

# Mathematical Models and Kinetic Parameters of the Oxidation of *Leonotis nepetifolia* Oil.

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## ARTICLE INFO

## ABSTRACT

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The objective of this study was to evaluate the kinetic parameters of oxidation of *Leonotis nepetifolia* oil using mathematical models to determine its stability and shelf life. The oil was extracted by cold pressing and analyzed using the Rancimat method under a constant airflow of 15 L·h<sup>-1</sup> at temperatures of 100, 110, 120, 130, and 140 °C. Kinetic parameters were calculated by applying the Arrhenius equation and the activated complex theory. To estimate the oil's shelf life, three mathematical models were used: logarithmic, exponential, and Malthusian, with model validation based on the coefficient of determination (R<sup>2</sup>). The results showed a decrease in the oxidative stability index with increasing temperature. The obtained values were Q<sub>10</sub> = 2.22, activation energy (E<sub>a</sub>) = 102.19 kJ·mol<sup>-1</sup>, frequency factor (A) = 2.14·10<sup>12</sup> h<sup>-1</sup>, enthalpy (ΔH) = 98.94 kJ, entropy (ΔS) = -19.53 J·K<sup>-1</sup>, and Gibbs free energy (ΔG) = 106.59 kJ. The estimated shelf life was 6.22 years at 20 °C, 4.18 years at 25 °C, and 2.8 years at 30 °C. All three models showed excellent fit to the experimental data (R<sup>2</sup> = 0.999). These findings provide valuable insights into the oxidative stability and storage behavior of *Leonotis nepetifolia* oil, supporting its potential application in the food and cosmetic industries.

**Keywords:** Activation energy, extrapolation, Rancimat, shelf life.

## 1. INTRODUCTION:

*Leonotis nepetifolia*, known as "dagga" or "lion's ear," is a medicinal plant from the Lamiaceae family native to South Africa and now widespread in tropical regions. Traditionally, it has been used to treat ailments such as asthma, fever, flu, cough, epilepsy, and skin diseases, owing to its phytochemical profile rich in alkaloids, flavonoids, terpenoids, and other bioactive compounds with antioxidant and anti-inflammatory properties. Its seeds contain vegetable oils with nutritional and therapeutic value. Cold pressing is preferred over solvent or thermal extraction methods because it preserves heat-sensitive bioactives. Assessing oxidative stability is essential for industrial applications. The Rancimat method determines the oxidative stability index (OSI), which indicates the oil's resistance to oxidation under accelerated conditions of temperature and airflow. This study aimed to evaluate the oxidation kinetics of *L. nepetifolia* oil to estimate its stability and shelf life. Mathematical models (logarithmic, exponential, and Malthusian) were applied to data obtained using Rancimat at 100–140 °C. Kinetic parameters such as Q<sub>10</sub>, E<sub>a</sub>, ΔH, ΔS, and ΔG were calculated, and the estimated shelf life was 6.22 years at 20 °C, 4.18 years at 25 °C, and 2.8 years at 30 °C. All models showed excellent fit (R<sup>2</sup> = 0.999). These findings provide valuable insight into the potential use of this oil in the food and cosmetic industries.

## 2. RESEARCH OBJECTIVES

- To evaluate the oxidation kinetic parameters of *Leonotis nepetifolia* oil through the use of mathematical models, in order to establish its stability and shelf life.
- To determine the Oxidative Stability Index (OSI) of *Leonotis nepetifolia* oil using the Rancimat method under different temperature conditions.
- To determine the kinetic parameters associated with the oxidation process of *Leonotis nepetifolia* oil.
- To develop mathematical models to predict the shelf life of *Leonotis nepetifolia* oil under various

temperature conditions.

### 3. RESEARCH METHODOLOGY:

This study was carried out at the Bromatology Laboratory of the Universidad Estatal Amazónica, located at kilometer 2 ½ on the road to Tena, in the canton and province of Pastaza, at an altitude of 940 meters above sea level, with geographic coordinates of 00° 59' -1" latitude and 77° 49' 0" west longitude.

#### 3.1 Data Collection and Processing of Raw Material:

D. The seeds of *L. nepetifolia* were freshly collected between 8:00 a.m. and 3:00 p.m. in the canton of Guano, Chimborazo province, Ecuador, located at 2700 meters above sea level, at the coordinates 1°32'49.1"S and 78°38'25.4"W. Uniform seeds in good physical condition and measuring between 2 and 3 mm in length were selected. The seeds were dried in an oven (Memmert brand, model SFE700) for 72 hours, and the moisture content was determined by weight difference using Equation (1) (Martínez et al., 2024).

$$\%H = 100 - \frac{m_s}{m_f} \cdot 100$$

Where  $m_s$  represents the initial mass (g) of the seeds and  $m_f$  the mass (g) of the seeds after drying.

