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Estimation of coffee shelf life under accelerated storage conditions using mathematical models – Systematic review

María Alina Cueva Ríos[1,2], *Frank Fernández Rosillo*[1,2], *Lenin Quiñones Huatangari*[2]*, *Eliana Milagros Cabrejos Barrios*[1]

[1]*Institute of Food Science and Technology, National University of Jaén, Jaén, Peru*
[2]*Data Science Research Institute, National University of Jaén, Jaén, Peru*

**Corresponding author: lenin.quinones@unj.edu.pe*

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Abstract: The shelf life of a food product is a finite period after manufacturing and packaging, during which it retains a required and acceptable level of quality for consumption. The objective was to characterise and describe the transparent and comprehensible processing process to collect, select, critically evaluate and summarise available evidence regarding the use of mathematical models in the estimation of the shelf life of coffee under accelerated storage conditions. Of the 183 articles identified, nine studies were included in the review: four evaluated various types of packaging containing roasted and ground coffee, three coffee-based beverages, one infusion and one in bean format; the models frequently used were Weibull-Hazard Analysis, first-order, and zero-order kinetic model, which requires the decay kinetic constant, the same as that acquired by the Arrhenius model or a proposed model. Quality descriptors and mathematical models have been identified that allow estimating the shelf life of coffee and its derivative products under accelerated storage conditions, in addition to primary sources with experimental designs.

Keywords: coffee variety; modelling coffee; prediction; accelerated shelf-life testing; packaging

According to FAO, almost one-third of the food produced for human consumption is lost or wasted, which has an impact on the security and sustainability of food systems (Nuñez de Villavicencio et al. 2017a, b). Food security is an important aspect of meeting the demands of the growing population (Khoo et al. 2021). Without food preservation, human life is at risk because there are serious diseases that are transmitted through spoiled food, called foodborne illnesses, such as meningitis, diarrhoea and cancer, and can cause lasting disabilities and death (Desta et al. 2022; Shaker et al. 2022; Waltenburg et al. 2022; Zhao and Sun 2022; Rashid et al. 2023). Knowing how long food will last has become increasingly important, which can be explained by consumers' interest in taking care of their health (Inungaray and Munguía 2013).

Coffee is one of the leading beverages worldwide (Samoggia et al. 2020; Lee et al. 2022) and therefore represents a highly valued trade (Pabon et al. 2020). Since its discovery in Abyssinia (now Ethiopia), it has captivated aficionados for centuries with its unique aroma and flavour (Rim 2019); there is substantial evidence that coffee contains a number of bioactive compounds (Socała et al. 2020; Andrade et al. 2022; Patil et al. 2022)

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and antioxidants with potentially beneficial effects on human health (Massey 2016; Açıkalın and Sanlier 2021; Barrea et al. 2021; Chieng and Kistler 2021; Aroufai et al. 2022; Gonçalinho et al. 2022; Pereira et al. 2022; Tommerdahl et al. 2022) as well as its effects as a stimulant to improve mental performance (Lim et al. 2019). 900 volatile compounds have been identified, although less than 20 have been considered relevant to coffee aroma (Buffo and Cardelli-Freire 2004). The word coffee encompasses a number of different products, from roasted coffee (Nakilcioğlu-Taş and Ötleş 2019), from whole and ground to a wide variety of prepared and semi-processed products (Nicoli et al. 2009; Alves et al. 2017; Singh et al. 2020; Da Silva et al. 2022; Yildirim and Karaca 2022), such as instant coffee, coffee concentrates (Parvathy et al. 2018; Gerasimov et al. 2020; Alencar Lopes et al. 2022; Almahasheer 2022) and ready-to-drink coffee beverages (Rianto et al. 2021; Gunel et al. 2022; Kyroglou et al. 2022; Lomolino et al. 2022; Zhang et al. 2022).

Shelf life is a finite period after manufacture and packaging, during which the food product retains a level of safety and quality required and acceptable for consumption (Nicoli 2012), depending on the level of technology used in the processing and on 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 simulation, implying knowledge by each member of the food chain. The number of food products whose shelf life depends on sensory properties is greater than those whose shelf life depends on microbiological and/or nutritional properties (Hough and Garitta 2012). The labels used on food products provide consumers with an approximate guide to their shelf life, as they assume that a product only experiences a limited range of predefined handling and storage conditions and do not take into account conditions that may shorten the shelf life of a product (Corradini 2018).

