that sensory analysis is a multisensory experience, which also takes sensory memory into account. The new experience and the decoding and breakdown of concepts such as acid, which is generalized in a coffee, but which expands into two more edges in combination with salty and sweet.

Figure 4.33, shows the first step of CLUSCATA, the hierarchical algorithm to obtain a dendrogram. Three classes were obtained from this algorithm. Cluster 1 has 6 assessors, Cluster 2 has 7 assessors, Cluster 3 has 21 assessors. k+1 Cluster has 6 assessors with 0.737 Rho parameter.



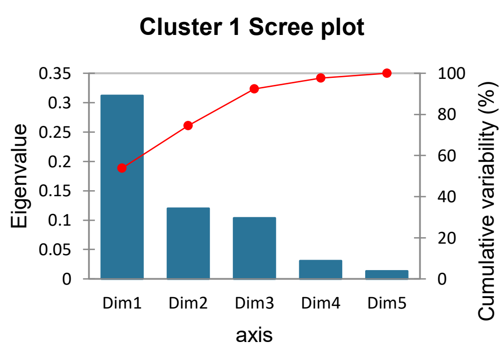
Number of assessors per cluster:

	Value
Cluster 1	6
Cluster 2	7
Cluster 3	21
K+1 cluster	6

Threshold for the noise cluster K+1 (Computed Rho parameter:0,737)

Figure 4.33. Dendrogram given by the CLUSCATA technique.

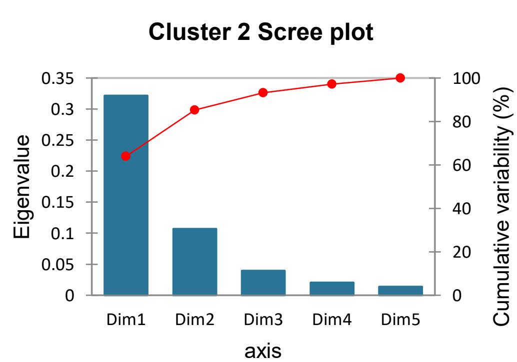
The quality of the analysis can be evaluated by consulting the eigenvalues or the corresponding scree plot, Figure 4.34.



Eigenvalues and percentages of inertia:

	Dim1	Dim2
Eigenvalue	0.312	0.120
Variability %	53.838	20.682
Cumulative %	53.838	74.520

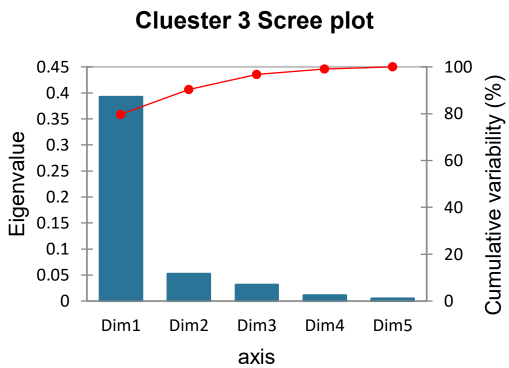
(a)



Eigenvalues and percentages of inertia:

	Dim1	Dim2
Eigenvalue	0.322	0.107
Variability %	63.957	21.293
Cumulative %	63.957	85.250

(b)



Eigenvalues and percentages of inertia:

	Dim1	Dim2
Eigenvalue	0.392	0.052
Variability %	79.749	10.617
Cumulative %	79.749	90.366

(c)

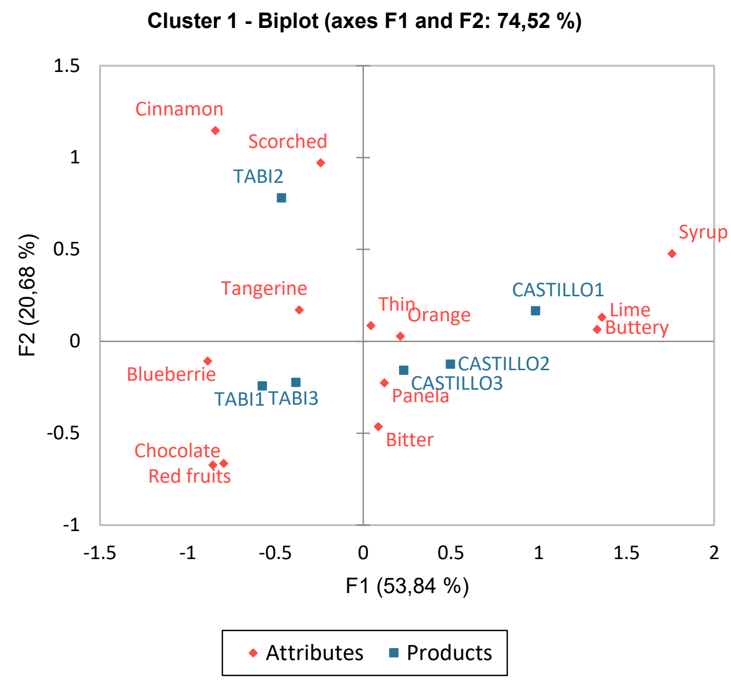
Figure 4.34. Scree plot for (a)Cluster 1, (b) Cluster 2, and (c) Cluster 3.

The scree plot indicates that the two first dimensions are sufficient to interpret relationships between attributes. Symmetric plots present the correspondence analysis for CLUSCATA analysis.

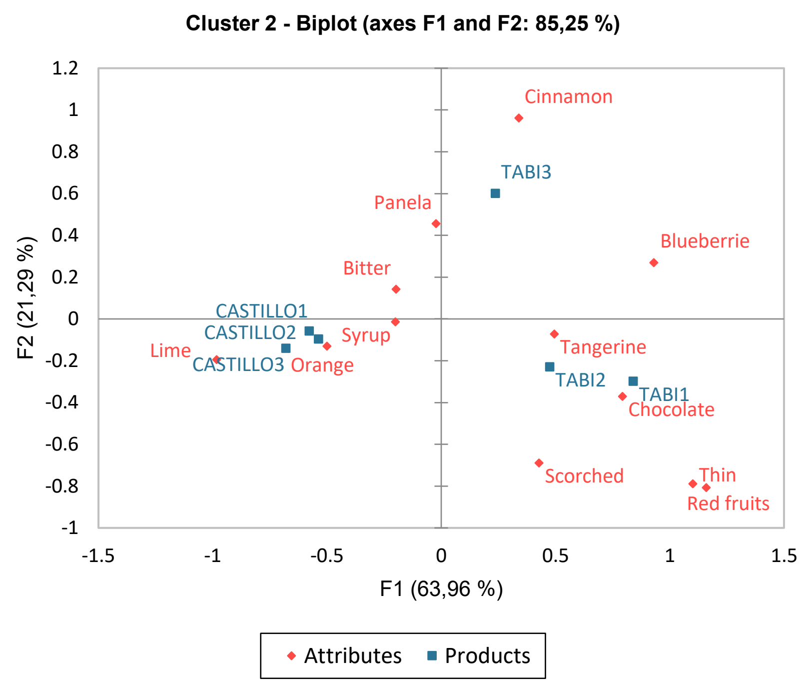
In the Figure 4.35a, six consumers of cluster 1, could assign the attributes for Tabi and Castillo coffees. Tabi1 and Tabi3 coffees as blueberries, tangerine, chocolate, and red fruits. Tabi2 with cinnamon and scorched descriptors. On the other hand, Castillo2 and Castillo3 was related with panela, bitter, orange descriptors. Castillo1 is close to lime, syrup, and buttery attribute. The quality of the analysis is acceptable (74,52% of explained total inertia on the first two dimensions).

In contrast, in cluster 2, Figure 4.35b, 7 assessors could assign the attributes of all Castillo1, Castillo2, and Castillo3 with orange, lime for acidity and syrup as medium body and bitter perception. Tabi1 and Tabi2 with Scorched, chocolate, tangerine, thin, and red fruits. Tabi3 with cinnamon and panela descriptors. The quality of the analysis is good (85.25% of explained total inertia on the first two dimensions).

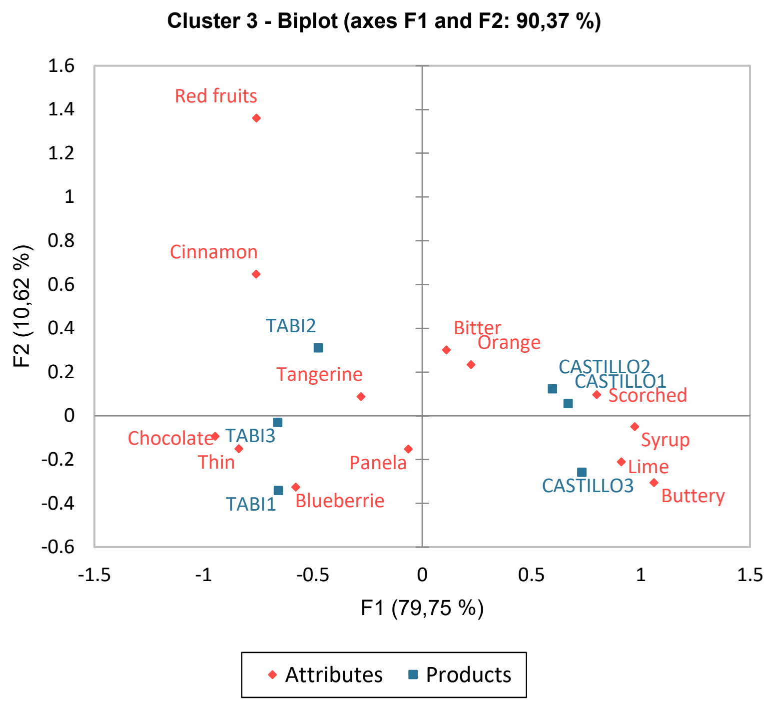
Figure 4.35c shows the cluster 3 biplot that presents the twenty-one assessors more emphasized relations. Tabi1 with Blueberries, Tabi2 with tangerine and Tabi3 with chocolate descriptors. Panela descriptor was present for all Tabi samples. In Castillo1 and Castillo2 samples the scorched, orange, and bitter attributes are present. Castillo 3 presents lime syrup descriptors. The quality of the analysis is good (90.37% of explained total inertia on the first two dimensions).


Cluster 1 - Biplot (axes F1 and F2: 74,52 %)
F2 (20,68 %)
F1 (53,84 %)
Cinnamon
Scorched
TABI2
Syrup
Tangerine
Thin
Orange
CASTILLO1
Lime
Buttery
CASTILLO2
CASTILLO3
Blueberrie
TABI1
TABI3
Panela
Bitter
Chocolate
Red fruits
Attributes
Products

(a)


Cluster 2 - Biplot (axes F1 and F2: 85,25 %)
F2 (21,29 %)
F1 (63,96 %)
Cinnamon
TABI3
Panela
Blueberrie
Bitter
CASTILLO1
CASTILLO2
Syrup
Lime
CASTILLO3
Orange
Tangerine
TABI2
TABI1
Chocolate
Scorched
Thin
Red fruits
Attributes
Products

(b)



(c)

Figure 4.35. Biplot representation of the products on the first two components of (a)Cluster 1, (b)Cluster 2, and (c)Cluster 3.

According to descriptive plots, its necessary to know the consensus between consumer's cluster. Table 4.32 presents the consensus configurations in clusters. Consensus configurations corresponds to the weighted average of the assessor's data. The greater the weight, the more the assessor contributed to the consensus. If the weighting is higher, the consumer will have contributed more to the consensus. A weighting that is too much lower than the others will mean that the evaluator is an outlier.

Table 4.32. Consensus configuration in clusters.

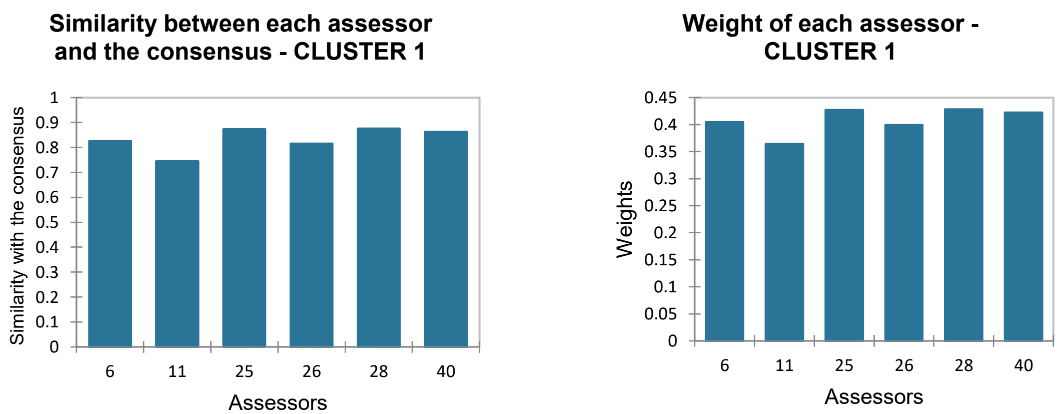
CLUSTER 1	TABI1	TABI2	TABI3	CASTILLO1	CASTILLO2	CASTILLO3
Lime	0.000	0.000	0.000	0.497	0.251	0.085
Tangerine	0.412	0.410	0.497	0.165	0.168	0.081
Orange	0.076	0.247	0.421	0.246	0.412	0.331
Blueberries	0.421	0.164	0.255	0.000	0.000	0.000
Thin	0.497	0.497	0.497	0.421	0.497	0.497
Syrup	0.000	0.000	0.000	0.076	0.000	0.000
Buttery	0.000	0.000	0.000	0.081	0.078	0.000
Bitter	0.327	0.000	0.247	0.089	0.329	0.421
Panela	0.157	0.076	0.343	0.166	0.242	0.235
Cinnamon	0.081	0.262	0.078	0.000	0.000	0.000
Scorched	0.000	0.087	0.000	0.000	0.000	0.078

Red fruits	0.078	0.000	0.165	0.000	0.000	0.000
Chocolate	0.164	0.000	0.161	0.000	0.000	0.000
CLUSTER 2	**TABI1**	**TABI2**	**TABI3**	**CASTILLO1**	**CASTILLO2**	**CASTILLO3**
Lime	0.000	0.000	0.068	0.375	0.379	0.454
Tangerine	0.531	0.531	0.463	0.078	0.297	0.075
Orange	0.000	0.375	0.221	0.386	0.531	0.386
Blueberries	0.376	0.150	0.377	0.000	0.000	0.000
Thin	0.152	0.219	0.000	0.000	0.000	0.000
Syrup	0.379	0.312	0.531	0.531	0.531	0.463
Buttery	0.000	0.000	0.000	0.000	0.000	0.000
Bitter	0.145	0.233	0.454	0.152	0.454	0.301
Panela	0.075	0.078	0.308	0.078	0.074	0.145
Cinnamon	0.000	0.149	0.382	0.077	0.000	0.000
Scorched	0.075	0.078	0.000	0.000	0.000	0.068
Red fruits	0.068	0.068	0.000	0.000	0.000	0.000
Chocolate	0.234	0.156	0.074	0.078	0.000	0.000
CLUSTER 3	**TABI1**	**TABI2**	**TABI3**	**CASTILLO1**	**CASTILLO2**	**CASTILLO3**
Lime	0.127	0.044	0.000	0.691	0.604	0.736
Tangerine	0.741	0.827	0.656	0.165	0.869	0.126
Orange	0.163	0.738	0.434	0.558	0.787	0.467
Blueberries	0.612	0.427	0.474	0.130	0.000	0.215
Thin	0.910	0.826	0.871	0.080	0.000	0.080
Syrup	0.000	0.084	0.039	0.830	0.910	0.830
Buttery	0.000	0.000	0.000	0.000	0.083	0.085
Bitter	0.206	0.609	0.179	0.519	0.349	0.177
Panela	0.607	0.554	0.432	0.350	0.423	0.478
Cinnamon	0.043	0.386	0.213	0.041	0.000	0.000
Scorched	0.000	0.043	0.000	0.086	0.082	0.084
Red fruits	0.000	0.041	0.000	0.000	0.000	0.000
Chocolate	0.343	0.337	0.265	0.000	0.000	0.000