#### 3.2 Obtaining the oil:

The oil extraction process was carried out using the cold-pressing technique, which better preserves the bioactive properties of the oil by avoiding the use of high temperatures (Kjyu, 2023). For this procedure, a CGOLDENWALL brand screw press with a power of 1500 W and a constant temperature of 40 °C was used. After extraction, the oil was filtered using Whatman No. 4 filter paper to remove impurities and obtain a purer product. Subsequently, the filtered oil was stored in dark glass bottles to protect it from light and prevent oxidation. It was kept at a temperature of  $4 \pm 1$  °C until further analysis. The extraction yield was calculated as the ratio between the mass of oil obtained and the total mass of seeds processed, using Equation (2) for its determination (Chávez et al., 2022).

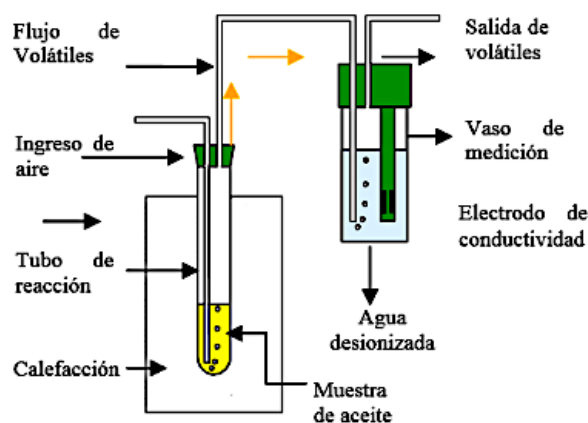
$$\%R = \frac{m_a}{m_s} \cdot 100$$

Where  $m_a$  is the mass of the oil (g), and  $m_s$  is the mass of the seeds (g).

#### 3.3 Determination of the Oxidative Stability Index (OSI):

The Rancimat method was used (Metrohm equipment, model 892, Switzerland), following the procedures established by AOCS Cd 12b-92 (2022). A constant airflow of 15 L·h<sup>-1</sup> was set and passed through a 2.5 ± 0.2 g oil sample placed in a reaction tube. This tube was positioned in a heating block and subjected to temperatures of 100, 110, 120, 130, and 140 °C. The volatile organic acids released from the sample were absorbed by a polycarbonate vessel containing 60 mL of distilled water, and the electrical conductivity (μS·cm<sup>-1</sup>) of the water was continuously measured during the process (Figure 1). The Oxidative Stability Index (OSI) was expressed in hours.

**Figure 1.** Principle of the Rancimat Method



**Source:** Rodríguez et al. (2019)

### 3.4 Calculation of Kinetic Parameters: Temperature Acceleration Factor (Q<sub>10</sub>)

This factor is a measure that describes how the oxidation rate of the oil changes when the temperature increases by 10 °C. The Q<sub>10</sub> was calculated using the following mathematical model:

$$Q_{10} = 10^{-10T_c}$$

Where  $T_{<sub>c</sub>}$  represents the temperature coefficient (°C<sup>-1</sup>).  $T_{<sub>c</sub>}$  was obtained from the slope of the line generated by plotting the logarithm of the OSI against temperature (°C), using the following equation:

$$\text{Log}(\text{OSI}) = mT + b$$

Where  $m$  is the slope of the line, which corresponds to  $T_{<sub>c</sub>}$ , and  $b$  is the y-intercept.

### 3.5 Reaction Rate Constant (k), Activation Energy (E<sub>a</sub>), and Frequency Factor (A):

Kelvin The parameter  $k$  represents the oxidation rate of the oil, i.e., the speed at which the oil decomposes due to the action of oxygen and temperature. It was calculated as the inverse of the OSI value, according to Ali et al. (2022):

$$K = \frac{1}{\text{OSI}}$$

$k$  is expressed in h<sup>-1</sup>.

On the other hand, the activation energy ( $E_a$ , kJ·mol<sup>-1</sup>) and the frequency factor ( $A$ , h<sup>-1</sup>) were determined using the Arrhenius equation:

$$k = A \cdot e^{\frac{-E_a}{R \cdot T}}$$

Where  $R$  is the universal gas constant (8.314 J·mol<sup>-1</sup>·K<sup>-1</sup>), and  $T$  is the absolute temperature in Kelvin.