Shelf life estimation of food and beverage products has become increasingly important due to technological advances and consumers' growing interest in consuming fresh, safe and high-quality products (Giménez et al. 2012). A food, like coffee, is a complex system in which different reactions occur, so the modelling, in this case, is applied not to a particular component but to a quality characteristic that reflects these reactions (González-González et al. 2016). To estimate food shelf life, methodologies based on Weibull analysis are used (Rovira et al. 2019; Quevedo et al. 2020; Reyes-Álvarez and Lanari 2020; Tamarit-Pino et al. 2020; Singh et al. 2022) to risk techniques and the method of accelerated storage by temperature abuse (Nuñez de Villavicencio et al. 2017a, b; Darniadi et al. 2021; Benjamas and Theprugsa 2022; Brilliantina et al. 2022; Hayati et al. 2022; Iwansyah et al. 2022; Li et al. 2022; Nurhasanah et al. 2022; Sadli et al. 2022; Xiao et al. 2022). These are the most commonly used mathematical models, and their use will depend on the nature of the particular product (Cincotta et al. 2020). The second method is used because the deterioration of the quality of some foods occurs quite slowly under actual storage conditions. Therefore, test methodologies can be adopted to determine shelf life under accelerated storage conditions; this methodology is called accelerated shelf life testing (ASLT) and reduces the time needed to estimate the product's shelf life (Calligaris et al. 2019). The Weibull Hazard method is one of the graphical methods used to determine the shelf life of foods (Cardelli and Labuza 2001). This method uses the cumulative hazard function of the Weibull distribution (Equation 1) (Keklik et al. 2017).

$$H(t) = \int_0^t h(x)dx = \left(\frac{t}{\alpha}\right)^{\beta} \tag{1}$$

where: $h(x)$ – cumulative risk function; $H(t)$ – risk function is time t; α –scale parameter; β – shape parameter.

When the logarithm of time is plotted against the logarithm of the cumulative risk values, the resulting plot is linear, as shown in Equation 2.

$$\log(t) = \left(\frac{1}{\beta}\right)\log H + \log\alpha \tag{2}$$

Shelf life is when the cumulative hazard value is equal to 69.3%, determined as the time when cumulative hazard value is equal to 69.3%, corresponding to a critical failure probability of 50% (Fu and Labuza 1997). The rate of deterioration of food quality can be described by Equation 3 (Basilio-Atencio and Paduro-Contreras 2021):

$$\pm\frac{\mathrm{d}Q}{\mathrm{d}t} = KQ^n \tag{3}$$

where: Q – quality attribute; t – time; n – reaction order; K – constant rate of deterioration of quality; + sign – attributes with increasing values with time (wilting, browning, odour); – sign – attributes with decreasing values (overall appearance, total cup test score).

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However, the Arrhenius model describes the relationship of the reaction rate constant with temperature; this dependence is shown in Equation 4:

$$K = K_0 e^{\frac{-E_a}{RT}} \quad (4)$$

where: K – speed constant (day^{-1}); K_0 – pre-exponential factor (day^{-1}); E_a – activation energy (cal·mol^{-1}); R – universal gas constant (1.986 cal·mol^{-1}·K^{-1}); T – absolute temperature (K).

The E_a for each decay kinetics is obtained from the slope of the graph of ln K *vs* 1/T (Equation 5).

$$\ln K = \ln K_0 - E_a / RT \quad (5)$$

Four different methods of storing roasted whole beans after opening the container are compared: transferring the beans to an airtight jar, sealing the original container with tape, closing it with a paper clip, and using a container with an integrated screw cap (Smrke et al. 2022). The shelf life of an artisanal ice cream flavoured with coffee infusion packaged in 250 mL polypropylene pots was determined (Boumba et al. 2016). Developed artificial neural engineering models and regression models to predict the shelf life of instant coffee beverages, research revealed that the multiple linear regression model was superior to the radial basis model for forecasting the shelf life of instant coffee beverages (Goyal and Goyal 2011). Determined the shelf life of cold coffee flavoured with pistachios using the Weibull hazard analysis method (Polat and İbanoğlu 2021). The influence of variety on the shelf life of Arabica and Robusta coffee capsules packaged to correctly indicate the minimum durability date was evaluated (Cincotta et al. 2020).A cold coffee beverage different from the existing products on the market in terms of flavour was developed. Its shelf life was determined according to consumer expectations using the Weibull Hazard model (Karahan and Keklik 2018).