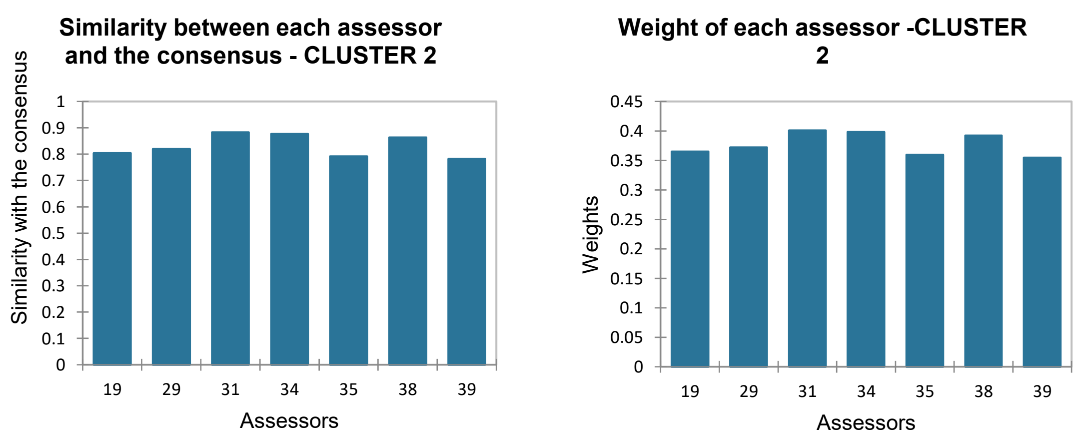
According to Table 4.32, in cluster 1, thin (body) and tangerine (acidity) attributes have the high values of consensus between assessors for TABI1, TABI2 and TABI3. It means, coffee brewing's according to consensus is nice to have these attributes. In fact, lime acidity and Bitter attributes have a consensus for Castillo samples. In the same way Blueberries acidity attribute show a consensus for only Tabi Samples. Tangerine and orange acidity attributes show a variable value of consensus in both, Tabi, and Castillo samples.

In Cluster 2, Lime (acidity), orange (acidity) and Syrup(body) attributes have the high values of consensus for Castillo1, Castillo2 and Castillo3 samples. Blueberries, and tangerine (acidity) and thin (body) attributes have a consensus only for Tabi samples. Tangerine acidity attribute show a high of consensus in Tabi coffee samples. Bitter as consensus in both Castillo and Tabi coffee samples.

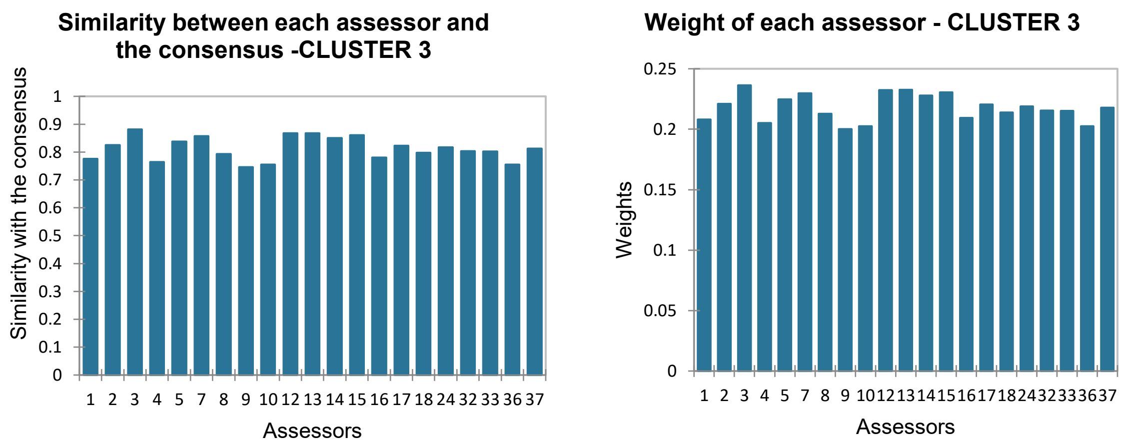
In Cluster 3, by example shows Lime, orange (acidity) and Syrup (body) attributes consensus for Castillo samples, and Blueberries (acidity) and Thin(body) attributes consensus for TABI samples. Bitter, Panela and Cinnamon descriptors are transversal to consensus, because values vary in a weak but representative range in both Castillo and Tabi samples. Table 4.32 also allow to explain the similarity of each evaluator and the consensus, as well as the weight associated with each consumer. Figure 4.36 shows these coefficients allow to detect atypical assessors. The advantage of similarity coefficients is that they are between 0 and 1, so they are easier to interpret than the weights. From the data matrix containing the pairwise similarity coefficients, CLUSCATA calculates the largest eigenvalue, which, once divided by the number of consumer evaluators, yields a homogeneity index.



(a)



(b)



(c)

Figure 4.36. Similarity between each assessor and the consensus and the weight of each assessor for (a)Cluster 1, (b)Cluster 2, and (c)Cluster 3.

The homogeneity index is a value between 1/n to 1, where n is the number of assessors in the class. This value increases with the homogeneity of the evaluators. The global homogeneity, which is a weighted average of the homogeneity of each class, was calculated HI=67.5%. This value reflects good agreement among consumers, through the CATA format, for both Castillo and Tabi coffees from the optimized roasting process. Table 4.33 shows the homogeneity indices for each cluster and the total index already mentioned.

Table 4.33. Homogeneities index - HI CLUSCATA:

	Before consolidation	After consolidation	%HI CLUSCATA
Cluster 1	0.696	0.696	69.6%
Cluster 2	0.664	0.693	69.3%
Cluster 3	0.630	0.663	66.3%
Global	**0.647**	**0.675**	**67.5%**
Global error/Within-cluster variance (Gerr)	14.122	11.059	

On the other hand, the error of the CLUSCATA criterion, called the overall error/intra-class variance was Gerr=11.059, corresponds to the within-class variance.

The segmentation demonstrates that a cluster of consumers present good homogeneities index. That result could be relevant for decision-making in the description of acidity and body for specialty coffee products, both in Castillo and tabi. Although consumers do not know how to differentiate by quality, it is observed that a panel of untrained consumers manages to reveal the attributes of acidity and body, expressing it in terms of acceptability in the drink.

4.4.4. Penalty analysis results

Penalty analyses are used to identify (positive and negative) drivers of consumer liking. A first analysis based on incongruence in which the attribute is missing in the real but not the ideal product allows to identify the must have attributes (Addinsoft, 2019; Gastón Ares, Dauber, et al., 2014).

Must have attributes: Figure 4.37 indicates the frequencies with which P(No)|(Yes) (0 in consumer and 1 in ideal) and P(Yes)|(Yes) (1 in both, consumer, and IDEAL) occurs for each attribute. Also, CATA percentage is shown graphically considering this P(No)|(Yes) vs P(Yes)|(Yes) for each attribute for the 280x18 dataset. According to Figure 4.37, the must have attributes analysis penalized the Blueberries (acidity) and thin (body), Bitter, and scorched descriptor. This analysis consider must have 33% of orange (acidity), 37% tangerine(acidity), 19% lime (acidity) and 47 % Syrup (body) descriptors. Must have panela in 35%, cinnamon 9%, red fruits 2% and chocolate 8%.

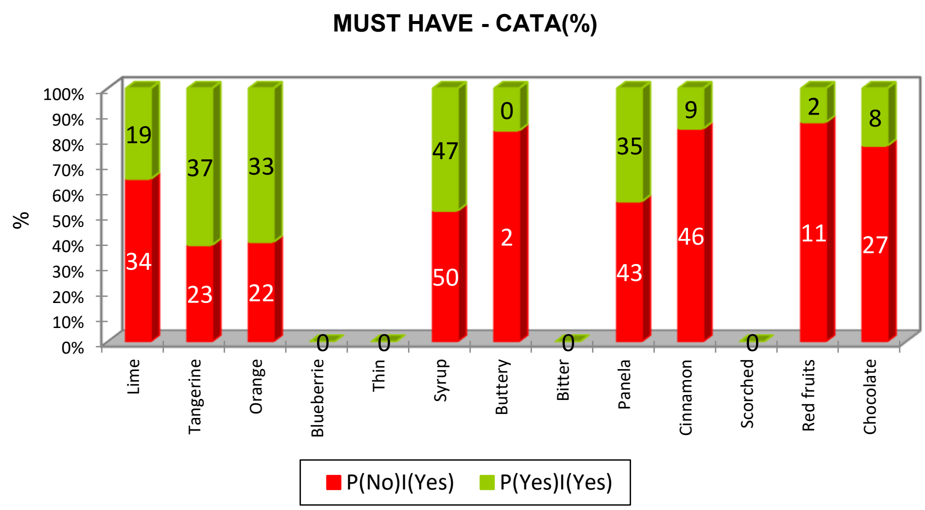


Figure 4.37. Analysis of the must have attributes

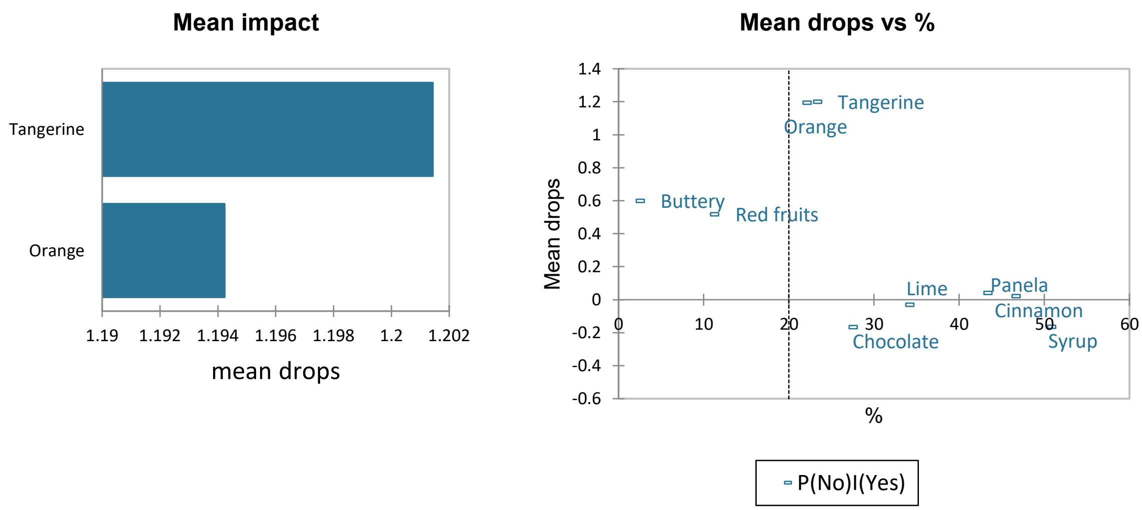
The comparison table for penalty analysis in must have attributes is shown in Table 4.34. Only Orange(acidity) and tangerine(acidity) are significant to must have attributes (p-value<0.0001). Tangerine attribute implies an increase of 1,201 Liking points between the tested products and the ideal product. This increase is significant at 0.05 ($p < 0.0001$). Orange attribute implies an increase of 1.194 liking points.

Table 4.34. Comparison table for must have attributes – penalty analysis

Variable	Level	Frequencies	%	Sum(Liking)	Mean(Liking)	Mean drops	Standardized difference	p-value	Significant	Penalties
Lime	P(No)I(Yes)	81	33.75%	591.000	7.296	-0.030	-0.132	0.990	No	
	P(Yes)I(Yes)	45	18.75%	327.000	7.267					0.021
Tangerine	P(No)I(Yes)	55	22.92%	356.000	6.473	**1.201**	6.273	<0.0001	**Yes**	
	P(Yes)I(Yes)	89	37.08%	683.000	7.674					0.674
Orange	P(No)I(Yes)	52	21.67%	337.000	6.481	**1.194**	5.964	<0.0001	**Yes**	
	P(Yes)I(Yes)	80	33.33%	614.000	7.675					0.638
Syrup	P(No)I(Yes)	121	50.42%	886.000	7.322	-0.163	-1.033	0.303	No	
	P(Yes)I(Yes)	113	47.08%	809.000	7.159					-0.171
Buttery	P(No)I(Yes)	5	2.08%	37.000	7.400	0.600				
	P(Yes)I(Yes)	1	0.42%	8.000	8.000					0.753
Panela	P(No)I(Yes)	103	42.92%	744.000	7.223	0.042	0.235	0.970	No	
	P(Yes)I(Yes)	83	34.58%	603.000	7.265					0.023
Cinnamon	P(No)I(Yes)	111	46.25%	801.000	7.216	0.022	0.076	0.997	No	
	P(Yes)I(Yes)	21	8.75%	152.000	7.238					-0.013
Red fruits	P(No)I(Yes)	26	10.83%	188.000	7.231	0.519				
	P(Yes)I(Yes)	4	1.67%	31.000	7.750					0.508
Chocolate	P(No)I(Yes)	65	27.08%	476.000	7.323	-0.165	-0.525	0.859	No	
	P(Yes)I(Yes)	19	7.92%	136.000	7.158					-0.100

Other analysis can be explained with the mean impact display, Figure 4.38a, and mean drops vs percentage (%) Figure 4.38b. The mean impact chart shows the attributes with a significant mean impact, Tangerine, and Orange. The mean drops vs % chart also allows to clearly identify the must have attributes.

The Y-axis corresponds to the differences in product perception when consumers check both a product and the ideal product and when they check only the ideal product. The X-axis represents the percentage of entries including a check for the ideal product without the actual product being checked. This corresponds to a situation where the attribute describes the ideal product well but is relatively little felt in the actual products (Addinsoft, 2019; Gastón Ares, Dauber, et al., 2014). Thus, attributes that are associated to high coordinates on both the X and Y axes (tangerine, orange, Syrup, Lime) appear here again to be must have.



(a) (b)

Figure 4.38. Must have attributes (a)mean impact and (b) mean drops vs % plots.

Nice to have and negative attributes: Considering the same, the nice to have and negative attributes were evaluated. A second analysis allow to identify the “nice to have” attributes. It is similar to the procedure Must Have Attributes but is based on incongruence in which the attribute is missing in the ideal but not the real product. Figure 4.39, show the analysis with summary table.