A plot of  $\ln(k)$  versus the inverse of temperature ( $1/T$ ) based on the linearized form of Equation (6) was used to determine the values of  $E_a$  and  $A$ .

$$\text{Ln}(k) = \text{Ln}(A) - \frac{E_a}{R \cdot T}$$

### 3.6 Determination of Enthalpy (ΔH) and Entropy (ΔS):

The values of  $\Delta H$  and  $\Delta S$  were obtained through linear regression of the plot of  $\log(k/T)$  versus the inverse of temperature ( $1/T$ ), using the equation derived from the activated complex theory (Almir et al., 2023):

$$\log\left(\frac{k}{T}\right) = \log\left(\frac{k_B}{h}\right) + \left(\frac{\Delta S}{2,303R}\right) - \left(\frac{\Delta H}{2,303RT}\right)$$

Where  $h$  is Planck's constant (6.626×10<sup>-34</sup> J·s) and  $k_{<sub>B</sub>}$  is Boltzmann's constant (1.381×10<sup>-23</sup> J·K<sup>-1</sup>).

### 3.7 Gibbs Free Energy

Gibbs free energy was determined as the difference between  $\Delta H$  and  $\Delta S$ , using the following equation:

$$\Delta G = \Delta H - T\Delta S$$

Where  $T$  is the temperature expressed in Kelvin.

### 3.8 Shelf Life

The shelf life of the oil was estimated at typical storage temperatures (20, 25, and 30 °C) using the extrapolation method. Various mathematical models were employed to relate exposure temperature and OSI values.

### 3.9 Logarithmic Model

This model describes the variation of OSI as a function of temperature, based on the observation that their relationship follows a logarithmic trend (Mendoza, 2024). The mathematical model used was:

$$\log(\text{OSI}) = a + bT$$

Where  $a$  and  $b$  are oil-specific constants determined experimentally through linear regression based on OSI data at different temperatures, and  $T$  is the temperature in °C.

### 3.10 Exponential Model

This model was used to directly calculate the shelf life of the oil as a function of temperature, using an exponential relationship based on OSI:

$$t_{OSI} = t_0 \cdot e^{BT}$$

Where  $t_0$  is the shelf life at a reference temperature,  $B$  is a parameter determined experimentally, and  $T$  is the temperature in °C. The equation can be linearized as:

$$\ln(t_{OSI}) = \ln(t_0) + BT$$

### 3.11 Malthusian Model

This model assumes that the rate at which OSI decreases with temperature follows an inverse relationship. As temperature increases, OSI declines more sharply, indicating an accelerated oxidation process. The model is expressed by the following separable differential equation:

$$\frac{dOSI}{dT} = -k \cdot OSI$$

By integrating this equation from an initial  $OSI_0$  to a given OSI and from an initial temperature to a given  $T$ , the following equation is obtained:

$$\ln(OSI) = -k(T - T_0) + \ln(OSI_0)$$

Where  $k$  is the degradation rate. Solving for OSI gives:

$$OSI = OSI_0 \cdot e^{-k(T-T_0)}$$

### 3.12 Validation of Mathematical Models

The correlation between experimental results and those predicted by the mathematical models was evaluated using the coefficient of determination ( $r^2$ ), calculated with the following equation:

$$r^2 = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

Where  $y_i$  represents the experimental OSI values,  $\hat{y}_i$  are the values predicted by the model,  $\bar{y}$  is the mean of the experimental values, and  $n$  is the number of samples.

### 3.13 Analysis of Results

All tests were performed in triplicate to minimize experimental errors and improve result accuracy. Data were expressed as mean  $\pm$  standard deviation ( $n = 3$ ) to adequately reflect measurement variability. Graphical representation of the results was generated using Excel 2016, providing a clear and detailed visualization of the data (Lazar et al., 2022).

## 4. DATA VISUALIZATION AND INTERPRETATION:

### Practical Research

This study is classified as practical research due to its experimental and applied focus. The main objective was to evaluate the oxidative stability of *L. nepetifolia* oil and determine its shelf life using mathematical modeling. The oil was extracted by cold pressing and analyzed with the Rancimat method, which measures the Oxidative Stability Index (OSI) at 100 °C to 140 °C under constant airflow. From this, kinetic parameters such as activation energy ( $E_a$ ) and temperature acceleration factor ( $Q_{10}$ ) were calculated. Logarithmic, exponential, and Malthusian models were applied to predict shelf life across various temperatures.

### Application of the Study

This research combines experimental data with kinetic and thermodynamic tools—such as the Arrhenius equation, enthalpy, entropy, and Gibbs free energy—to estimate the oxidative behavior of the oil. Experiments were conducted in a specialized lab using Rancimat equipment. Data were processed using Excel for regression modeling and shelf-life prediction. This approach offers a reliable, replicable method to evaluate the stability of vegetable oils, supporting improved storage strategies and potential applications in the food and cosmetics industries.

