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Shelf-Life Prediction of Specialty Coffees using the Arrhenius Model

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Abstract: The study estimated the shelf life of roasted and ground specialty coffees in bi-laminated and tri-laminated packaging concerning cup score, using the Acceleration Test at temperatures of 40, 50, and 60°C. The sensory evaluation was carried out by Q Grader tasters. Based on the higher value of the coefficient of determination of the regressions resulting from the cup and temperature profiles, it was determined that the order of the reaction was of the first order, with a second regression adjusted to the Arrhenius equation. The activation energy and the pre-exponential factor were obtained, variables with which the degradation rate constant was determined for each package and temperature of study. Employing the first-order kinetic equation, the results of shelf life at storage temperatures for 10, 15, 20, 25, 30, 40, 50, and 60°C were estimated at 26.9, 21.9, 17.8, 14.7, 12.2, 8.5, 6.1 and 4.4 days for bi-laminated packaging and 137.9, 93.8, 64.6, 45.1, 31.8 16.4, 8.8 and 4.9 days for tri-laminated, using a good performance prediction technique to determine quality descriptors of specialty coffees.

Keywords: Coffee Variety, Modelling, Prediction, Test Accelerated

Introduction

From its discovery in Abyssinia (now Ethiopia) to becoming one of the world's most widely consumed beverages, coffee has captivated fans with its unique aroma and flavor (Lim *et al*., 2019). It contains a variety of chemical compounds responsible for its sensory quality and physiological effects, such as caffeine, which is a central nervous system stimulant (Gotteland and de Pablo, 2007). The word coffee encompasses a range of products, from roasted coffee (Nakilcioğlu-Taş and Ötleş, 2019), whole and ground to a wide variety of prepared and semi-processed products (Alves *et al*., 2017; da Silva *et al*., 2022; Nicoli *et al*., 2009; Singh *et al*., 2020; Yildirim and Karaca, 2022), such as instant coffee, coffee concentrate (Alencar Lopes *et al*., 2022; Almahasheer, 2022; Gerasimov *et al*., 2020; Parvathy *et al*., 2018) and drinks derived from coffee fit for consumption (Gunel *et al*., 2022; Kyroglou *et al*., 2022; Lomolino *et al*., 2022; Pimpley *et al*., 2022; Rianto *et al*., 2021; Zhang *et al*., 2022).

The impact of coffee storage variables on coffee quality has been reviewed (Pazmiño-Arteaga *et al*., 2022). It is difficult to retain the aroma compounds in coffee once the roasting process is complete and it is difficult to store the beans for longer with the volatile compounds retained, as these are easily lost in the grinding of the roasted coffee beans and the storage of the ground coffee (Rattan *et al*., 2015). Proper packaging and storage are necessary to preserve freshness (Smrke *et al*., 2022). Atmosphere estimation of roasted coffee packaging was presented as a case study (Lee *et al*., 2022).

Shelf life is a finite period after manufacture and packaging, during which the food product retains a level of quality required and acceptable for consumption (Nicoli, 2012). It depends on the level of processing techniques used and the packaging-food-environment system (Espinoza Atencia, 1996). It represents an important parameter in the processing of fresh, semi-processed, and processed foods, moreover, it is estimated by experimental tests and by simulation; implying knowledge by each member of the food chain. Because the deterioration of the quality of some foods occurs rather slowly under real storage conditions, therefore, test methodologies are adopted to determine the shelf life under accelerated storage conditions. This methodology is called Accelerated Shelf-Life Testing (ASLT) and allows us to reduce the time needed to estimate the shelf life of the product (Calligaris *et al*., 2019). The ability to predict the shelf life of the product in different materials can help select the optimal packaging (Witik *et al*., 2019).