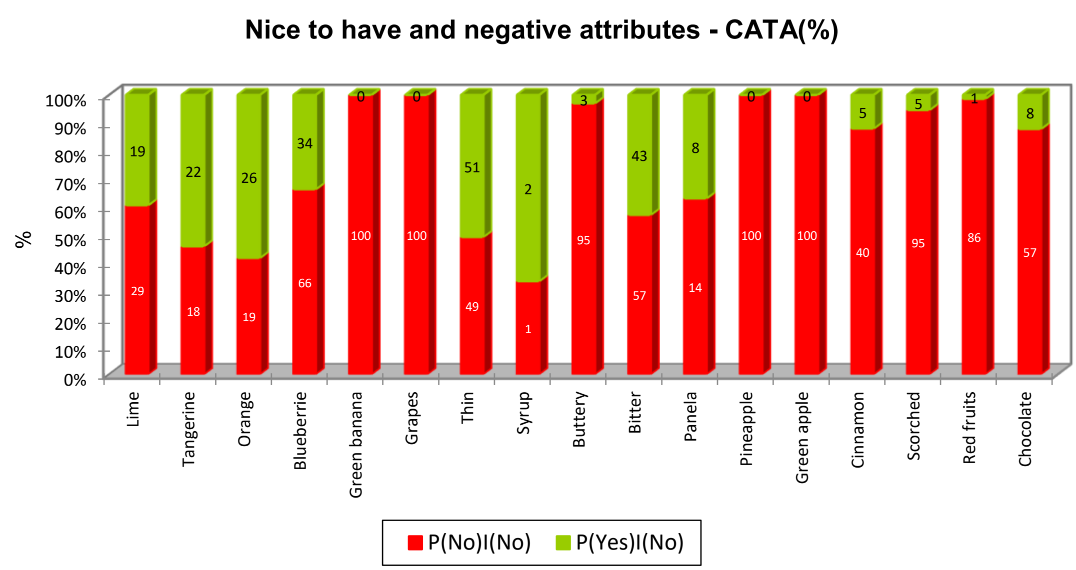


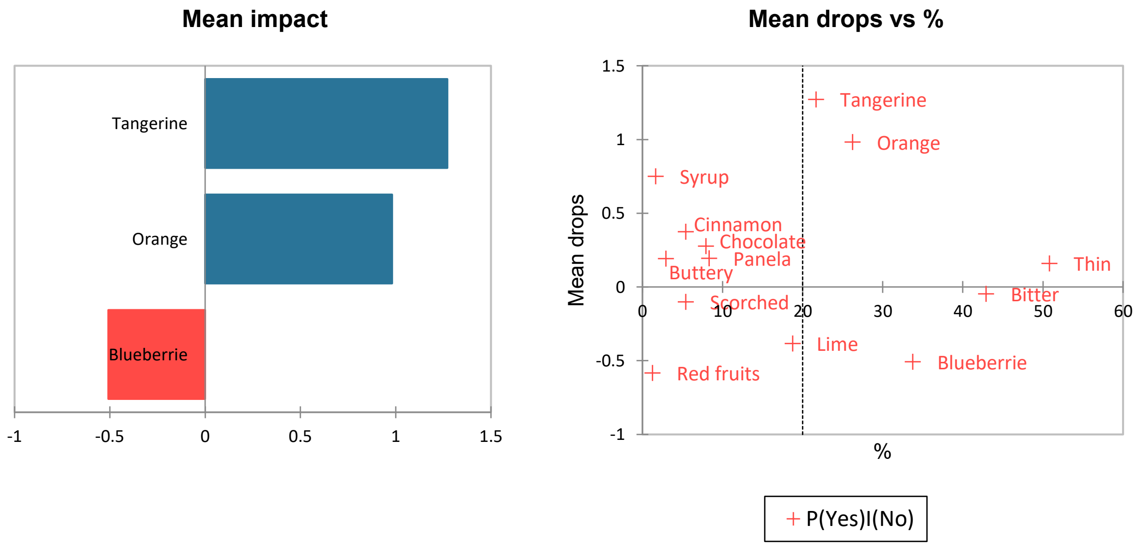
Figure 4.39. Analysis of the nice to have and negative attributes with summary table.

In this penalty indicator, 19 % lime, 22% tangerine, 26% orange, 34% blueberries, 51% thin, 2% syrup, 43% Bitter, 5% cinnamon, 8% panela, 8% chocolate and 5% scorched descriptors were considering nice to have attributes, in relation to the ideal product. From another point of view, green banana, grapes, buttery, pineapple, green apple, scorched, red fruits and chocolate descriptors were considered negative attributes, because unchecked percentage >70% of the attribute occurs in the CATA session. The comparison table for penalty analysis in nice to have and negative attributes is shown in Table 4.35.

Table 4.35. Comparison table for nice to have and negative attributes – penalty analysis.

Variable	Level	Frequencies	%	Sum(Liking)	Mean(Liking)	Mean drops	Standardized difference	p-value	Significant	Penalties
Lime	P(No)I(No)	69	28.75%	508.000	7.362					0.158
	P(Yes)I(No)	45	18.75%	314.000	6.978	-0.385				
Tangerine	P(No)I(No)	44	18.33%	291.000	6.614					-0.779
	P(Yes)I(No)	52	21.67%	410.000	7.885	**1.271**	5.460	<0.0001	**Yes**	
Orange	P(No)I(No)	45	18.75%	303.000	6.733					-0.636
	P(Yes)I(No)	63	26.25%	486.000	7.714	**0.981**	4.331	<0.0001	**Yes**	
Blueberries	P(No)I(No)	159	66.25%	1,180.000	7.421					
	P(Yes)I(No)	81	33.75%	560.000	6.914	**-0.508**	-3.154	0.002	**Yes**	0.000
Green banana	P(No)I(No)	240	100.00%	1,740.000	7.250					
	P(Yes)I(No)	0	0.00%							0.000
Grapes	P(No)I(No)	240	100.00%	1,740.000	7.250					
	P(Yes)I(No)	0	0.00%							0.000
Thin	P(No)I(No)	118	49.17%	846.000	7.169					
	P(Yes)I(No)	122	50.83%	894.000	7.328	0.158	1.021	0.308	No	0.000
Syrup	P(No)I(No)	2	0.83%	14.000	7.000					-0.252
	P(Yes)I(No)	4	1.67%	31.000	7.750	0.750				
Buttery	P(No)I(No)	227	94.58%	1,643.000	7.238					-0.224
	P(Yes)I(No)	7	2.92%	52.000	7.429	0.191				
Bitter	P(No)I(No)	137	57.08%	996.000	7.270					
	P(Yes)I(No)	103	42.92%	744.000	7.223	-0.047	-0.298	0.766	No	0.000
Panela	P(No)I(No)	34	14.17%	245.000	7.206					-0.051
	P(Yes)I(No)	20	8.33%	148.000	7.400	0.194				
Pineapple	P(No)I(No)	240	100.00%	1,740.000	7.250					
	P(Yes)I(No)	0	0.00%							0.000
Green apple	P(No)I(No)	240	100.00%	1,740.000	7.250					
	P(Yes)I(No)	0	0.00%							0.000
Cinnamon	P(No)I(No)	95	39.58%	688.000	7.242					-0.013
	P(Yes)I(No)	13	5.42%	99.000	7.615	0.373				
Scorched	P(No)I(No)	227	94.58%	1647.000	7.256					
	P(Yes)I(No)	13	5.42%	93.000	7.154	-0.102				0.000
Red fruits	P(No)I(No)	207	86.25%	1,501.000	7.251					0.009
	P(Yes)I(No)	3	1.25%	20.000	6.667	-0.585				
Chocolate	P(No)I(No)	137	57.08%	986.000	7.197					-0.123
	P(Yes)I(No)	19	7.92%	142.000	7.474	0.277				

From Table 4.35, penalty analysis can be explored from graphical view with the mean impact plot, in Figure 4.40a, and mean drops vs percentage (%) in Figure 4.40b. According with significant test the mean impact plot shows that tangerine an orange (acidity) descriptor increases 1.271 and 0.981 Liking points between the tested products and the ideal product, respectively. While blueberries descriptor decreases in -0.508 liking points.



(a) (b)

Figure 4.40. Nice to have and negative attributes (a)mean impact and (b) mean drops vs %, plots.

Finally, penalty analysis resume is presented in Figure 4.41. In this case of study, from statistically significant point of view, Tangerine and Orange, acidity descriptors, were selected as a must have attributes. Lime (acidity) and syrup(body), panela, and cinnamon descriptors were selected as Does not influence attributes. Thin (body) Buttery, Bitter, Scorched, Red fruits and Chocolate attributes has selected as Does not harm attribute. Blueberries (acidity) a descriptor has selected as a “must not have” attribute from consumers’ perception. Table 4.36 Summarizes the penalty analysis.

Table 4.36. Summary penalty analysis

Must have	**Nice to have**	**Does not influence**	**Does not harm**	**Must not have**
Tangerine		Lime	Thin	Blueberries
Orange		Syrup	Buttery	
		Panela	Bitter	
		Cinnamon	Scorched	
			Red fruits	
			Chocolate	

Here we can show that consumers used some characteristics that are considered defects by specialists to describe the special coffees (Buttery, Bitter, Scorched, red fruits), which reinforces the idea that the specialized sensory classification can be questioned and, many times, does not correspond to consumer preferences as reported in (Giacalone et al., 2019). There are no studies that meet consumer expectations for flavor descriptors. Our results contribute to understanding the context of consumers only in the context of acidity and body, within the framework of the proposed aroma triangle. Market researchers and product developers use penalty analysis (mean-drop) to learn which product attributes most influence liking, purchase interest or any other product-related metric. The Figure 4.41 presents these findings considering the subjects involved in the CATA experiment are generally not trained. Therefore, they may differ in the interpretation of the attributes or may have different perceptions of the products. Thus, the segmentation of these subjects is of paramount interest. This issue has not sufficiently been addressed in the literature.

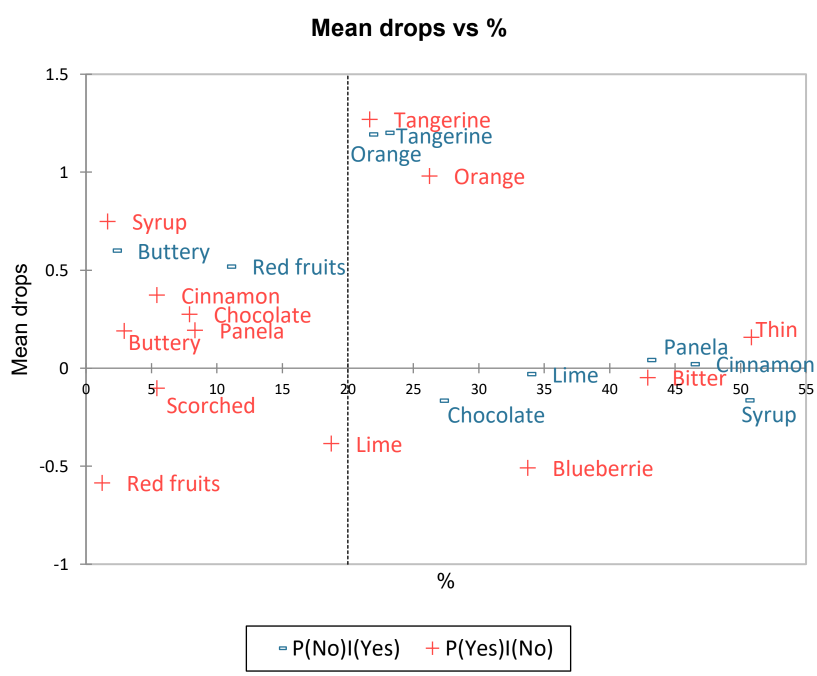


Figure 4.41. Penalty analysis for CASTILLO and TABI optimized samples resume

Penalty analysis is a valuable tool to determine tendencies for the improvement of coffee products, based on the assumption that each consumer has an ideal coffee flavor and aroma. It also proposes attributes that it should have, some that it would be good to have and on the other hand those that it should definitely not have, or they will be negative for the total description of acidity and body. Here it was obtained that the Castillo and Tabi coffees, through the processes of optimization of the roasting curve, in a global way should have orange and tangerine attributes. On the contrary, it should not have blueberries, which was evaluated as a negative attribute in comparison with the ideal of each consumer. The attribute with the most strength in the consumers' assessment was tangerine.

4.5. Final considerations for optimization scheme

For comparison purposes the contingency table of acidity and body intensities in the 0-15 scale and 25-95 for color perception from CASTILLO1, CASTILLO2, CASTILLO3, and TABI1, TABI2, and TABI 3, are presented in table 4.37 for the 40 consumers in optimization samples.

Table 4.37. Contingency table for acidity, body and color perceived by consumers for optimized samples.

Sample	**Acidity 0-15 scale**	**CLUSCATA Cluster 3**	**Body 0-15 scale**	**CLUSCATA Cluster 3**	**Color 25-95**
CASTILLO 1	8	Orange	6	Syrup	65
CASTILLO 2	10	Orange	4	Buttery	65
CASTILLO 3	8	Lime	4	Buttery	65
TABI 1	8	Blueberries	6	Thin	65
TABI 2	6	Tangerine	6	Thin	65
TABI 3	6	Chocolate	6	Thin	65

Acidity, body, and color values were calculated from the median from forty consumer perceptions. Descriptor are associated from CLUSCATA cluster 3 which contain the largest number of segmented consumers 90.27% variability.

Considering results of table 4.37, the consumers we can related the intensity values with the possible descriptors of acidity and body presented in CATA experiment.

In this work, three clusters were generated to evaluate the performance of optimized samples, and to analyze the homogeneity of consumer assessments using the CATA questionnaire. It was found acceptable global homogeneity=0.647. With this, a valuable tool was obtained to study the consumer's perceptions of a coffee beverage. Consumers perceived the acidity and body descriptors, and can be related with its predicted intensity. Limitations of the tool were also visualized, such as the dependence on a pre-training of coffee consumers in terms of acidity and body intensity and of the sensory memory that can establish significant differences between one cup of coffee and another, or as in this case, to propose a tool that allows differentiating between acidity intensities and body levels of coffee according to their optimizing roasting profile. We found that consumers were unable to differentiate between coffee varieties for the optimized samples. However, two tools have been promoted, a quality tool based on consumer preferences with the CATA questionnaire and the intensity scale with the 0-15 scale for both acidity and body. On the other hand, nothing can be concluded about the color of the bean coffee perceived by consumers, the optimized samples had the same color and the consumers perceived it in the 65-medium-dark tone, both for tabi and Castillo. Regarding the parameterization process, it is important to mention that a medium-high roast enhances the attributes of acidity and body in the Castillo variety from the perception of untrained consumers. The literature refers to this expression in the Castillo variety to for medium roasts from the perception of tasters (trained consumer)(Alvarado-Alvarado et al., 2005; Osorio & Pabón, 2022). This is important due to the potential of the optimized roasting curves obtained to develop new market segments.

The proposed optimization scheme made it possible to establish the time and temperature conditions of the roasting process to accentuate the desired attributes (acidity and body) and to study its consistency through sensory perception methods applied to coffee consumers. The proposed scheme included: (i)The physical properties data set according to the SCA protocol. (ii)To perform the roasting profiling process. (iii)Performing the consumers' perception of intensity using roasted coffee through the CCD - RSM methodology and the 0-15 lexicon scale. (iv)Preparation of homogeneous beverages with the French press. (v)To calculate Fleiss' kappa and Cronbach's alpha statistics to validate the strength of inter-consumer agreement and the reliability measure of the 0-15 intensity scale. (vi)To calculate mathematical models to predict acidity and body. (vii)Optimize model’s trough desirability function to obtain coffee samples for confirmatory experiments. (viii)Prepare coffee beverages with optimized profile samples. (ix)Implement CATA to obtain consumer preference data, including the 1-9 hedonic scale. (x)Run the CLUSCATA algorithm to segment consumers, define consumer homogeneity assessment, linking with 0-15 intensity scale and study the penalty analysis using ideal descriptors to identify potential directions for improving Cauca coffees.