The objective of the research was to characterise and describe the transparent and comprehensible elaboration process to collect, select, critically evaluate, and summarize available evidence regarding the use of mathematical models in the estimation of the shelf life of coffee under accelerated storage conditions.

MATERIAL AND METHODS

Bibliographic searches. For the systematic review (Letelier et al. 2005; Moher et al. 2014), the Preferred Reporting Items for Systematic Reviews and Meta-Analyses (PRISMA) reporting guidelines were followed (Page et al. 2021). Between April 11 and July 16, 2022, the databases EBSCO Host, Scopus, Wiley Online Library, Scielo, IEEE Xplore and Google Scholar were searched for scientific articles published between January 1990 and July 2022 using standardised search terms. The search terms used were: 'Shelf life modelling coffee', or 'Shelf life model coffee', or 'estimation shelf life coffee', or 'coffee shelf life accelerated tests', or 'coffee shelf life prediction', or 'coffee shelf life arrhenius', or 'coffee shelf life weibull', or 'Shelf life model coffee'. Titles and abstracts were searched and screened, and relevant full-text articles were independently reviewed. Disagreements were resolved by consensus.

Inclusion and exclusion criteria. We included studies that met each of the following criteria: *i*) original scientific articles with experimental design; *ii*) analysed of any of the two coffee families, either robusta or arabica; *iii*) used coffee as raw material for the elaboration of products and/or derivatives; *iv*) used mathematical models to determine the shelf life of the product elaborated from coffee; *v*) used the accelerated storage method by temperature abuse; *vi*) published in English or Spanish; and *vii*) the type of publication was full text and peer-reviewed. Scientific articles were excluded if: *i*) they did not predict the shelf life of coffee or its derivatives of using mathematical models; *ii*) in the estimation of the processed product or derivatives, the base of the product was not coffee; *iii*) they were descriptive studies such as systematic reviews or meta-analyses; and *iv*) errata or editorials.

Data extraction. The authors independently extracted the following characteristics using a standardised spreadsheet in Excel software: manuscript title, year of publication, database, topic or search mix, browser used, date of search, keywords, abstract, stable URL (drive or similar) to the full text, journal name, authors' names, country, university, type of research, a methodological perspective, techniques used, procedure, limitations, subjects, sample selection criteria, contents, sample selection criteria, contents, objective, hypothesis/research questions, variables used and main findings.

RESULTS AND DISCUSSION

The systematic review identified 183 potentially relevant manuscripts, from which nine full-text articles were extracted by selecting titles and abstracts (Figure 1). Coffee has different presentations (five evaluated coffee-based beverages, four different types

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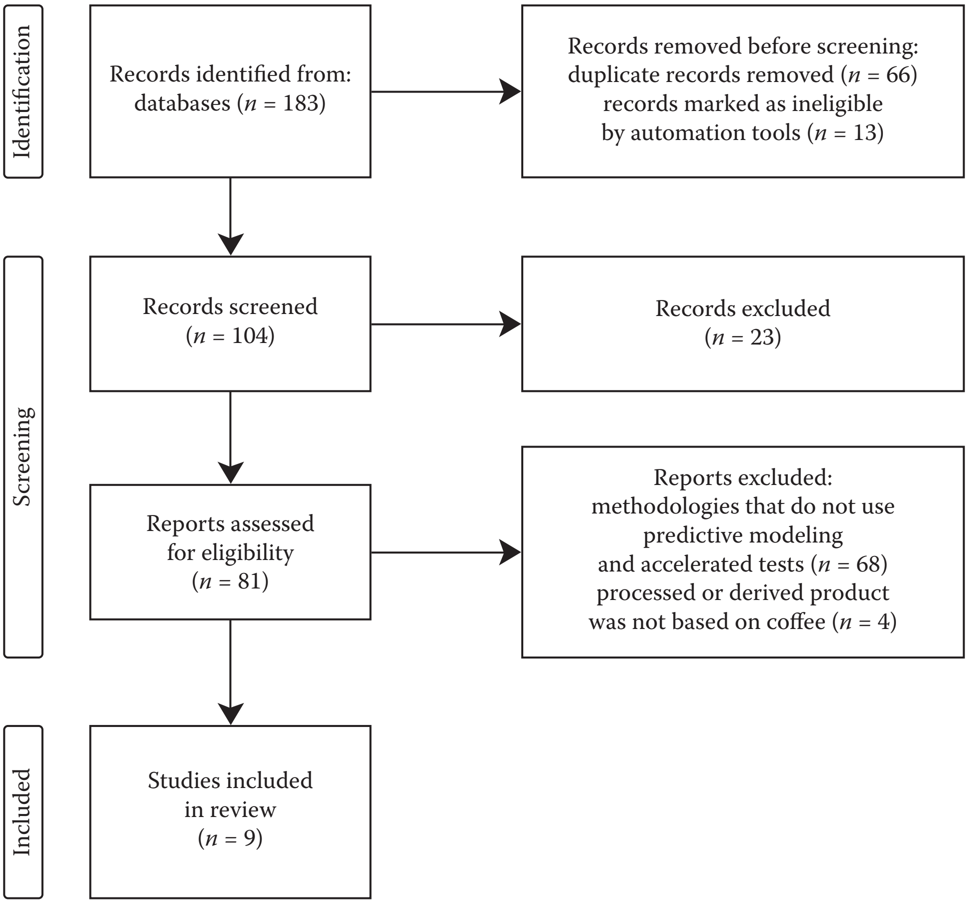