Science Publications

Coffee produced in the provinces of Jaen and San Ignacio in Peru needs a boost to increase local and international consumption. However, more than 200 coffee organizations and cooperatives participated in the FICAFE 2019 Specialty Coffee Fair, which allowed them to showcase the best of their production to establish a direct business in the short and medium-term (GORECAJ, 2022). The business was estimated at 13 million soles, with buyers of specialty coffees from the United Arab Emirates, South Korea, Japan, Hong Kong, USA, Argentina, and Chile (Perú 21, 2019).

The objective was to estimate the shelf life of roasted and ground specialty coffees in bi-laminated and tri-laminated packaging concerning cup score, using the Temperature Acceleration Test with the Arrhenius approach.

Materials and Methods

Tools and Materials

Coffea arabica was evaluated roasted (medium dark) and ground (medium grind, particle size 10) packaged in 250 g bi-laminated (LDPE, Aluminium) and tri-laminated (PET, Aluminium, Polyethylene) packages, with a degassing valve. The product came from the production units of the members of the Cooperativa Agraria Cafetalera "La Prosperidad" de Chirinos, San Ignacio, Cajamarca, Peru; corresponding to the 2021 harvest. Faithful, WGLL 125B equipment was used to accelerate the process of deterioration of the cup score.

Research Methods

The study was conducted in three stages: Accelerated conditions, cup score assessment, and service life estimation (Mardjan and Hakim, 2019). Accelerated conditions: The samples constituted 30 hermetically sealed 250 g packages, 15 bi-laminated and 15 tri-laminated, duly coded. These were placed in an oven with a relative humidity of 80% at three temperatures 40, 50, and 60°C as storage simulation. The evaluations were carried out every 48 h for 8 days, for the three temperatures.

Evaluation of the cup score: Carried out by three Q Arabica Graders of the Specialty Coffee Association (SCA) tasters, using the SCA tasting protocol. Sample preparation, sensory evaluation, and respective assessment were considered. The first step consisted of preparing and extracting the essence to be evaluated. The second step was the sensory evaluation and the respective assessment in the SCA format. The evaluation consisted of assigning a score from 0 to 10 for each attribute: Fragrance/aroma, flavor, residual flavor, acidity, body, balance, uniformity, clean cup, sweetness, and taster score. With the cumulative score, the coffee was rated according to the SCA (Table 1).

Table 1: Coffee grades based on cup score

Cup score	Quality	Classification
90-100	Outstanding	Specialty
85-89.99	Excellent	
80-84.99	Very good	
<80.0	Below specialty quality	Not specialty

Estimated shelf life: Using ASLT, the loss of the cup profile during storage was simulated and observed and the data obtained was systematized in a data matrix. Utilizing linear regression, the value of the coefficient of determination (R^2) was calculated, with which the order of the reaction was determined (zero or one). Once the order of the reaction was obtained, it was plotted using the slopes and temperatures. A second regression to match the linearized Arrhenius model, from which the activation energy is obtained (Ea) and the pre-exponential factor (K_0), variables that help to find the decay rate constant (K). The Arrhenius model shows the dependence of the rate of decay reaction on temperature, Eq. 1 to 2:

$$K = K_0 e - \left(\frac{Ea}{RT}\right) \tag{1}$$

$$\ln K = -\left(\frac{Ea}{R}\right)\frac{1}{T}\ln\left[K_0\right] \tag{2}$$

where:
T = Absolute temperature (°K)
R = Gas constant (1.986 cal/moL °K).

Estimating the shelf life of roasted-ground coffee shall be obtained by entering the deterioration rate in Eq. 3 or 4 of the deterioration kinetics of order zero or one depending on the result, with losses of desirable compounds:

$$order\,1t = \frac{A_0 - A}{K} \tag{3}$$

$$order\,1t = t = \frac{\ln A_0 - \ln A}{K} \tag{4}$$

where:
A_0 = The initial value of the cup score of the roasted-ground coffee

However, coffee is considered not to be included in the specialty category if the cup score value is less than 80 and this value is assumed to be the limit of acceptability A = 79.75.