CHAPTER 5

5. Conclusions and future work

5.1. Conclusions

To date, this study represents the pioneering effort in incorporating consumer perception of acidity and body into the construction of prediction models, specifically focusing on specialty coffee grade samples and the modulation of the coffee roasting curve at critical points. Additionally, this study explores the validation of consumer perception for optimized samples, combining a sensorial techniques approach to gain insights into how consumers perceive optimized profiles of Castillo and Tabi Cauca coffees. The findings of this research contribute to the advancement of understanding consumer preferences and optimizing coffee profiles in specialty coffee.

The optimization of coffee roasting conditions allows for achieving the desired outcome by different paths, while reaching the same roasting point. The CCD-RSM experimental design demonstrated its effectiveness in generating variations in critical points along the coffee roasting curve, leading to consistent perceptions of acidity, body, and color among consumers. This study revealed a quantitatively inverse relationship between acidity and body, as perceived by consumers on a 0-15 intensity scale. Moreover, a strategy based on the desirability function was employed to optimize this relationship. It became evident that key factors to consider were the physical properties of green coffee beans, along with monitoring the roasting process at critical points including charge, turning, drying, Maillard reaction, caramelization, first crack, development time, and the drop in the coffee roaster protocol. Two significant quadratic models were calculated for acidity and body, that can be used by roasters to conduct experiments focusing on the optimum roasting region for roasting coffee products with an acidity/body consistency with the desired quality properties of Cauca coffees like the Castillo and Tabi variety.

Furthermore, this thesis has demonstrated that incorporating numerical optimization based on consumer perception provides a systematic tool for roasters to avoid common trial-and-error experiments when aiming to achieve specific coffee characteristics with desired profiles. The optimized roasting curves for the Castillo and Tabi varieties, obtained through mathematical models, exhibited distinct characteristics primarily due to genetic differences reflected in the physical properties of the green coffee beans. By linking consumer perception to mathematical models, it becomes possible to determine the precise roasting time and temperature points, providing a competitive advantage for roasters to focus on a specific roasting stage, typically after the first crack, and attain a harmonious balance between acidity and body for each variety.

This work expands our understanding of consumer perceptions of acidity and body in specialty coffees, specifically the Castillo and Tabi Cauca varieties, through the application of different methods such as CATA (Check-All-That-Apply), CLUSCATA, and penalty analysis. It supports the notion that a panel of pre-trained consumers can discern differences among specialty coffees. By incorporating common attributes for acidity (lime, orange, tangerine, blueberries, grapes, green apple, green banana), body (water, thin, syrup, buttery), and overall flavor and defects (chocolate, cinnamon, pineapple, panela, bitter, scorched), it becomes possible to identify trends for enhancing coffee products. It is assumed that each consumer has an ideal coffee flavor and aroma, making their preferences an ongoing subject of research. Sensory and consumer research, aided by technological tools, serve as a bridge to narrow the gap, and facilitate the dissemination of research findings to the wider community.

5.2. Future work

The check-all-that-apply approach may be employed to understand consumer preferences in practical applications of the coffee industry 4.0. This research can provide further insights into the use of consumer profiles for evaluating the sensory characteristics of products, in comparison to a trained sensory panel. Additionally, the results can validate the potential replacement of a trained panel with an untrained consumer panel in situations where a detailed sensory profile, along with precise definitions and subsequent quantification of sensory attributes, is not essential, as reported by (Oliver et al., 2018).

Most of the results from coffee roasting time-temperature profile modulation experiments focus on reporting the effects on bean chemistry, lacking descriptive sensory analysis or consumer test data. There is a need for new research in intelligent systems to effectively utilize this information, as coffee professionals face difficulties in practically interpreting a list of aromatic precursors solely based on coffee's chemical compounds. The problem of reliably predicting the flavor of coffee remains open, as it depends on various factors including the agronomic process, bean origin, chemical composition, type of processing, fermentation process, roasting, grinding, preparation, and beverage. Addressing these challenges and developing comprehensive models to predict coffee flavor require further exploration in the field of intelligent systems.

Sensory and consumer science reveals that the concept of quality varies not only among experts but also between experts and consumers. When quality is well-defined within the specialty coffee community, it becomes easier for researchers and developers to establish and measure quality objectives. This valuable information can serve as the foundation for defining parameters to be incorporated into subsequent models of consumer perception in controlling the quality of roasted coffee. An effective approach to achieve this is through a hybrid technique combining artificial neural networks (ANN), genetic algorithms (GA), and response surface methodology (RSM). The hybrid ANN-GA technique acts as an implementation tool, utilizing RSM-ANN generated data points to initialize the algorithm, as report by (Aung et al., 2022).

The development of new sensors and actuators to support the coffee chain is important and warrants further research. Additionally, integrating electronic instrumentation, such as the electronic nose, electronic eye, and electronic tongue, as analytical tools in stages like fermentation and roasting, has the potential to create unique and high-value coffees for future coffee research.

In the coffee 4.0 industry, quality is a concept that should not solely be entrusted to experts. Despite coffee experts and consumers being seen as distinct, establishing synergy between them is necessary to enhance the value chain of coffee (Thomas et al., 2017). Sensory and consumer research, facilitated by technological tools, can serve as a bridge to close the gap between experts and consumers. Future research is committed to incorporating smart data capture throughout the various stages of coffee production, including raw material selection, fermentation, grading, pulping, roasting, cupping, and brewing. This endeavor requires infrastructure, commitment, and rigor to ensure that the coffee of Cauca continues to showcase its full potential, owing to our diverse range of offerings.

A. Appendix. Dataset of Physical properties of Coffee

Table A.1 and Table A.2 show the physical assessment protocol and expert sensory assessment for specialty coffee industry (SCA>80). TECNiCAFÉ.

Table A.1. Dataset of physical assessment protocol for specialty coffee.

MUESTRAS C=CAFÉ 1 T=CAFÉ 2	Humedad CPS =café pergamino seco	Densidad CPS= café pergamino seco	Peso Muestra (g)	Peso despues de trilla(g)	Merma Trilla	Humedad Verde (%)	Defectos (g)	% Defectos	MALLAS (n/64) pulgadas							Almendra Sana(g)	Factor Rendimiento	Densidad Excelso(g/L)
									18	17	16	15	14	13	12			
C1	10	206	1000	343.8	65.6%	11	36.7	3.7%	29.5	68.6	96	30.5	27.1	55.4	4.1	307.1	56.98	699
C2	11.6	208	1000	346.6	65.3%	10.8	30.2	3.0%	41.7	99.5	113.6	44.7	12	4.9	1.1	316.4	55.31	720
C3	10.2	195	1000	344.2	65.6%	10.6	35.3	3.5%	35.6	91.6	106.3	40	14.7	20.7	2.5	308.9	56.65	706
C4	12	215	1000	344.5	65.6%	11	35.4	3.5%	43.2	107.1	104.6	32.6	12.8	8.8	2.4	309.1	56.62	692
C5	10.2	520.0	250	196	21.6%	9.1	12.3	4.9%	13	45.3	61.8	42.5	18.6	2.5	0.7	183.7	95.26	846
C6	11.4	528.0	250	198.8	20.5%	11.3	8.9	3.6%	25.5	52.2	63.9	37.2	9.3	1.8	0.4	189.9	92.15	861
C7	10.7	539.0	250	195.2	21.9%	10.6	10.3	4.1%	12.9	41.5	69.2	42.9	16.8	1.6	0.6	184.9	94.65	848
C8	10.0	540.0	250	197	21.2%	9.2	14.5	5.8%	20.7	51.8	64.1	32.2	10.9	2.8	0.6	182.5	95.89	858
C9	10.9	502.0	250	193.2	22.7%	11.7	9.1	3.6%	20.3	56.8	65.5	29.1	10.9	1.5	0.3	184.1	95.06	825
C10	10.3	498.0	250	215.2	13.9%	11.4	15.4	6.2%	28.2	59.6	61.3	37.4	12.5	0.8	0.3	199.8	87.59	844
C11	9.8	446.0	250	204.6	18.2%	10.5	11.6	4.6%	27.5	51.3	63.8	38	11.1	1.3	0.4	193	90.67	861
C12	10.0	514.0	250	203.8	18.5%	9.9	16	6.4%	24	55	62.6	33.7	10.7	1.8	0.9	187.8	93.18	856
C13	10.5	218	1000	326.4	67.4%	9	35.3	3.5%	25.7	77.2	120.3	46.5	13.8	12.3	20.4	295.8	59.16	711
C14	10	217	1000	313.3	68.7%	9.1	52.4	5.2%	21.2	66.1	115.8	39.3	14	4.5	33.6	260.9	67.08	726
C15	10.8	214	1000	320.3	68.0%	9.1	29	2.9%	17.6	73.7	129.7	51.7	13.6	5	27	291.3	60.08	699
C16	10.5	209	1000	327.7	67.2%	9.4	28.3	2.8%	19.4	70.1	133	50.2	20.3	6.4	20.6	299.4	58.45	723
C17	8.1	511.0	250	198	20.8%	8.3	7.5	3.0%	10.7	54.2	68.6	41.6	13.1	2.3	0.5	190.5	91.86	845
C18	10.8	522.0	250	196.8	21.3%	8.2	4.3	1.7%	13.7	49.9	69.8	42.6	14.1	2.4	0.8	192.5	90.91	848
C19	10.6	504.0	250	197.6	21.0%	8.9	8	3.2%	13.4	45.7	68.3	44.3	15.1	2.8	1	189.6	92.30	851
C20	10.8	530.0	250	196.6	21.4%	10.5	6.4	2.6%	16.3	53.2	68.5	38	12.9	1.3	0.5	190.2	92.01	864
C21	9.2	510.0	250	203.0	18.8%	9.4	8.2	3.3%	18.2	53.8	74.3	34.8	11.9	1.8	0.8	194.8	89.84	847
C22	9.2	510.0	250	203	18.8%	9.1	6.9	2.8%	20.1	58.6	66.2	34.7	13.7	2.8	0.7	196.1	89.24	842
C23	8.0	520.0	250	202.4	19.0%	8.7	4.8	1.9%	17.7	51	73.3	39.9	13.7	2	0.5	197.6	88.56	846
C24	10.0	511.0	250	202.8	18.9%	10.5	8.8	3.5%	18.9	57.8	74.8	33.7	7.4	1.4	0.5	194	90.21	842
C25	10	196	1000	333.7	66.6%	9.9	47.2	4.7%	44	83.5	112	40.7	4	2.3	16.3	286.5	61.08	713
C26	10.5	203	1000	338.5	66.2%	9.8	41.4	4.1%	50.9	87.7	100.6	44.6	9.7	3.6	11.5	297.1	58.90	726
C27	10.6	198	1000	339.2	66.1%	9.8	31.9	3.2%	51.4	98.4	110.5	36.6	7.9	2.5	8.9	307.3	56.95	713
C28	10.5	192	1000	339.8	66.0%	9.4	38.8	3.9%	49.7	88.3	113.1	38.7	8.7	2.5	8.7	301	58.14	714
C29	10.0	513.0	250	197.4	21.0%	10.1	8.3	3.3%	40	51.2	60.2	28.6	7.3	1.5	0.3	188.8	92.69	849
C30	10.8	520.0	250	197	21.2%	10.2	8.5	3.4%	33.5	59.8	55.6	29.2	9.3	1.1	0.1	188.5	92.84	834
C31	10.5	497.0	250	190.8	23.7%	8.8	8.2	3.3%	32	52.5	59.4	29.5	7.9	1.3	0.3	182.6	95.84	849

C32	9.3	505.0	250	197	21.2%	9.4	7.2	2.9%	27.9	58.5	59.3	32.5	10	1.6	0.2	189.8	92.20	838
C33	10.4	495.0	250	203.4	18.6%	8.9	9.1	3.6%	37.2	63.7	60	24.9	7.2	1.3	0.2	194.3	90.07	833
C34	9.3	479.0	250	203.4	18.6%	8.7	5.4	2.2%	32.5	63.4	62	28.3	10.7	1.1	0.5	198	88.38	838
C35	10.7	507.0	250	203.4	18.6%	10.3	7.9	3.2%	41.2	57.4	62.3	25.4	7.9	1.3	0.5	195.5	89.51	849
C36	9.7	513.0	250	202.6	19.0%	10.2	8.4	3.4%	40.4	63.1	57.5	21.4	10.3	1.5	0.4	194.2	90.11	841
T1	10.5	214	1000	341.8	65.8%	8.8	42.4	4.2%	23.1	66.4	123.3	65.3	17.8	3.5	5.8	299.4	58.45	724
T2	10.2	209	1000	339.6	66.0%	8.9	45.7	4.6%	18.4	57.4	127.7	65.3	21.2	3.9	7.8	293.9	59.54	715
T3	10	215	1000	341.7	65.8%	9.1	45.6	4.6%	24.9	61.4	125.1	62.5	19.1	3.1	7.9	296.1	59.10	733
T4	10	221	1000	343	65.7%	9.6	28.3	2.8%	30.1	69	132.7	59.6	20.4	2.9	6.3	314.7	55.61	743
T5	8.6	528.0	250	197.6	21.0%	8.6	9.7	3.9%	15.7	39.3	60.1	48.2	21.6	3	0.6	187.9	93.13	854
T6	8.7	523.0	250	197.4	21.0%	8.5	10.7	4.3%	14.7	42.6	61.9	46.7	17.3	3.5	0.8	186.7	93.73	854
T7	8.6	515.0	250	197	21.2%	8.9	8.5	3.4%	14.8	36.4	65.1	49.5	21.4	1.3	0.8	188.5	92.84	847
T8	10.0	462.0	250	197.8	20.9%	9.4	6.3	2.5%	19.7	43	64.7	46.7	16.4	1	0.4	191.5	91.38	845
T9	10.8	476.0	250	203.2	18.7%	9	8	3.2%	16.6	45.3	60.4	52.2	18.3	2.4	0.6	195.2	89.65	839
T10	10.3	483.0	250	202.6	19.0%	10.1	7.1	2.8%	16.6	47.8	70.5	43.1	15.9	1.6	0.5	195.5	89.51	832
T11	9.8	472.0	250	201.6	19.4%	9.6	10.6	4.2%	15	50.9	65.8	41.5	15.9	1.9	0.4	191	91.62	854
T12	9.8	509.0	250	202.2	19.1%	10.2	8	3.2%	15.5	42.5	70.3	48.7	15.3	1.9	0.2	194.2	90.11	871
T13	10.2	205	1000	345	65.5%	10.1	33.1	3.3%	27.1	85.3	124	50.4	21.3	3.8	3.9	311.9	56.11	735
T14	10.4	210	1000	344.3	65.6%	9.5	43.4	4.3%	28.2	76.2	122.6	54.7	16.2	3	2.7	300.9	58.16	731
T15	10.5	211	1000	346.5	65.4%	9.9	46.5	4.7%	26.2	81.1	120	52.4	18.2	2.1	2.6	300	58.33	715
T16	10	210	1000	343.4	65.7%	10.1	39.8	4.0%	22.7	72	130.2	55.7	19.7	3.3	4.1	303.6	57.64	728
T17	9.8	505.0	250	191.4	23.4%	8.2	21.3	8.5%	2.9	26.4	56.2	54.3	27.4	2.9	1.3	170.1	102.88	825
T18	10.2	508.0	250	190.6	23.8%	8.6	25	10.0%	4.8	26.2	52.5	52.6	26.1	3.4	1.4	165.6	105.68	839
T19	10.5	503.0	250	195.8	21.7%	8.8	7.1	2.8%	28.3	48.6	58	38.2	13.2	2.4	1	188.7	92.74	853
T20	11.1	460.0	250	188.2	24.7%	10.1	8.6	3.4%	11.7	37.7	69.5	41.9	16.6	2.2	0.9	179.6	97.44	839
T21	10.5	492.0	250	198.2	20.7%	9	21.6	8.6%	5.2	29.5	63.2	55.2	21.5	2	0.9	176.6	99.09	844
T22	10.2	481.0	250	201.8	19.3%	9.7	9.8	3.9%	36.8	53.9	60.7	27.7	12.4	0.5	1.1	192	91.15	846
T23	10.2	479.0	250	201	19.6%	9.4	10.6	4.2%	25.4	45.4	64.6	40.3	12.9	1.8	0.4	190.4	91.91	843
T24	10.8	490.0	250	199.2	20.3%	9.7	9.9	4.0%	17.2	53.9	61.7	41.1	13.8	1.6	0.5	189.3	92.45	844
T25	10.6	195	1000	347.6	65.2%	9.8	71.5	7.2%	18.9	61.7	116.5	58.8	17.6	2.6	5	276.1	63.38	724
T26	10.8	186	1000	348.3	65.2%	9.5	62.3	6.2%	18.9	74.8	116.6	56.6	16.3	2.8	5.9	286	61.19	722
T27	10.8	200	1000	343.3	65.7%	10.5	43.9	4.4%	42.6	83	111.6	46.4	12.9	2.9	5.9	299.4	58.45	731
T28	10.7	200	1000	347.6	65.2%	10.3	54.2	5.4%	60.8	77.8	95.6	42.3	14.6	2.3	2	293.4	59.65	730
T29	10.8	495.0	250	195.4	21.8%	9.2	18.5	7.4%	43.2	69.1	33.9	26.2	4.2	0.3	1.2	176.9	98.93	821
T30	9.5	505.0	250	194.8	22.1%	8.9	15.5	6.2%	40.7	67.4	39.8	24.9	5.7	0.8	0.6	179.3	97.60	844
T31	9.8	509.0	250	195.6	21.8%	10.1	20.1	8.0%	13.7	56.7	51.3	47.3	5.8	0.7	1.3	175.5	99.72	831
T32	10.7	502.0	250	186.6	25.4%	10.1	21.7	8.7%	4.5	24.2	35.7	68.7	26.1	5.7	2.6	164.9	106.12	832
T33	10.2	496.0	250	203.6	18.6%	8.6	10.1	4.0%	46.4	73.7	34	32.6	5.9	0.9	0.5	193.5	90.44	851
T34	10.8	500.0	250	201.4	19.4%	9	14.9	6.0%	52.5	48.8	62.6	20.1	1.7	0.8	0.4	186.5	93.83	877
T35	11.0	489.0	250	196.8	21.3%	9	23.4	9.4%	11.1	50.3	43.9	53.8	12.9	1.4	1.7	173.4	100.92	855
T36	11.0	497.0	250	194.4	22.2%	8.6	22.7	9.1%	5.5	30.6	38.4	67.1	24.4	5.7	3.1	171.7	101.92	812