Figure 1. Selection process of studies that estimate the useful life of coffee using mathematical models

of packaging containing roasted and ground coffee, one in capsule form, one infusion and one in bean format), where various quality descriptors were addressed, and mathematical models were used, such as first and zero-order kinetics, Arrhenius, Weibull Hazard and others (Table 1).

The nine studies included in the review meet the inclusion and exclusion criteria of the systematic review. The practical implications allow the identification of mathematical models using accelerated tests that estimate the shelf life of coffee and its derivative products. It has led to identifying through primary sources with experimental designs accelerate,ted tests and mathematical models used.

Different presentations of coffee and its derivatives were identified, being coffee beverages sought after for their organoleptic characteristics, making it one of the most consumed in the world (Gotteland and de Pablo 2007). In addition, cold-brewed coffee is a new trend in the coffee industry (Kwok et al. 2020; Claassen et al. 2021) since drinking coffee is part of people's daily life and is qualified as a social event (Ramírez Prada 2010). In addition, the age of coffee consumers and several sociodemographic characteristics significantly affect coffee consumption (Alsafra et al. 2022). However, in coffee, packaging technologies are used (Aghaye Ghazvini et al. 2022; Chen et al. 2022; Sant'Anna et al. 2022; Smrke et al. 2022; Zarebska et al. 2022) that target value addition involving shelf life extension, prevention of microbial attack, adequate moisture barrier, use of carbon dioxide scavengers/emitters, ethylene scavengers, flavour absorbers, freshness indicators, biosensors and release of bioactive compounds during storage (Sharma and Ghoshal 2018), the influence of packaging design on taste impressions has even been examined (Becker et al. 2011) and the colour of coffee packaging is a factor used to attract consumer attention and generate sensory and hedonic expectations (Sant'Anna et al. 2022).

The quality of coffee results from processes that allow the development and conservation of its physical and chemical characteristics until its transformation and consumption (Parada et al. 2018). Also, oxidation is the most common event leading to the

Table 1. Characteristics of the samples, descriptors, and models of the 9 studies included