Statistical Analysis

The experiments were performed in triplicate and the results were expressed as means ± standard deviations. The software used was Python via Google coll laboratory.

Results

Accelerated Conditions Test

The coffee sample in the initial condition obtained different cup scores: 85.08, 81.83, and 81 for bi-laminated packaging for temperatures of 40, 50, and 60°C; 84.17, 83.17, and 81.75 for tri-laminated packaging for temperatures of 40, 50 and 60°C. Therefore, the samples were classified in the specialty category, Fig. 1.

The value of 10 in the uniformity attributes shows that this coffee flavor has a good consistency, while the value of 10 in the clean cup attribute and the default value of 0 shows that the processing of the coffee is done in a clean way so that no foul taste or aroma is found in the coffee.

Cup Score

The results of the simulation of the storage of packaged coffee at various temperatures with decreasing cup scores are presented in Table 2.

Shelf Life

After obtaining the cup score degradation data for each storage temperature and packaging material (Table 2). The order of the chemical reaction kinetics of sensory quality loss was determined, defined as first order by the highest R^2 value and linear regression was used with ln *K* and 1/T values.

The value of the degradation rate constant for each temperature and packaging type was obtained from the value of the slope of each first-order plot. The value of ln *K* was plotted on a semi-logarithmic graph and fitted to the Arrhenius model, where ln *K* is the ordinate and 1/T is the abscissa, to obtain the value of -Ea/R for each type of packaging. The linear regression for bi-laminated and tri-laminated packages, Fig. 2.

Referring to Fig. 2, the relationship of the straight-line equation between the values of ln K and the value of 1/T for each package was obtained. The value of slope of the equation is the value of -Ea/R for each equation. The activation energy for each packing has been obtained, in Table 3. The intercept value in the semi-logarithmic plot is the value of ln K_0 in the Arrhenius equation, so the results for ln K_0 and K_0 were obtained as shown in Table 4.

Once the Arrhenius model was obtained for each type of packaging, cup scores were calculated for roasted and ground coffee, as a function of storage temperature and packaging type, as shown in Table 5. The K-values obtained from the calculations with Eq. 1 and the estimated shelf life of roasted and ground coffee was obtained by entering the deterioration rate in Eq. 4.

The initial cup score value of 85 was established with the letter A_0. Coffee is considered to be in the specialty category if the cup score value is less than 80 or has reached the value of 79.75 and this value is hereinafter referred to as the critical cup score value (A). Shelf-life estimation results for roasted and ground coffee at storage temperatures of 40, 50, and 60°C were estimated at 8.5, 6.1, and 4.4 days for bi-laminated packages and 16.4, 8.8, and 4.9 days for tri-laminated packages, respectively. Shelf life was estimated at temperatures from 10 to 30°C, the results are presented in Table 6 and Fig. 3.