Table A.2. Dataset example of expert assessment in arabica SCA protocol

MUESTRAS	FRAGANCIA/ AROMA	SABOR	SABOR RESIDUAL	ACIDEZ	CUERPO	UNIFORMIDAD	BALANCE	TAZA LIMPIA	DULZOR	PUNTAJE CATADOR	PUNTAJE SCA TOTAL	DESCRIPTORES
Ensayo C1	8.0	8.3	8.0	8.0	8.0	10.0	8.0	10.0	10.0	8.3	**86.5**	Caramelo, cacao dulce
Ensayo C2	8.0	8.3	8.0	8.0	8.0	10.0	8.3	10.0	10.0	8.3	**86.8**	Caramelo, chocolate amargo
Ensayo C3	8.0	8.0	8.0	8.0	8.0	10.0	8.0	10.0	10.0	8.0	**86.0**	Melaza, caramelo,
Ensayo C4	8.0	8.3	8.0	7.8	7.8	10.0	7.8	10.0	10.0	8.0	**85.5**	cacao, mandarina
Ensayo C5	8.1	8.0	8.0	7.9	8.0	10.0	7.9	10.0	10.0	7.9	**85.8**	Panela, miel caramelo, moras
Ensayo C6	8.0	7.9	7.9	7.8	7.9	10.0	7.8	10.0	10.0	7.8	**84.9**	Frutos amarillos, caramelo
Ensayo C7	7.9	7.8	8.0	7.8	7.8	10.0	7.8	10.0	10.0	7.8	**84.6**	Panela, nuez moscada, chocolate amargo
Ensayo C8	8.0	7.9	7.9	7.8	7.8	10.0	7.8	10.0	10.0	7.6	**84.6**	Manzana, achocolatado, afrutado
Ensayo C9	7.9	7.9	7.9	7.8	7.8	10.0	8.0	10.0	10.0	7.8	**84.9**	Panela y cítrico, frutal piña
Ensayo C10	8.1	8.1	8.1	8.1	7.9	10.0	8.0	10.0	10.0	8.0	**86.4**	Caramelo, limón, avinado
Ensayo C11	8.0	8.0	7.9	7.8	7.8	10.0	7.8	10.0	10.0	7.8	**84.9**	afrutado, floral
Ensayo C12	8.3	8.4	8.4	8.1	8.0	10.0	8.0	10.0	10.0	8.0	**87.1**	panela, floral, dulce, caramelo
Ensayo C13	8.0	8.0	8.0	8.3	8.0	10.0	8.0	10.0	10.0	7.8	**86.0**	Avellana, caramelo
Ensayo C14	8.0	8.5	8.3	8.0	8.0	10.0	8.3	10.0	10.0	8.3	**87.3**	achocolatado, frutos rojos, avellana
Ensayo C15	8.3	7.8	7.8	8.0	8.0	10.0	8.0	10.0	10.0	7.8	**85.5**	caramelo, fresas
Ensayo C16	8.3	8.0	8.0	8.0	8.0	10.0	8.0	10.0	10.0	7.8	**86.0**	manzana, achocolatado
Ensayo C17	7.8	7.9	7.9	7.8	7.9	10.0	7.9	10.0	10.0	7.6	**84.6**	Melocoton, panela
Ensayo C18	7.9	7.9	7.9	8.0	8.0	10.0	8.0	10.0	10.0	7.9	**85.5**	Frutal, achocolatado, miel, pimienta, herbal, vinoso
Ensayo C19	8.0	8.0	7.9	7.9	7.9	10.0	7.9	10.0	10.0	7.9	**85.4**	Chocolate afrutado
Ensayo C20	7.8	7.9	8.0	7.8	7.8	10.0	7.8	10.0	10.0	7.8	**84.6**	Frutos secos, achocolatado, afrutado, Avellana
Ensayo C21	7.8	8.0	8.3	8.0	8.0	10.0	7.8	10.0	10.0	8.0	**85.8**	Chocolate afrutado, melaza
Ensayo C22	8.0	7.5	7.5	7.8	7.8	10.0	7.4	10.0	10.0	7.3	**83.1**	Caramelo, intenso. Se repite porque la tostión no fue la ideal
Ensayo C23	8.0	7.9	7.9	8.0	7.9	10.0	8.0	10.0	10.0	8.0	**85.6**	caramelo intenso
Ensayo C24	7.6	8.0	8.0	7.8	7.8	10.0	7.8	10.0	10.0	7.9	**84.8**	Vinoso, afrutado, frutos secos
Ensayo C25	8.0	7.8	7.8	7.8	8.3	10.0	7.8	10.0	10.0	7.5	**84.8**	caramelo, flor de jamaica
Ensayo C26	8.0	8.0	8.0	8.3	8.3	10.0	8.0	10.0	10.0	7.8	**86.3**	afrutado
Ensayo C27	8.3	7.5	7.5	8.3	8.3	10.0	7.5	10.0	10.0	7.3	**84.5**	frutos amarillos, caramelo
Ensayo C28	8.3	8.0	8.0	8.0	8.3	10.0	8.3	10.0	10.0	8.0	**86.8**	Manzana, miel, chocolate amargo
Ensayo C29	7.8	8.0	8.0	7.8	7.8	10.0	8.0	10.0	10.0	8.0	**85.3**	Afrutado
Ensayo C30	7.8	7.8	7.8	7.8	7.8	10.0	7.5	10.0	10.0	7.5	**83.8**	Canela, mora
Ensayo C31	7.3	7.5	7.5	8.0	7.5	10.0	7.5	10.0	10.0	8.0	**83.3**	Frutal, intenso
Ensayo C32	7.5	7.5	7.5	7.5	7.5	10.0	7.5	10.0	10.0	7.5	**82.5**	Afrutado
Ensayo C33	8.0	7.8	7.8	7.5	7.5	10.0	8.0	10.0	10.0	8.0	**83.0**	Afrutado suave
Ensayo C34	7.3	7.5	7.5	7.8	7.8	10.0	7.5	10.0	10.0	7.5	**82.8**	Frutos rojos, frutal
Ensayo C35	7.5	7.5	7.5	7.8	7.8	10.0	7.8	10.0	10.0	7.8	**83.5**	Dulces poco intensos

Ensayo C36	7.8	7.8	7.8	8.0	8.0	10.0	7.5	10.0	10.0	7.5	**84.3**	Afrutado kiwi
Ensayo T1	8.0	8.3	8.3	8.0	8.0	10.0	8.0	10.0	10.0	8.0	**86.5**	cacao
Ensayo T2	8.0	8.0	8.0	8.0	8.3	10.0	8.0	10.0	10.0	8.0	**86.3**	caramelo, miel
Ensayo T3	8.0	8.0	8.0	8.3	8.0	10.0	7.8	10.0	10.0	7.8	**85.8**	caramelo, miel
Ensayo T4	8.0	8.0	8.0	8.3	8.0	10.0	8.0	10.0	10.0	8.0	**86.3**	avellana, afrutado
Ensayo T5	8.0	7.5	7.5	7.6	7.6	10.0	7.6	10.0	10.0	7.5	**83.4**	Frutal, moras, fresa, uvas pasas
Ensayo T6	8.0	8.0	8.0	7.9	8.0	10.0	7.8	10.0	10.0	7.9	**85.5**	Frutos rojos dulces, melaza, durazno, intenso
Ensayo T7	8.0	7.9	7.8	7.9	8.0	10.0	7.9	10.0	10.0	7.8	**85.1**	intenso achocolatado amargo
Ensayo T8	8.3	8.1	7.9	8.0	7.9	10.0	7.5	10.0	10.0	7.5	**85.1**	Chocolate afrutado, dulce, caramelo, uvas
Ensayo T9	8.3	8.1	7.9	8.0	7.9	10.0	7.5	10.0	10.0	7.5	**85.1**	Chocolate afrutado, dulce, caramelo, uvas
Ensayo T10	8.0	7.9	7.8	7.9	8.0	10.0	7.9	10.0	10.0	7.8	**85.1**	Afrutado, miel
Ensayo T11	8.0	7.9	7.9	8.0	8.0	10.0	7.9	10.0	10.0	7.9	**85.5**	Suave, fino, melaza, frutos dulces
Ensayo T12	7.8	7.9	7.8	7.8	7.9	10.0	8.0	10.0	10.0	8.0	**85.0**	Dulce, frutal, miel
Ensayo T13	8.3	8.0	8.0	8.0	8.0	10.0	7.8	10.0	10.0	7.8	**85.8**	cítrico, avellanas
Ensayo T14	8.0	8.0	8.0	8.0	8.0	10.0	7.8	10.0	10.0	7.8	**85.5**	frutos amarillos, chocolate, miel
Ensayo T15	7.8	8.0	8.0	8.0	8.0	10.0	7.8	10.0	10.0	7.5	**85.0**	chocolate, avellanas
Ensayo T16	8.0	8.3	8.3	8.0	8.0	10.0	8.0	10.0	10.0	8.0	**86.5**	frijol, poco intenso, cacao, afrutado
Ensayo T17	8.3	8.4	8.1	8.0	8.3	10.0	8.0	10.0	10.0	8.1	**87.1**	Achocolatado, afrutado durazno
Ensayo T18	8.0	7.3	7.5	7.5	7.8	10.0	7.5	10.0	10.0	7.3	**82.8**	Se repite porque la tostión no fue la ideal
Ensayo T19	7.9	7.9	7.9	7.9	7.9	10.0	7.6	10.0	10.0	8.1	**85.1**	Chocolate amargo afrutado, caramelo, miel
Ensayo T20	7.9	7.9	7.9	8.0	7.8	10.0	8.0	10.0	10.0	8.0	**85.4**	Afrutado, citrico, frutos rojos, caramelo
Ensayo T21	8.0	8.0	7.9	7.6	7.9	10.0	7.8	10.0	10.0	7.9	**85.0**	afrutado, dulce, miel
Ensayo T22	7.0	7.5	7.5	7.5	7.4	10.0	7.4	10.0	10.0	6.8	**81.0**	Se repite porque la tostión no fue la ideal
Ensayo T23	8.0	8.0	8.0	7.8	7.8	10.0	8.0	10.0	10.0	8.0	**85.5**	Caramelo, chocolate
Ensayo T24	8.0	7.8	7.8	7.5	8.0	10.0	7.8	10.0	10.0	7.8	**84.5**	Dulce
Ensayo T25	7.8	8.0	8.0	8.0	8.3	10.0	8.0	10.0	10.0	7.8	**85.8**	Afrutado intenso, moras, cítrico
Ensayo T26	7.8	7.3	7.3	8.0	8.3	10.0	7.0	10.0	10.0	6.3	**81.8**	Se repite porque la tostión, no fue la ideal
Ensayo T27	8.3	8.5	8.5	8.5	8.3	10.0	8.5	10.0	10.0	8.3	**88.8**	Caramelo, avellana
Ensayo T28	8.3	8.3	8.0	8.0	8.3	10.0	7.8	10.0	10.0	7.8	**86.3**	Chocolate amargo, manzana
Ensayo T29	8.0	7.8	7.8	7.8	7.8	10.0	8.0	10.0	10.0	8.0	**85.0**	Afrutado dulce
Ensayo T30	8.3	7.8	7.5	7.5	7.8	10.0	7.8	10.0	10.0	7.8	**84.3**	Frutal intenso
Ensayo T31	7.8	7.5	7.5	7.8	7.8	10.0	7.5	10.0	10.0	7.5	**83.3**	Caramelo, nuez, suave
Ensayo T32	7.8	7.5	7.5	7.5	7.8	10.0	7.5	10.0	10.0	7.5	**83.0**	Caramelo, chocolate, afrutado, complejo
Ensayo T33	7.8	7.8	7.8	7.8	7.5	10.0	7.5	10.0	10.0	7.5	**83.5**	Dulce afrutado
Ensayo T34	8.0	7.8	7.3	7.8	7.5	10.0	7.5	10.0	10.0	7.5	**83.3**	Chocolate afrutado
Ensayo T35	8.0	7.8	7.3	7.5	7.5	10.0	8.0	10.0	10.0	7.8	**83.8**	Chocolate avellana
Ensayo T36	8.0	7.8	7.8	7.5	8.0	10.0	7.8	10.0	10.0	7.8	**84.5**	Panela, caña, caramelo, chocolate seco

B. Appendix. Roast profiling protocol

The physical properties of the raw coffee were used to define the reference roasting curve in the roaster. 250g of specialty coffee beans were used to obtain the reference trials in a PROBAT sample roaster gas driven. Reference S curve sets the loading temperature and gives guidelines for the ranges of volume gain and mass loss of roasted coffee beans that guarantee consistency in the process. The desired roasting profiles was recreated by matching the temperatures and times of the current roast with the temperatures and times in the reference. Consistent results can be obtained if a certain amount of heat is applied to a batch at a given time. The roasting reference profiles trials ranged from high temperature short time (HTST) to low temperature long time (LTLT) roasting, and from medium to dark roast degree according to (Gloess et al., 2014). HTST profiles aims to accentuate the acidity and the LTLT to accentuate the body.