Title	Sample/features	Quality descriptor	Model	Reference
Characterisation of the lipid oxidation process of Robusta green coffee beans and shelf life prediction during accelerated storage	Robusta green coffee beans. The coffee beans were harvested in 2018/2019 in Wanning, China. The harvested raw coffee beans were obtained by mechanical dehulling, degumming, shelling and drying.	peroxide values	First-order kinetic models. Arrhenius.	Cong et al. 2020
Greek coffee quality loss during home storage: Modelling the effect of temperature and water activity	Greek coffee drink. Weighing 2 g of Greek coffee per 60 mL cup.	sensory analysis	Weibull-Hazard Analysis	Orfanou et al. 2019
Prediction shelf life of Arabica Java preanger coffee beans under hermetic packaging using Arrhenius method	Airtight and non-airtight plastic containers containing parchment coffee.	the total score of the cup test	Zero-order kinetic model. Arrhenius.	Mardjan and Hakim 2019
The evaluation of the shelf life of Arabica mixed coffee drinks using the accelerated shelf life testing method	Mixed beverage of husk extract, green coffee and roasted coffee added with sugar, maltodextrin, and whole milk.	pH, TDS (ppm), TSS (Brix), Total Color Difference, TPC ($CFU \cdot mL^{-1}$)	First-order and zero-order kinetic model. Arrhenius.	Cempaka et al. 2019
Modelling of Greek coffee aroma loss during storage at different temperatures and water activities	Blend of Arabica and Robusta coffee varieties, roasted and ground.	Sensory analysis, coffee aroma	Proposes a model. First order and zero order kinetic model.	Makri et al. 2011
Coffee brew shelf life modelling by integration of acceptability and quality data	The coffee beverage was found to have a solids concentration of 1.8% (*w*/*w*).	H_3O^+	Zero-order kinetics. Linear regression analysis	Manzocco and Lagazio 2009
Modelling the Secondary shelf life of ground roasted coffee	Dark roasted fresh ground coffee (*Arabica cv.*) from Italy in airtight containers.	water activity	propos-esa model	Anese et al. 2006
Application of Weibull Hazard Analysis to the Determination of the Shelf Life of Roasted and Ground Coffee	Roasted and ground Arabica coffee from Colombia.	sensory analysis	Analysis Weibull Hazard	Cardelli and Labuza 2001
Changes in coffee brews in relation to storage temperature	Coffee infusion: The coffee powder to water ratio was 1 : 10. A 50 : 50 dark roast blend of Coffea arabica and Canephora var Robusta .	pH	zero-order kinetics	Rosa et al. 1990

TDS – total dissolved solids; TSS (Brix) – total suspended solids; TPC – total plate count

end of the shelf life of microbiologically stable foods (Calligaris et al. 2016). Likewise, professional cupping is a reliable methodology for the coffee industry and its professionals; however, it faces barriers to its application on an industrial scale (Baqueta et al. 2021). Therefore, food spoilage, in general, involves physicochemical, sensory, microbiological and nutritional changes (González-Aguilar et al. 2007). From

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the systematic review, four papers used the quality descriptor of sensory analysis (Table 1) through the attributes fragrance, aroma, acidity, body, uniformity, balance, clean cup, residual flavour, sweetness, and overall impression standardised by the Specialty Coffee Association of America (SCAA). Two papers used pH to determine the acidity of the beverages studied. One report considered water activity as a quality descriptor to assess shelf life in fresh ground dark roast coffee. They also evaluated the antioxidant capacity of raw coffee beans obtained by mechanical hulling, degumming, peeling and drying. In the study, articles have been found that have used zero-order kinetics (Rosa et al. 1990; Manzocco and Lagazio 2009; Makri et al. 2011; Cempaka et al. 2019; Mardjan and Hakim 2019), first-order kinetics (Makri et al. 2011; Cempaka et al. 2019; Cong et al. 2020) to the various quality descriptors (Table 1).

ASLTs apply to any deterioration process with a valid kinetic model, whether chemical, physical, biochemical, microbiological, or even sensory, as shown in Table 1. There are several approaches to ASLT, but the most common method is the kinetic model approach, more specifically, the Arrhenius model, which is demonstrated in the study since these are the models that have been found the most. The temperatures used in the studies are diverse such as 25, and 45 °C (Orfanou et al. 2019), also 27 and 37 °C (Cempaka et al. 2019), 40, 50, and 60 °C (Mardjan and Hakim 2019), 25 and 45 °C (Makri et al. 2011); diversity of temperatures is related to the quality descriptor and the product used in the experiment.

Adopting predictive mathematical models to assess microbial behaviour under different environmental conditions is a tool for food industries to maximise production and reduce waste (Giarratana et al. 2022). The nine articles use three models to determine the service life: the first group of four articles uses the Arrhenius model to determine the deterioration constant and chemical kinetics to estimate the service life. The second group of three articles proposed new models for the deterioration constant and also used chemical kinetics as in group 1. Finally, the third group (two articles) used Weibull analysis by sensory analysis.