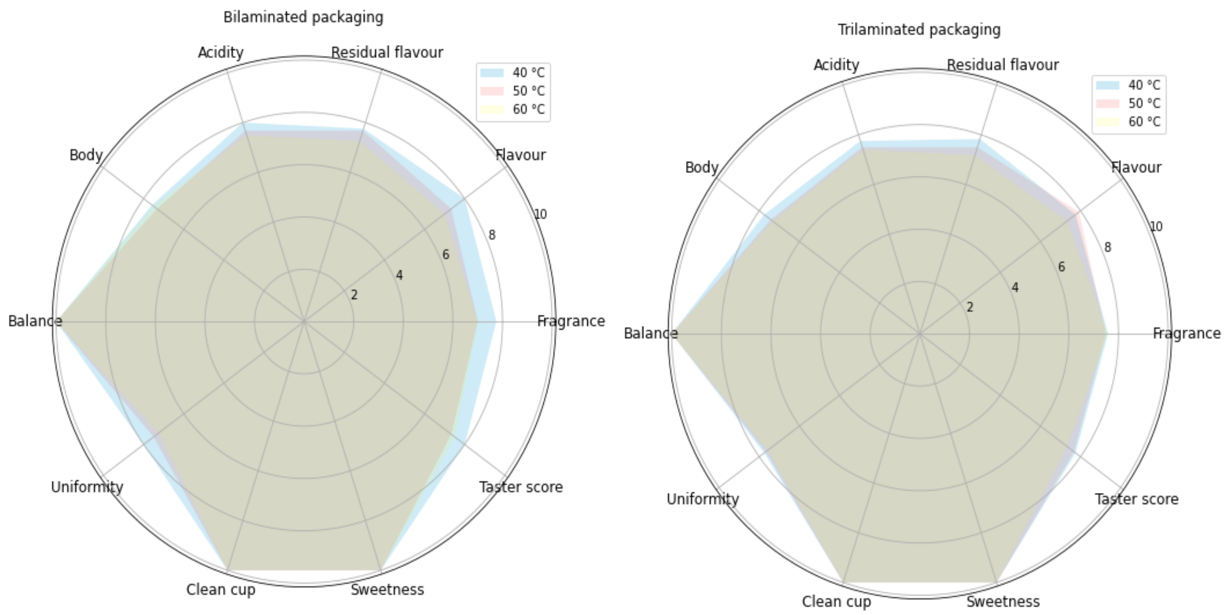

Fig. 1: Cup score results for unprocessed roasted and ground coffee

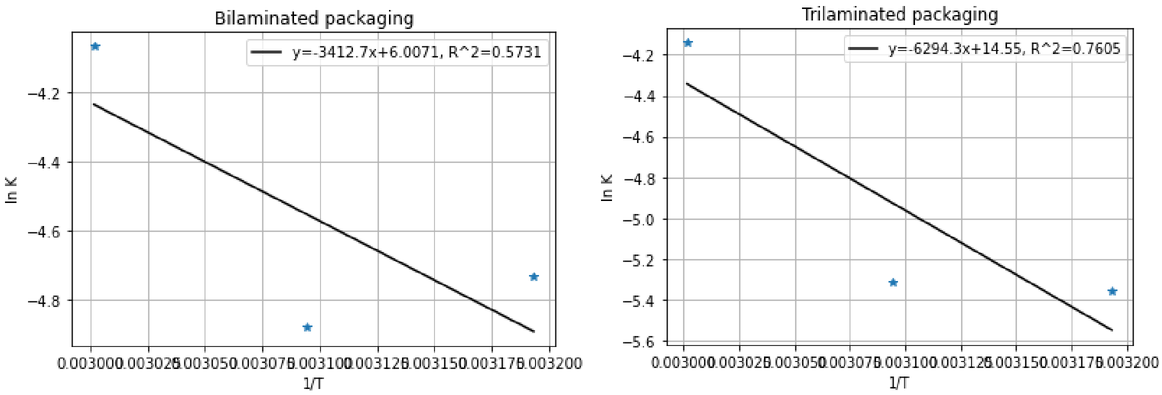

Fig. 2: Relationship between ln *K* with 1/T for roasted and ground coffee

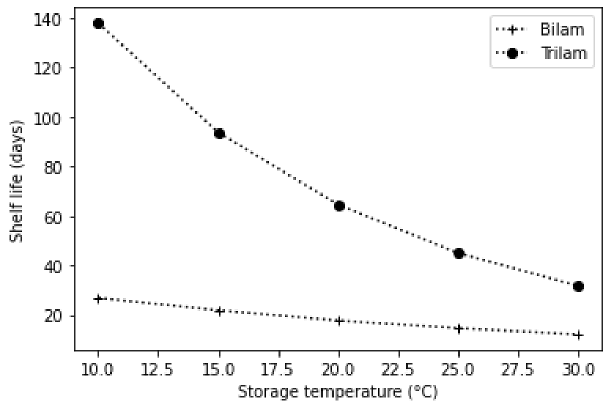

Fig. 3: Estimated shelf life concerning storage temperature

Table 2: Data on the decrease in cup score during storage

	40°C		50°C		60°C	
Days	Bi-laminated	Tri-laminated	Bi-laminated	Tri-laminated	Bi-laminated	Tri-laminated
0	85.08±0.12	84.17±0.24	81.83±0.24	83.17±0.24	81.00±0.00	81.75±0.20
2	84.42±0.12	83.75±0.20	80.42±0.31	81.25±0.35	79.08±0.12	80.25±0.20
4	82.33±0.24	83.33±0.24	79.58±0.12	80.58±0.12	75.00±0.00	76.00±0.00
6	81.00±0.00	82.17±0.24	78.42±0.43	80.08±0.12	73.17±0.24	74.00±0.00
8	79.50±0.00	81.00±0.00	77.42±0.32	79.58±0.12	71.00±0.00	72.33±0.12

Table 3: Determination of the reaction order

T °C	Presentation	Order	Regression	R^2	Selection
40	Bi-laminated	0	y = -0.7250x + 85.3000	0.969	1
		1	y = -0.0088x + 4.4465	0.969	
	Tri-laminated	0	y = -0.3875x + 4.3000	0.961	0
		1	y = -0.0047x + 4.4345	0.960	
50	Bi-laminated	0	y = -0.6000x + 81.7000	0.973	1
		1	y = -0.0076x + 4.4032	0.975	
	Tri-laminated	0	y = -0.4000x + 82.4000	0.877	1
		1	y = -0.0049x + 4.4116	0.881	
60	Bi-laminated	0	y = -1.3000x + 81.0000	0.983	1
		1	y = -0.0171x + 4.3954	0.985	
	Tri-laminated	0	y = -1.2250x + 81.6500	0.976	1
		1	y = -0.0159x + 4.4033	0.978	