The coffee profiling allowed us to obtain a general panorama of the behavior of green coffee in relation to the roaster technology and its way of transferring heat. To conduct this profiling, 8 samples were prepared using 250 g per sample. Then, the samples for the profiling assay were roasted following the references of the 8 Agtron SCA discs, to obtain 8 roasting colors: 25-Very Dark, 35-Dark, 45-Moderately Dark, 55-Medium, 65-Light Medium, 75-Moderately Light, 85-Light, and 95-Very Light. The samples were labeled as M1, M2, M3, M4, M5, M6, M7, M8, respectively. Considering that the region of interest for this project is the mid-tones, samples 35-85 were analyzed, removing the least roasted (95) and the most roasted (25). The exclusion criterion for profiling is based on the fact that the less browned sample will have an underdevelopment defect and the more browned one will have an overdevelopment defect (Giacalone et al., 2019).

The samples of roasted and ground coffee have variation factors: producing region, species, variety, postharvest process, drying conditions, transport, storage, coffee composition, roasting process, coffee blend, and intra and inter batch variations. To characterize the beans and ground coffee for the experimental scheme a Near infrared spectroscopy - NIR, Hyperspectral images and industrial colorimetry was used.

NIR-Spectroscopy

The objective of the near infrared spectroscopy was to correlate the sensory attributes of the coffee with the spectral bands and thus classify the samples by SCA disc roasting levels (From dark to light color samples M8=25, M7=35, M6=45, M5=55, M4=65, M3=75, M2=85, M1=95). This technique was used as a pilot test to study the phenomena associated with the development of the roasting curve. For this test, the NIR Hamamatsu 896-1684 nm system of the physical properties laboratory TAGRALIA research group -Técnicas Avanzadas en Agroalimentación of the Polytechnic University of Madrid, Spain, was used. The test consisted of 3 trials for each coffee sample, however, we proceeded to exclude the less roasted 95 and the more roasted 25 samples, because, according to their characteristics in the SCA protocol, in the less roasted one some important sensory characters in the aroma and flavor of coffee have not been developed and in the more roasted one the defects can be masked. Therefore, 6 samples per coffee batch were left, M2 to M7, both roasted coffee beans and roasted ground coffee. Samples were prepared in triplicate, using 5 g of roasted coffee in 10 cm^3 containers.

Hyperspectral images

To complement the roasted coffee profiling information, including the color for roasted coffee, a hyperspectral camera was used, which combines the infrared and visible spectrum band to obtain a spectrum or fingerprint of the product, in a wider range, particularly for the spectral fingerprint of interest for coffee. An EMCCD Luca-R camera (AndorTM Technology, Northern Ireland) equipped with a Hyperspec® VNIR- HS-VNIR 1002A-00451 spectrograph (spectral range: 400-1,000 nm) from TRAGALIA- UPM spain lab was used for this test.

Hyperspectral system was configured to obtain 189 wavelengths (spectral resolution 3.17 nm). Image acquisition and storage were performed through a specific software algorithm using Endviread in MATLAB. Illumination was provided by two halogen lamps in the physical property's laboratory TAGRALIA research group -Técnicas Avanzadas en Agroalimentación of the Universidad Politécnica de Madrid- Spain. A generalized RAW file was obtained, which was processed with the MATLAB digital image processing tool, and a script developed to obtain the calibrated hyperspectral profile of the system by analyzing the samples in triplicate. Hyperspectral images were used for samples profiling classification by roasting degrees. Each of the photographs was processed and the spectra of the coffee samples at the six roasting levels were consolidated, taking 200 pixels for each, in the 189 bands studied.

Industrial colorimetry

One of the challenges in the traceability of the industrial roasting process is to measure coffee bean color and validate the quantification of roasted coffee color. The Konica Minolta CM700d colorimeter of the physical property's laboratory TAGRALIA- Técnicas Avanzadas en Agroalimentación of the Polytechnic University of Madrid-Spain was used to characterize the color of coffee beans and ground coffee. The technique of this colorimeter is based on a 2° observer protocol and a standard diffuse illumination known as D65 or d6,500 coupled to a spectrophotometer. For roasted coffee, the colorimeter configuration emphasizes the CIELAB color planes, and the 800 nm band of the near infrared.

COLORIMETRIC PROTOCOL FOR COFFEE SAMPLES

The infrared absorption bands for water result from rotational and vibrational transitions, and are found around 1,200 and 1,450 nm, as shown in Figure B.1.

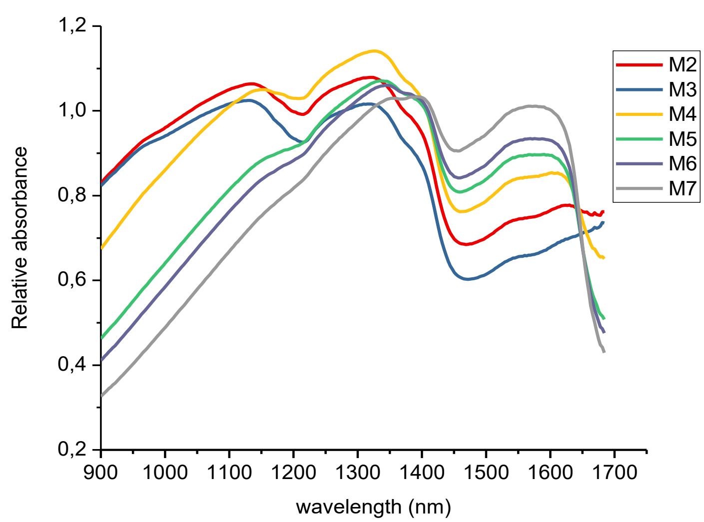


Figure B.1. NIR spectra obtained for roasted coffee.

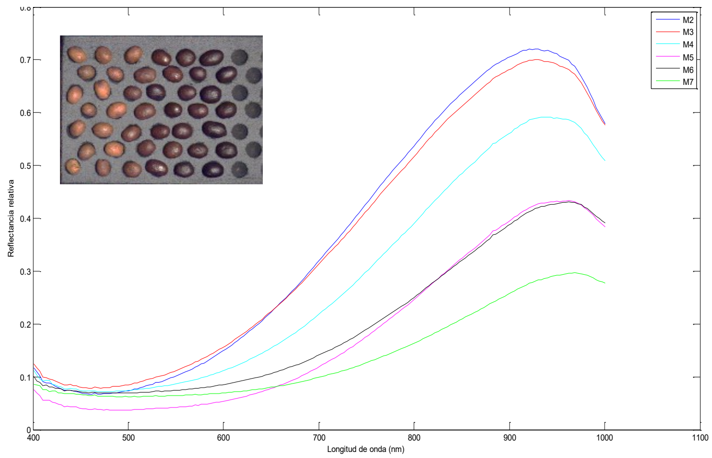
The preliminary results of the NIR test for the 6 samples, it is observed that in the band from 900 nm to 1,100 nm approximately, a linear region with a change of slope can be distinguished for each of the roasting levels studied. The less roasted, the higher the relative infrared reflectance and the more roasted, the lower the received signal.

The gradual reduction of the intensity in the water-related bands is related to the decrease in moisture content due to the process of increased heat transfer. Here it is observed that the lighter colored samples M2, M3 and M4 still have presence of the water band, however, this is due to structural water. The spectral regions for observing sucrose content, for example, is 1,600-1,680 nm (Catelani et al., 2018), where a decomposition of the sugar bands is observed for the samples with the highest level of roasting (M5, M6, M7), suggesting that they have undergone the process of sugar reduction to a certain degree, which is reflected in the caramelization process. In addition, several important compounds related to the quality of roasted coffee are spectrally active in these regions as a result of the decomposition of amino acids, the reduction of sugars, the degradation of chlorogenic acids and the formation of esters, aldehydes and other volatile and non-volatile compounds as reported in the literature (Catelani et al., 2018; Giacalone et al., 2019; Yang et al., 2016).

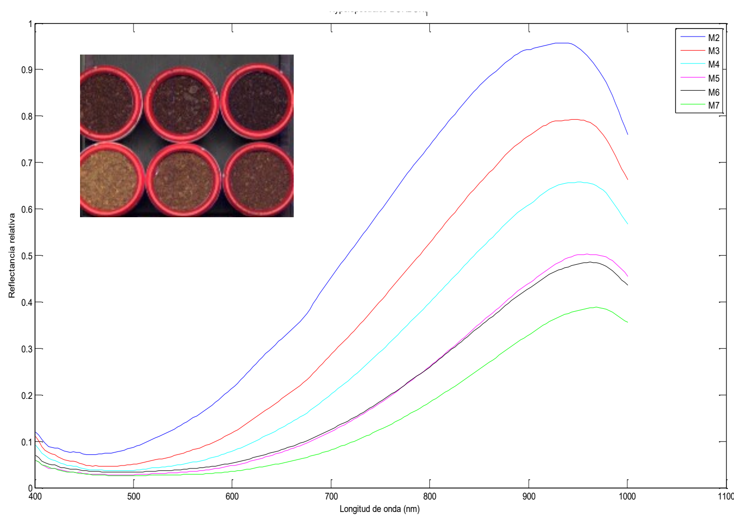
In the region from 900 to 1,100 nm, the linear region can be observed, to distinguish between each roasting level. In the ANOVA analysis of the NIR spectrum in this range, with $p<0.05$ level, significant differences were found that would allow identifying the level of roasting of the sample based on calculations of the slope of the spectrum, for example, associated to time and temperature conditions. These variables correspond to previous data that were used as input for the roasting protocol of the project samples.

Hyperspectral Imaging Technique

The results of the hyperspectral imaging experiment are shown in Figure B.2.



(a)



(b)

Figure B.2. Hyperspectral profiles of roasted (a) whole bean and (b) ground coffee images in 189 bands from 400 to 1,000 nm, for roast levels M2-M7.

The differences between each spectrum can be observed in two areas: the steep valley between 400 and 750 nm and the peak at 900 and 1,000 nm. The visible region of the spectra (400-750 nm) depends on the absorbance of the different compounds generated by the development of the Maillard and caramelization reactions, however, in this region it is very narrow. On the other hand, in the infrared region, a greater differentiation between the tones of roasted coffee is displayed and a region between 800 and 900 nm can be noted where a study of the slope of the profile can be carried out to differentiate each level of roasting. The sample with the highest relative reflectance is M2 (blue) and the one with the lowest reflectance is

M7 (green). M2 represents the light roasting level sample and M7 a dark roasting level. When ANOVA analysis was performed, with significance level $p<0.05$, it was found that there were significant differences in the range (750-1,000 nm) in the roasted and ground samples. Particularly, for the grain samples, significant differences were only found in M2, M4, and M7, this effect is since the surface of the grain samples is not homogeneous. The preparation protocol for roasted and ground samples is taken as a reference to avoid this inconvenience.

Due to the complexity of defining the color of roasted coffee beans, the multispectral images in the 900-1,000 region are left as a reference for future work.

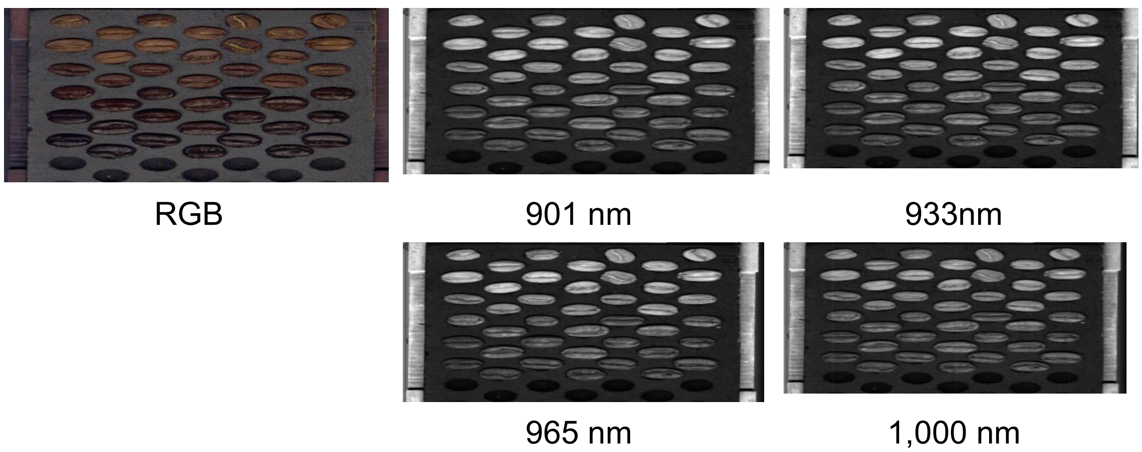


Figure B.3. Underside spectral images from 900-1,000 nm tabi coffee roasted beans.

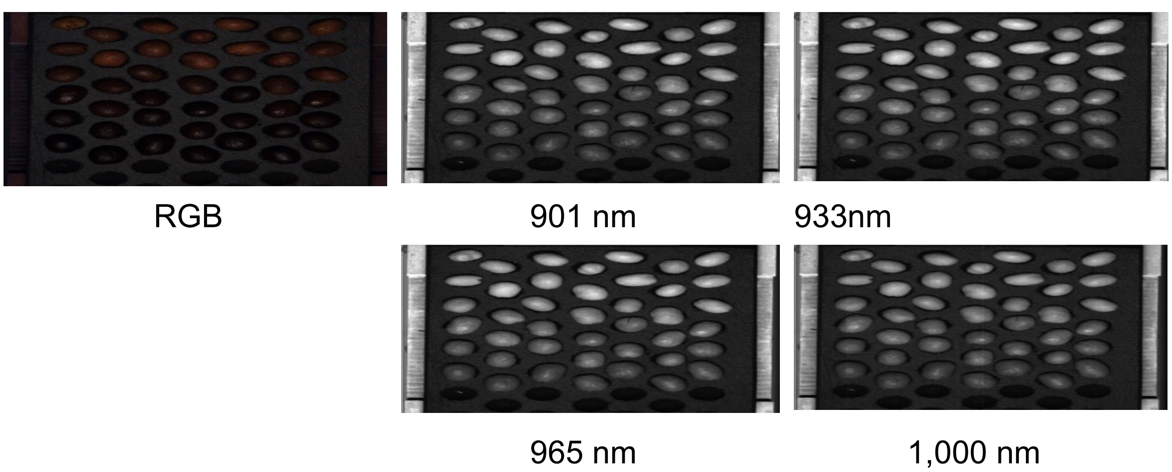


Figure B.4. Top side spectral images from 900-1000 nm tabi samples. Only 4 bands extracted.

Industrial Colorimetry Techniques

The exploratory results of this test for the roasted coffee samples are presented in Table B.1 below.

Table B.1. Konica Minolta data of 6 roasted coffee samples.