Cong et al. 2020 characterised the lipid oxidation process of green Robusta coffee beans during accelerated storage for 20 days at 40, 50, and 60 °C. They evaluated conventional oxidation rates and fatty acid compositions; where the estimated shelf life using the Arrhenius model for zero and one order reactions was 57.39, 44.44, and 23.12 days when stored at 40, 50, and 60 °C, respectively. The accelerated storage simulation was carried out at temperatures of 40, 50, and 60 °C, with 80% relative humidity using airtight and non-airtight packaging, using the Arrhenius equation to predict shelf life. The shelf life of coffee beans packaged in airtight and non-airtight plastic was 232 and 45 days (10 °C), 113 and 26 days (15 °C), and 57 and 16 days (20 °C), 29 and 10 days (25 °C), respectively (Mardjan and Hakim 2019). They made a blended beverage of husk extract, green and roasted coffee added with sugar, maltodextrin, and whole milk; samples were stored at temperatures of 4, 27, and 37 °C. The quality descriptors evaluated were pH, total dissolved solids, total sugar, total colour difference and total plate count. They estimated the shelf life by Arrhenius for each parameter and obtained that if stored at 4 °C it would be 4 days, the time of the lowest value of the parameters (Cempaka et al. 2019). They tested an aseptically bottled coffee beverage; sensory analysis allowed to define a lower pH limit at which the shelf life of the product ended, and knowledge of the kinetic rate constants of pH decrease at different temperatures allowed to correlate the shelf life of the product with its storage temperature (Rosa et al. 1990).

They used chemical kinetics with different reaction orders; however, for the estimation of the decay kinetics constant, they proposed mathematical models: They evaluated the acceptability of brewed coffee, during storage, by consumers through acceptability scoring and consumer rejection through survival analysis, the equations provided information to produce shelf-life models that took into account consumer response (Manzocco and Lagazio 2009). They found that furfural was a good aromatic marker for the rancidity of Greek coffee during storage; the shelf life of 0.52 a_w coffee stored at temperatures of 25 and 45 °C was 82–92 and 20–23 days, respectively. At 45 °C, the decrease in a_w from 0.52 to 0.33 led to an increase in shelf life from 20–23 to 36–41 days obtained through the zero-order kinetics equation (Makri et al. 2011). They studied the secondary shelf life of roasted ground coffee, using fresh samples with a_w up to 0.44 and stored at 30 °C for up to 1 month, simulated domestic storage conditions, periodically disturbed the atmosphere by briefly opening and closing the container; developed a mathematical model that allows the secondary shelf life of coffee to be calculated as a function of its a_w at a temperature (Anese et al. 2006).

Coffee samples were stored at 25, 35, and 45 °C in simulated home storage conditions; Greek coffee infusions were prepared and served fresh during

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sensory evaluation. The use of Weibull hazard analysis determined the secondary shelf life (SSL) as a function of water temperature and activity (a_w). SSL values ranged from 20 (45 °C, a_w = 0.52) and 104 days (25 °C, a_w = 0.15) (Orfanou et al. 2019). The roasted and ground coffee was stored at partial pressure of O_2 constant (0.5–21.3 kPa), a_w (0.106–0.408), and temperature (4–35 °C). Product acceptability was monitored using a mixed Weibull Hazard sensory method, where the end of shelf life was the time at which the product was 50% of consumers considered the product unacceptable. The activation for shelf life was: 13 kJ·mole^{-1}, indicating that diffusion within the glass matrix controls deterioration (Cardelli and Labuza 2001).

The contribution of the work is that using mathematical models obtained from the systematic review and the same ones that can be developed in software would allow a limited use of expensive and time-consuming experiments with physically prepared foods to reliably estimate shelf life (Mengucci et al. 2022). This will enable research to be carried out in the coffee supply chain (primary production, transformation process, transportation and distribution, and distribution to the final consumer) since these stages impact the useful life of the raw material or derived product.

CONCLUSION

The information obtained on mathematical models used, quality descriptors and experimental trials from the nine articles of the systematic review can serve as an orientation to estimate the shelf life of coffee and its diverse derived products that have their specifications in their form of preparation, type of roasting, type of packaging, storage conditions, variety, etc. It could help establish policies for estimating the shelf life of specialty coffees (total cup score greater than 80) and identify problems to guide future research such as using conduct, data mining algorithms or the Internet of Things (IOT) in the various components of the coffee production chain.

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