Table 4: Values of -Ea/R, Ea, ln K_0 and K_0 for each packaging type

	-Ea/R	R (cal/mol°K)	Ea (cal/mol°K)	ln K_0	K_0
Bi-laminated	-3412.7	1.986	6777.6222	-3412.7	1.986
Tri-laminated	-6294.3	1.986	12500.4798	-6294.3	1.986

Table 5: K-values and shelf life for each temperature and packaging type

Type of packaging	Storage temperature	K	T (days)
Bi-laminated	40°C o 313.15 K	0.00751	8.5
	50°C o 323.15 K	0.01053	6.1
	60°C o 333.15 K	0.01446	4.4
Tri-laminated	40°C o 313.15 K	0.00389	16.4
	50°C o 323.15 K	0.00724	8.8
	60°C o 333.15 K	0.01299	4.9

Table 6: K-values and lifetime estimation for different temperatures

Type of packaging	Storage temperature	K	T (days)
Bi-laminated	10°C o 283.15 K	0.00237	26.9
	15°C o 288.15 K	0.00292	21.9
	20°C o 293.15 K	0.00357	17.8
	25°C o 298.15 K	0.00434	14.7
	30°C o 303.15 K	0.00525	12.2
Tri-laminated	10°C o 283.15 K	0.00046	137.9
	15°C o 288.15 K	0.00068	93.8
	20°C o 293.15 K	0.00099	64.6
	25°C o 298.15 K	0.00141	45.1
	30°C o 303.15 K	0.00200	31.8

Discussion

Various coffee quality and presentation descriptors have been studied using accelerated testing and the Arrhenius approach (Anese *et al*., 2006; Cardelli and Labuza, 2001; Pacheco Alfaro, 2016; Rivera Barzola, 2016). However, it is the first study in South America to use specialty roasted ground coffee and to use the quality descriptor "cup score" determined by certified assessors.