Sample	L*(D65)	a*(D65)	b*(D65)
M2	28.87	9.22	9.71
M3	28.99	9.32	9.94
M4	25.22	7.74	4.82
M5	20.01	4.34	-1.39
M6	19.69	3.53	-2.31
M7	17.98	2.3	-4.01

The data show a decrease in the L-plane with increasing degree of browning. The a* and b* parameters can evaluate hue and chroma in these controlled illumination conditions and in the visible and infrared regions configured. It is necessary to consider the particle size and distance to the sensor to ensure measurement consistency, based on the manufacturer's measurement scheme for coffee. This represents an input to determine that the standard illumination factor, particle size and measurement distance should be considered for color measurement, according to the standards recognized by the SCA. The variables associated with the color of roasted coffee and evaluated so far are Wavelength of radiation used for color measurement. Red band in the visible (700 nm) and infrared (800 to 1,100 nm). L, a* and b* parameters in the CIELAB color space and color indicators Chroma, Hue, Browning index (BI) (Benitez & Campo-Ceballos, 2018).

Roast profiling protocol for accepted samples

Coffee profiling is the first way to know the potential of a specialty coffee. After selecting the coffee and guaranteeing its homogeneity and known physical properties, we proceed to roast it in eight different profiles, standardized by the SCA, to know its organoleptic potential. The final assessment is given by a certified q-grader expert as a basis for optimizing any attribute later. The profiling analysis was carried out with samples M1-M8, both in beans and ground. According to SCA standards, 8 samples were roasted with light to dark profiles and correlate with the spectral bands and the degree of roasting of the samples. Figure B.5 shows the roasted coffee beans after profiling.

Figure B.5. Samples of roasted coffee beans.

Currently coffee roasters use a series of visual standards developed by the SCA to grade the roast level of their coffee products. This crude visual scale, figures B.5 and B.6 works well for classifying the color of coffee, but at only eight grades, it does not offer great resolution for grading the roast of coffee in process. In addition, as with any visual grading system, human subjectivity introduces a level of error. In this work NIR-spectroscopy, hyperspectral images and industrial calorimetry correlation was obtained. The images of roasted and ground coffee are shown in Figure B.6.

In the follow-up of roasting based on color, we developed a coffee colorimetric device and its software called PICAFÉ - registered with the national copyright office - DNDA #:13-73-33 to measure the color of the coffee bean, adopting the results of profiling. PICAFÉ works with the correlation between NIR spectroscopy, Hyperspectral imaging, and industrial colorimetric techniques to evaluate the color of roasted coffees in this work. The main result of this process was to correlate the SCA color disc with NIR, hyperspectral and CIE Lab color space.

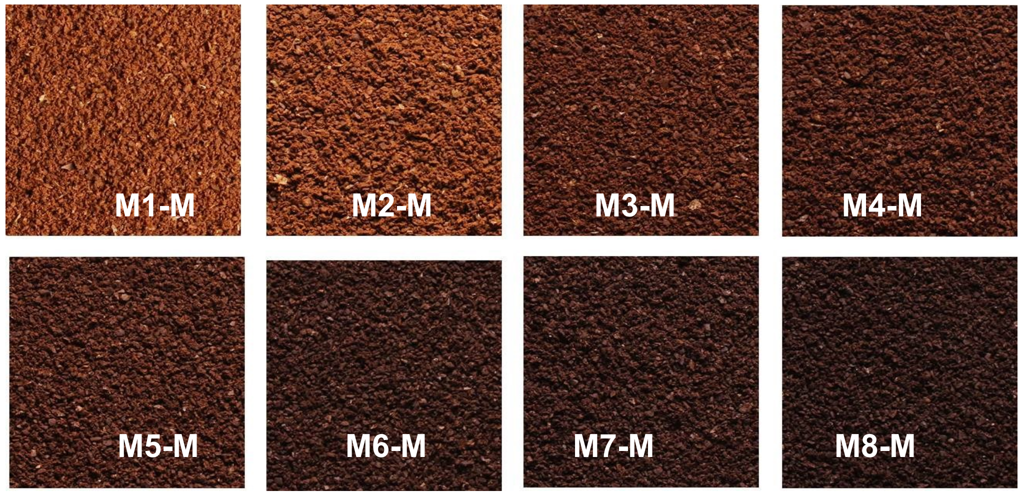


Figure B.6. Samples of roasted ground coffee.

Table B.2 presents six samples characterized with colorimetric techniques. Appendix B presents all NIR & hyperspectral spectra and industrial colorimetric data. The spectra highlight wavelength (NIR 1,000 nm and 1,600 nm. Hyperspectral images 800 nm) bands and trends allowing a clear separation among the different coffee samples.

Table B.2. Six ground coffee samples from SCA profiles correlated with NIR, Hyperspectral images and industrial colorimetric technique.

SCA DISC	NIR (abs) 1000 nm	NIR (abs) 1600 nm	Hyperspectral (reflectance 800 nm)	L*	a*	b*
M2=35	0.96	0.76	0.74	28.87	9.22	9.71
M3=45	0.94	0.67	0.52	28.99	9.32	9.94
M4=55	0.86	0.85	0.40	25.22	7.74	4.82
M5=65	0.64	0.89	0.26	20.01	4.34	-1.39
M6=75	0.58	0.93	0.26	19.69	3.53	-2.31
M7=85	0.48	1.00	0.18	17.98	2.3	-4.01

In this study we set out to understand how the relative absorbance in the NIR spectrum correlates to SCA (Agtron) roast numbers and how the reflectance % in the Hyperspectral band 800 nm compares to the CIE Lab industrial colorimetric range of roasted coffee samples. This result allowed us to evaluate the degree of roasting of Castillo and Tabi coffee as a new tool proposed to support the quality control of coffee. Figure B.7 show that a strong correlation between the measurements exists and support the premise that either wavelength will provide suitable results.

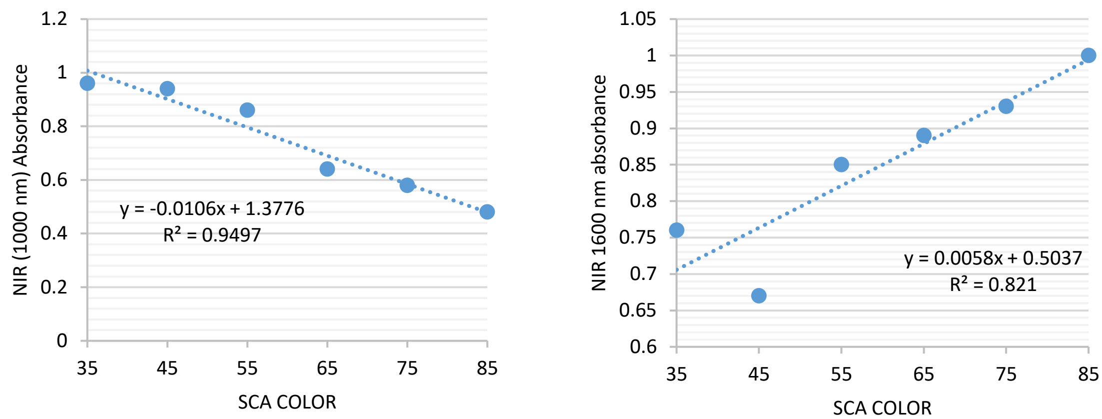


Figure B.7. Correlation between SCA number and NIR absorbance at 1,000 nm and at 1,600 nm for 6 ground coffee samples.

Also, for Hyperspectral 800 nm reflectance and CIE Lab industrial colorimetry.

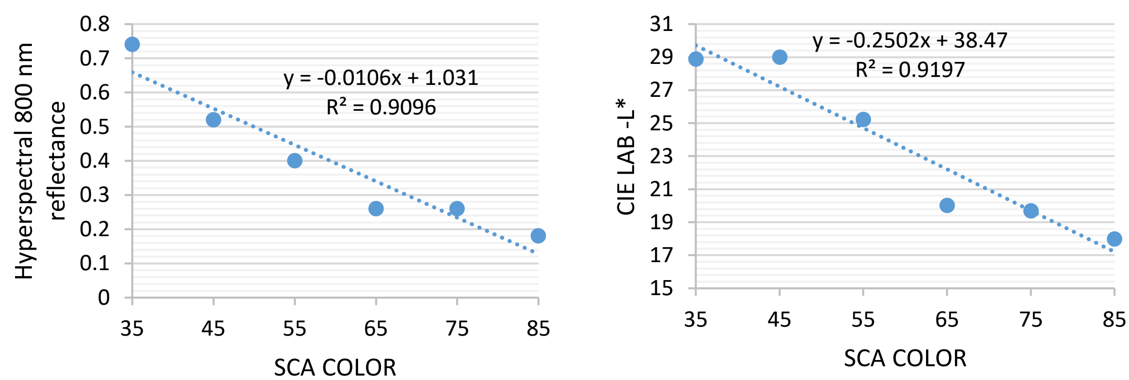


Figure B.8. Hyperspectral 800 nm reflectance and CIE Lab- L coordinate correlation with SCA color

PICAFÉ system provide more objective and precise color measurement results for determining the degree of roasting coffee. These results were presented in CIIMA 2019, international congress of mechatronics engineering.

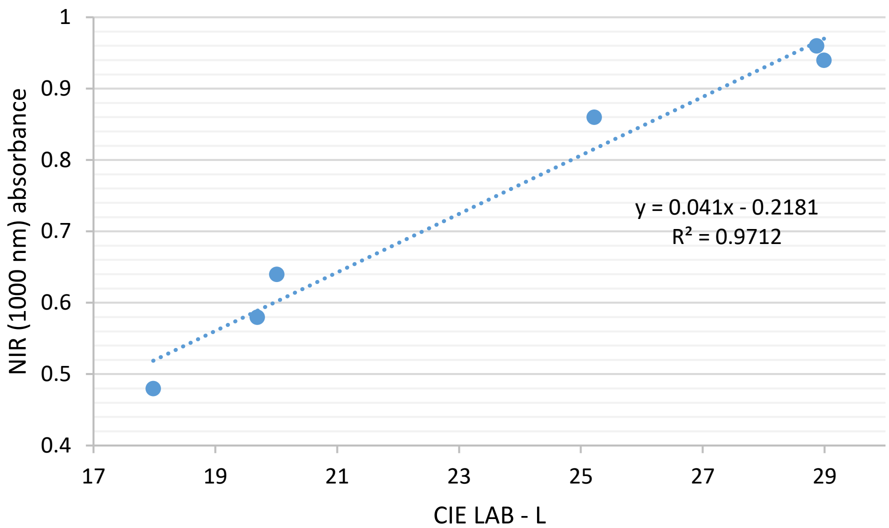


Figure B.9. Industrial CIE Lab correlation witn NIR 1,000 nm band.

Color is an indicator of coffee quality and could affect the perceived sensory characteristics. Although this result is not new in coffee, our results suggest that proper control of the roasting level could produce the desired colors for new coffee products.

In the coffee industry, sensory analysis has become a highly valuable tool, due to its capacity to correctly process an enormous number of variables related to product attributes. Depending on the objectives of the project or research, the profile of the tasters may vary, as well as the level and time of training (Gutiérrez G. & Barrera B., 2016). As part of the project, the criteria of a panel of CQI experts with a Q-Grader level from the departmental committee of coffee growers of Cauca, CAFICAUCA, were used as a reference to evaluate the coffee samples studied, aligned with the protocols of the association of specialty coffees SCA. Figure B.10 shows the 10 attributes evaluated by the SCA format, corresponding to the sensory perception of the panel of experts.

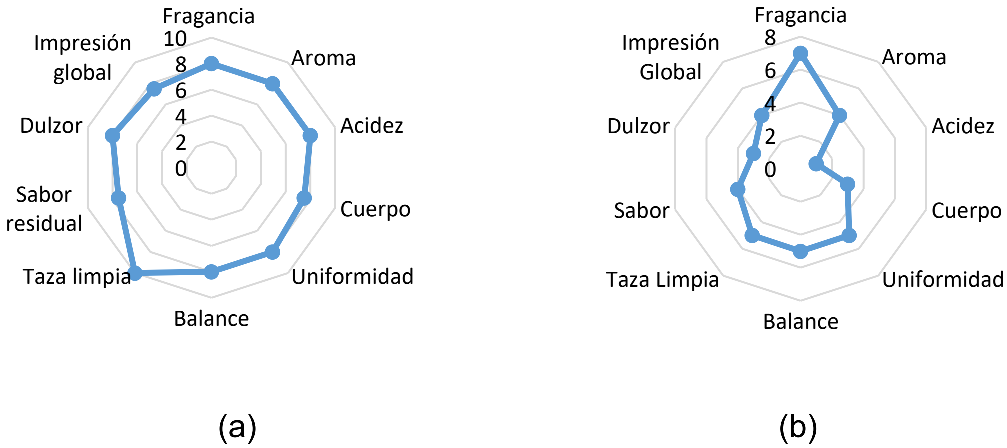


Figure B.10. Sample cup profile (a) M4 (medium) and (b) M7 (high).

For example, for medium roasts M3-M4, the attributes of acidity and body, which are the objective of the assessment, are maintained at intermediate levels (score 8) related to the roasting curve of the sample.

C. Appendix. Intensity survey for consumers assessment

Universidad del Cauca	**TITULO DE LA INVESTIGACIÓN:** Estudio de la percepción del consumidor de café Castillo y Tabi. Se darán a probar 13 bebidas de café. Se solicita evaluar la intensidad percibida en la escala de 0-15. Los atributos a medir son acidez, cuerpo y color **RESPONSABLE:** Diego Andrés Campo Ceballos - Doctorado en Ciencias de la Electrónica- FIET-UNICAUCA. **Director:** PhD. Carlos Alberto Gavíria López

Yo (Nombre)		**Edad**		**Sexo**	M	F

Autorizo el uso y la divulgación de mi información para el desarrollo de la investigación descrita anteriormente. Acepto voluntariamente participar y sé que tengo el derecho de terminar mi participación en cualquier momento. Al firmar esta hoja de consentimiento Informado no he renunciado a ninguno de mis derechos legales.

Para constancia, firmo a los ______ dias del mes de ______ del año __________

FIRMA: ________________________ CC/TI: _________________

APRECIADO PARTICIPANTE

1. Realice el proceso de inducción a la prueba. Practique con la escala 0-15.
2. Por favor marque evalúe el nivel de intensidad percibido según la referencia para acidez, cuerpo y color.

(0=nada, 2=apenas detectable, 4=Identificable, pero poco intenso, 6=Ligeramente intenso, 8=Medianamente intenso, 10=Intenso, 12=Muy intenso y 15=Extremadamente intenso)

25-Muy oscuro, 35-Oscuro, 45-Medio oscuro, 55-Medio, 65-Medio claro, 75-Medio claro, 85-Luz y 95-Muy claro

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15) — **Compare el Color del café en grano/molido**

Acidez	**Cuerpo**	**Color (25-95)**

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15) — **Compare el Color del café en grano/molido**

Acidez	**Cuerpo**	**Color (25-95)**

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15) — **Compare el Color del café en grano/molido**

Acidez	**Cuerpo**	**Color (25-95)**

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15) — **Compare el Color del café en grano/molido**

Acidez	**Cuerpo**	**Color (25-95)**

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15) — **Compare el Color del café en grano/molido**

Acidez	**Cuerpo**	**Color (25-95)**

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

TAZA ____

¿Escriba el nivel de intensidad percibido? Escala (0-15)

Compare el Color del café en grano/molido

Acidez	Cuerpo	Color (25-95)

D.Appendix. Warm Up a Roaster Protocol

This research recommend the following procedure to determine an effective warm-up protocol for the roaster, to obtain consistency in the roasting samples (Rao, 2019).

1. Set the airflow to the average level you will use during your roasts.
2. Using a medium-to-high gas setting, warm up the machine until the bean probe indicates 50°F (28°C) above your intended charge temperature.
3. Idle the machine at that temperature for 20 minutes.
4. Lower the gas setting so the temperature drops gradually.
5. Once the probe displays the charge temperature, idle the machine at that temperature for 10 minutes.
6. Charge the first batch.
7. Roast the first batch, using the same gas and airflow settings you would for a batch later in the day.
8. Compare this batch to the results you would typically get later in a roast session. If this batch roasted faster than desired, lower the peak warm-up temperature next time. If this batch was slow, idle at the peak warm-up temperature for a longer time.
9. Repeat step 8 each day, until your first batch behaves exactly as batches later in a roast session do.

Between-Batch Protocol

To maintain protocol between batches, an identical procedure should be followed after each batch to restore the roaster's thermal energy to the desired level before loading the next batch.

1. Decrease the airflow to the lowest level you will use during a roast batch.
2. Turn off the gas for 1 minute after dropping a roast batch. Adjust the gas to a setting that will bring the temperature probe to the intended charge temperature in 60-90 s.
3. Once the charge temperature is reached, idle there for 1 minute.
4. Charge the next batch.

Based on experimentation, these protocols should allow anyone to produce roasts that follow the expected profiles almost identically in each batch, with total roasting times varying no more than 5-10 s per batch.

Consumers protocol for perception (Rao, 2019)

Consumers were pre-trained with a perception protocol in CATA test.

1. Recognize the cups, taking a moment to smell each one.

2. After 4 minutes have elapsed, “break the crust” of the cups in the order in which they were poured. To break the crust, dip the bowl of a cupping spoon halfway into the coffee, push aside the crust of grounds with the back of the spoon, and bring your nose close to the surface of the coffee without touching the grounds with your nose. Sniff the aromatics released as you break each crust.

3. Inhale slowly and deeply as you break each crust. Long, slow inhalations provide better aroma detection than short sniffs. Take notes on your impressions.

4. After breaking all the crusts, remove the grounds, foam, and oils from the surface of the cups. An efficient method is to skim the surface using two cupping spoons simultaneously.

5. At 9:00 min, begin tasting the coffees. Dip a cupping spoon just below the surface of the coffee, raise it to your lips, and vigorously slurp the coffee, spraying it throughout your mouth. Tasting the coffees at the highest temperature you can comfortably tolerate, but not before 9 minutes have elapsed.

6. Focus on the coffee’s aromatics, mouthfeel, flavor, and other impressions. Take notes.

7. Spit out the coffee. If you are not sampling too many coffees in the session, consider swallowing the occasional spoonful. Swallowing promotes retro nasal olfaction and ensures the cupper exposes his farthest-back taste buds to a sample.

8. Move on to the other coffees, slurping and spitting as needed to get sufficient impressions of all of them. There is no need to “cleanse the palate” between each slurp, but swishing some water in the mouth every few minutes may help refresh the taste buds and forestall palate fatigue.

9. Record copious notes while cupping.

10. Take a break for five minutes. Slurp and spit the coffees again when they are lukewarm.

11. Allow the coffees to cool to room temperature, about 15-30 minutes, and repeat the process of slurping and spitting. You will find the coffees offer much new information after they have cooled.

All process of cupping coffees occurs 24 hours after coffee samples were roasted.

E. Appendix. MATLAB script to extract ALOG roasting files information.

```
function [d_timex,d_temp1,d_temp2] = alog2excel(filename)

input_filename = filename(1:end-4);
output_filename = [input_filename,'.xlsx'];
sheet = 1;
cell = 'A1';
%% Lectura de campos del archivo

[fid,errmsg] = fopen(filename);
if fid < 0
    disp(errmsg);
    return;
end
% Cadena timex
tline = fgetl(fid);
cad_timex = 'computed';
scadena = size(cad_timex,2);
ind = strfind(tline,cad_timex);
fseek(fid,ind(1)-1,'bof');
tline2 = fgetl(fid);
ind2 = strfind(tline2,'}');
fseek(fid,ind(1)+scadena+3,'bof');
tline3 = fgets(fid,ind2(1)-scadena-5);
d_timex = str2num(tline3)';

% Cadena temp1
% frewind(fid);
% tline = fgetl(fid);
% cad_temp1 = 'temp1';
% scadena = size(cad_temp1,2);
% ind = strfind(tline,cad_temp1);
% fseek(fid,ind(1)-1,'bof');
% tline2 = fgetl(fid);
% ind2 = strfind(tline2,']');
% fseek(fid,ind(1)+scadena+3,'bof');
% tline3 = fgets(fid,ind2(1)-scadena-5);
% d_temp1 = str2num(tline3)';

% Cadena temp2
frewind(fid);
tline = fgetl(fid);
cad_temp2 = 'temp2';
scadena = size(cad_temp2,2);
ind = strfind(tline,cad_temp2);
fseek(fid,ind(1)-1,'bof');
tline2 = fgetl(fid);
ind2 = strfind(tline2,']');
fseek(fid,ind(1)+scadena+3,'bof');
tline3 = fgets(fid,ind2(1)-scadena-5);
d_temp2 = str2num(tline3)';
fclose(fid);
names = {cad_timex,cad_temp2};
data = num2cell([d_timex,d_temp2]);
A = [names;data];
xlswrite(output_filename, A, sheet, cell);
```

F. Appendix. Check-All-That-Apply (C.A.T.A) surveys

Universidad del Cauca	**INVESTIGACIÓN:** Optimización de las condiciones de tiempo y temperatura en el tostado de café de cauca, teniendo en cuenta la percepción del consumidor. Se darán a probar 6 bebidas de café codificadas. Se solicita marcar con una x si percibe cualquiera de las características listadas. Igualmente, después de la prueba con cada taza se pide marcar su impresión global y la taza ideal (solo puede ser una) **RESPONSABLE:** Diego Andrés Campo Ceballos - Doctorado en Ciencias de la Electrónica-FIET-UNICAUCA **Director:**PhD. Carlos Alberto Gavíria López

Yo (Nombre)		**Edad**		**Sexo**	M	F

Autorizo el uso y la divulgación de mi información para el desarrollo de la investigación descrita anteriormente.
Acepto voluntariamente participar y sé que tengo el derecho de terminar mi participación en cualquier momento. Al firmar esta hoja de consentimiento Informado no he renunciado a ninguno de mis derechos legales.
Para constancia, firmo a los ______ días del mes de ______ del año __________

FIRMA:________________________ CC/TI:_________________

APRECIADO PARTICIPANTE

1. Realice el proceso de inducción a la prueba.
2. Por favor marque con una X, en caso de que perciba alguno de las características listadas
3. Por favor marque solo una opción en la percepción global de la bebida

TAZA ____
IDEAL? ___

¿Qué percibe en la taza de café?
selección múltiple

GLOBAL
Marque solo una opción

☐	Lima	☐	Naranja	Me gustó extremadamente	☐
☐	Arándanos	☐	Mandarina	Me gustó mucho	☐
☐	Uvas	☐	Plátano Verde	Me gustó moderadamente	☐
☐	Bebida ligera/refrescante	☐	Agua	Me gustó ligeramente	☐
☐	Bebida pesada/viscosa	☐	Bebida Jarabe	Ni me gustó ni me disgustó	☐
☐	Amargo	☐	Panela	Me disgustó levemente	☐
☐	Piña	☐	Manzanas verdes	Me disgustó moderadamente	☐
☐	Canela	☐	Quemado	No me gustó mucho	☐
☐	Chocolate	☐	Frutos rojos	Me disgustó en extremo	☐

TAZA ____
IDEAL? ___

¿Qué percibe en la taza de café?
selección múltiple

GLOBAL
Marque solo una opción

☐	Lima	☐	Naranja	Me gustó extremadamente	☐
☐	Arándanos	☐	Mandarina	Me gustó mucho	☐
☐	Uvas	☐	Plátano Verde	Me gustó moderadamente	☐
☐	Bebida ligera/refrescante	☐	Agua	Me gustó ligeramente	☐
☐	Bebida pesada/viscosa	☐	Bebida Jarabe	Ni me gustó ni me disgustó	☐
☐	Amargo	☐	Panela	Me disgustó levemente	☐
☐	Piña	☐	Manzanas verdes	Me disgustó moderadamente	☐
☐	Canela	☐	Quemado	No me gustó mucho	☐
☐	Chocolate	☐	Frutos rojos	Me disgustó en extremo	☐

TAZA ____
IDEAL? ___

¿Qué percibe en la taza de café?
selección múltiple

GLOBAL
Marque solo una opción

☐	Lima	☐	Naranja	Me gustó extremadamente	☐
☐	Arándanos	☐	Mandarina	Me gustó mucho	☐
☐	Uvas	☐	Plátano Verde	Me gustó moderadamente	☐
☐	Bebida ligera/refrescante	☐	Agua	Me gustó ligeramente	☐

☐	Bebida pesada/viscosa	☐	Bebida Jarabe	Ni me gustó ni me disgustó	☐
☐	Amargo	☐	Panela	Me disgustó levemente	☐
☐	Piña	☐	Manzanas verdes	Me disgustó moderadamente	☐
☐	Canela	☐	Quemado	No me gustó mucho	☐
☐	Chocolate	☐	Frutos rojos	Me disgustó en extremo	☐

TAZA ____
IDEAL? ___

¿Qué percibe en la taza de café? selección múltiple

GLOBAL Marque solo una opción

☐	Lima	☐	Naranja	Me gustó extremadamente	☐
☐	Arándanos	☐	Mandarina	Me gustó mucho	☐
☐	Uvas	☐	Plátano Verde	Me gustó moderadamente	☐
☐	Bebida ligera/refrescante	☐	Agua	Me gustó ligeramente	☐
☐	Bebida pesada/viscosa	☐	Bebida Jarabe	Ni me gustó ni me disgustó	☐
☐	Amargo	☐	Panela	Me disgustó levemente	☐
☐	Piña	☐	Manzanas verdes	Me disgustó moderadamente	☐
☐	Canela	☐	Quemado	No me gustó mucho	☐
☐	Chocolate	☐	Frutos rojos	Me disgustó en extremo	☐

TAZA ____
IDEAL? ___

¿Qué percibe en la taza de café? selección múltiple

GLOBAL Marque solo una opción

☐	Lima	☐	Naranja	Me gustó extremadamente	☐
☐	Arándanos	☐	Mandarina	Me gustó mucho	☐
☐	Uvas	☐	Plátano Verde	Me gustó moderadamente	☐
☐	Bebida ligera/refrescante	☐	Agua	Me gustó ligeramente	☐
☐	Bebida pesada/viscosa	☐	Bebida Jarabe	Ni me gustó ni me disgustó	☐
☐	Amargo	☐	Panela	Me disgustó levemente	☐
☐	Piña	☐	Manzanas verdes	Me disgustó moderadamente	☐
☐	Canela	☐	Quemado	No me gustó mucho	☐
☐	Chocolate	☐	Frutos rojos	Me disgustó en extremo	☐

TAZA ____
IDEAL? ___

¿Qué percibe en la taza de café? selección múltiple

GLOBAL Marque solo una opción

☐	Lima	☐	Naranja	Me gustó extremadamente	☐
☐	Arándanos	☐	Mandarina	Me gustó mucho	☐
☐	Uvas	☐	Plátano Verde	Me gustó moderadamente	☐
☐	Bebida ligera/refrescante	☐	Agua	Me gustó ligeramente	☐
☐	Bebida pesada/viscosa	☐	Bebida Jarabe	Ni me gustó ni me disgustó	☐
☐	Amargo	☐	Panela	Me disgustó levemente	☐
☐	Piña	☐	Manzanas verdes	Me disgustó moderadamente	☐
☐	Canela	☐	Quemado	No me gustó mucho	☐
☐	Chocolate	☐	Frutos rojos	Me disgustó en extremo	☐

G. Appendix. Methods to analyze CATA data.

Due to the importance of the CATA methodology data for the proposed optimization scheme. It contains the most used methods to analyze CATA data, using the XLSTAT SOFTWARE. The questions can be divided into two types: Exploratory questions: allow the investigation of multivariate datasets without considering any hypothesis to validate. Exploratory multivariate data analysis tools often imply a reduction of the dimensionality of large datasets making data exploration more convenient. Decisional questions imply testing the relationship between two sets of variables (correlation) or explaining a variable or a set of variables by another set (causality).

Table G.1. CATA tools details

Question	Number of tables	Data description	Tool	Remarks
Exploratory	1	Quantitative variables only	Principal Component Analysis (PCA)	Considers all the variance in the data; components do not necessarily reflect real phenomena
Exploratory	1	Quantitative variables only	Factor analysis (FA)	Considers only the covariance between variables; latent factors reflect real phenomena
Exploratory	1	Proximity matrix	Multidimensional scaling (MDS) /Principal Coordinate Analysis(PCoA)	
Exploratory	1	Contingency table (2 qualitative variables)	Correspondence Analysis (CA)	
Exploratory	1	Qualitative variables only	Multiple Correspondence Analysis (MCA)	
Exploratory	1	Quantitative and qualitative variables	Factorial analysis of mixed data (PCAmix)	Contrary to MFA, the dataset is not structured in groups
Exploratory	≥2	Qualitative variables tables and-or quantitative variables tables and-or frequency table	Multiple Factor Analysis (MFA)	
Exploratory	≥2	Quantitative variables tables	Generalized Procrustes Analysis (GPA)	Could include an inferential part: the consensus test
Exploratory (clustering)	1	Quantitative variables only	Clustering tools (AHC, k-means...)	Classical clustering methods could be applied on a qualitative variables table indirectly, using row scores on the dimensions of a Multiple Correspondence Analysis
decisional (causality)	1	One dependent variable and several quantitative and-or qualitative explanatory variables	Statistical modeling tools(regression, ANCOVA…)	
decisional (correlation) or exploratory	2	Two quantitative variables tables	Canonical correlation analysis	Linear relationships between the two tables
decisional (causality) or exploratory	2	One contingency table Y (often a site-species data matrix) and one explanatory quantitative and-or qualitative variables table (X)	Canonical correspondence analysis	Unimodal relationships between X and Y; could be used to depict species niches along environmental gradients
decisional (causality)	2	One dependent quantitative variables table (Y) and one quantitative and-or qualitative explanatory variables table (X)	Redundancy analysis (RDA)	Linear relationships between X and Y
decisional (causality)	2	One dependent quantitative variables table (Y) and one quantitative and-or qualitative explanatory variables table (X)	Partial Least Square regression (PLS)	Especially used for prediction
decisional (causality)	≥2	Tables of manifest variables, each table representing a latent variable	Partial Least Square Structural Equation Modeling (PLS-PM)	

H. Appendix. Sensory software packages

In this work we used different computational packages that support data consistency analysis. R scripts were integrated into the excel interface for this study, through XLSTAT in its 2019 PREMIUM and 2020 trial versions.

CATA - R SOFTWARE

https://www.rdocumentation.org/packages/cata/versions/0.0.10.9

CLUSBLOCK - R SOFTWARE

https://www.rdocumentation.org/packages/ClustBlock/versions/3.0.0

CATATIS – R SOFTWARE

https://www.rdocumentation.org/packages/ClustBlock/versions/2.4.1/topics/catatis

XLSTAT CATA DATA

https://www.xlstat.com/es/soluciones/funciones/analisis-de-datos-cata

XLSTAT CLUSCATA

https://www.xlstat.com/en/solutions/features/cluscata

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