The evaluation of coffee quality cannot be separated from a sensory evaluation, although this practice is time-consuming and requires a trained professional panel (Liberto *et al*., 2019). However, temperatures and soil chemistry have a strong effect on coffee quality and biochemistry (Getachew *et al*., 2022). Therefore, coffee improvement requires combining sustainable productivity with the improvement of technological characteristics (Vega *et al*., 2021) and cup quality (Leroy *et al*., 2011).

According to the reaction rate theory, the increase in temperature will cause an increase in kinetic energy in the particles. This condition will accelerate the movement of the molecules and increase the number of collisions occurring between the particles so that the reaction will be faster. This also occurs in roasted and ground coffee in the package, where reactions can occur from the inside, such as oxidation of fat; the reaction of coffee with the package, where migration of substances from the package is absorbed by the product; and also, the reaction of coffee with substances outside the environment that can penetrate the package, such as absorption of moisture content, oxygen permeability, and growth of bacteria or fungi.

Emerging concepts of active and intelligent packaging technologies offer innovative solutions to extend shelf life and improve the quality and safety of food products (Han *et al*., 2018). As can be seen in Fig. 3, the tri-laminated plastic container has a higher capacity to maintain the quality of roasted and ground coffee than the bi-laminated plastic container. At storage temperatures of 10-30°C roasted and ground coffee can last up to 32-138 days for tri-laminated packaging and 12-27 days for bi-laminated packaging. The shelf life of specialty coffees is influenced by the rate of decline in the final flavor value score during storage, the lower the rate of decline in flavor, the longer the shelf life. The aroma of coffee begins to deteriorate after roasting and proper packaging and storage are necessary to preserve its freshness (Smrke *et al*., 2022).

The Peruvian technical standards (NTP) for roasted coffee beans or ground coffee NTP 209.028:2015 and specialty coffees NTP 209.311:2019 stipulate the characteristics and conditions that must be taken into account for the coffee to be evaluated to meet the requirements established in the standards and allow a given lot to be classified as specialty coffee. Weaknesses have been noted in the aforementioned NTP because it does not consider a study of the shelf life of specialty coffee based on the cup profile as a descriptor of quality and does not guarantee adequate information in the labeling and labeling to the consumer on the durability of the quality of the product, a fact that leads to offering a product lacking reliable and explicit information.

(INACAL, 2015; 2019). The effort in the production and to offer a final product of quality as exceptional coffee, merits a rigorous technological treatment from the harvest to the final consumer, where the standardized range of specialty coffee should be maintained for the longest possible time on the shelves, achieving that the product has similar organoleptic attributes to those obtained in a freshly roasted and ground coffee; a property that is highly valued by consumers of this type of coffees. It is for this reason that in this research the shelf life of specialty coffees was estimated based on the cup profile as a descriptor of quality through accelerated methods.

Suggestions for future research, estimate the shelf life of coffee products using the ASLT method and the Arrhenius approach, where the critical parameters used should represent the overall quality, including organoleptic tests.

Conclusion

The roasted and ground coffee in tri-laminated packaging had a slower rate of deterioration compared to bi-laminated packaging. Shelf-life estimation using the ASLT method with the Arrhenius model shows that the shelf life of coffee is 138 days with tri-laminated packaging at 10°C, 94 days at 15°C, 65 days at 20°C, 45 days at 25°C and 32 days at 30°C. With bi-laminated packaging the shelf life is shorter, 27 days at 10°C, 22 days at 15°C, 18 days at 20°C, 15 days at 25°C and 12 days at 30°C.

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Author’s Contributions

Frank Fernandez Rosillo: Writing, Investigation, and original draft preparation.

María Alina Cueva Ríos: Revision and edited, supervision.

Lenin Quiñones Huatangari: Revision and edited, validation and methodology.

Carla Guianella Samaniego Lalangui: Literature review and references.

Ethics

This article is original and contains unpublished material. The corresponding author confirms that all authors have read and approved the manuscript and that there are no ethical issues.

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