### Effect of Temperature on OSI Values

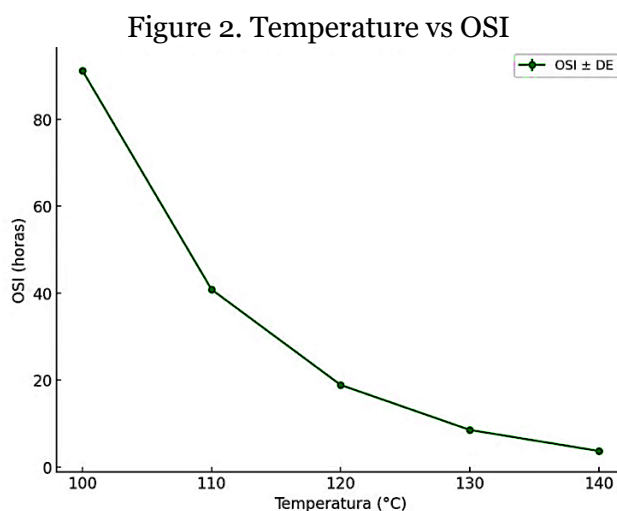
The Oxidative Stability Index (OSI) results in Table 1 show an inverse relationship with temperature, as illustrated in Figure 2. As temperature increased, OSI values decreased significantly, indicating reduced oxidative stability of the oil. Thermodynamically, higher temperatures provide energy to overcome the activation barrier of oxidation reactions, accelerating oil degradation.

This trend aligns with scientific literature, which reports that elevated temperatures increase the reactivity of free radicals and other intermediates, triggering oxidation chains that produce compounds like peroxides and aldehydes. These degrade oil quality and affect its nutritional and sensory properties.

**Table 1.** OSI values at different temperatures

Temperature (°C)	OSI $\pm$ DE (h)
100	91,16 $\pm$ 0,80
110	40,83 $\pm$ 0,61
120	18,87 $\pm$ 0,73
130	8,53 $\pm$ 0,72
140	3,68 $\pm$ 0,34

**Source:** Own elaboration.



**Source:** Own elaboration.

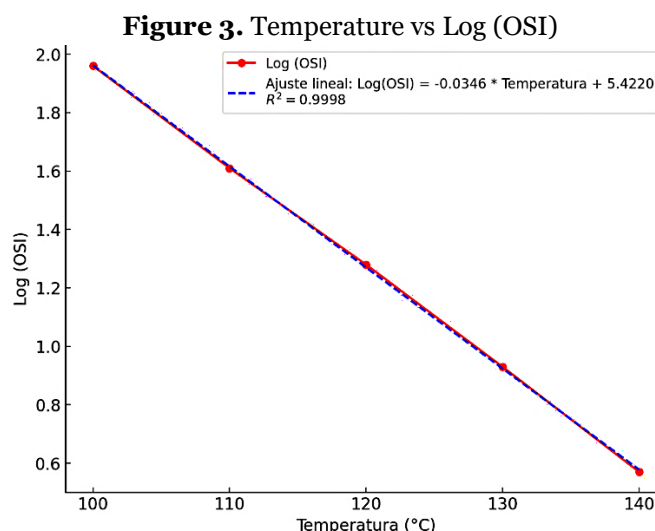
These results are consistent with various studies. For example, Bañares et al. (2019) emphasized that increasing temperature leads to a significant decrease in the induction time of edible oils due to the accelerated oxidation caused by increased free radical formation under high thermal conditions. Eudes et al. (2023) analyzed vegetable oils and concluded that oxidative stability decreases with rising temperatures, especially in oils rich in polyunsaturated fatty acids, which are particularly prone to oxidation. Furthermore, this behavior aligns with the principles of the Arrhenius equation, which describes how the rate of chemical reactions increases exponentially with temperature (Ma et al., 2024).

This supports the validity of the experimental approach based on the Rancimat method for evaluating the oxidative stability of vegetable oils. Rodríguez et al. (2020) emphasized that thermodynamic analysis based on induction time is essential for predicting the shelf life of oils and fats. On the other hand, Golmakani et al. (2020) noted that oils with higher concentrations of antioxidant compounds, such as tocopherols and polyphenols, tend to exhibit greater resistance to oxidation at moderately high temperatures.

### Kinetic Parameters — Temperature Acceleration Factor (Q<sub>10</sub>)

To calculate this parameter, a graph was created (Figure 3) showing the relationship between the logarithm of OSI and temperature, based on the values in Table 2. This relationship followed Equation (4), and the slope of the resulting linear regression was used to determine the temperature coefficient. The experimental data

showed excellent fit to the linear model, with a coefficient of determination ( $R^2$ ) of 0.9998.



**Source:** Own elaboration.

**Table 2.** Logarithmic values of OSI and Q10 calculation

Temperature (°C)	OSI ± DE (h)	Log (OSI)	Q10
100	91,16 ± 0,80	1,96	2,22
110	40,83 ± 0,61	1,61	
120	18,87 ± 0,73	1,28	
130	8,53 ± 0,72	0,93	
140	3,68 ± 0,34	0,57	

**Source:** Own elaboration.

The Q10 value obtained was 2.22, indicating that the oxidation rate of the oil more than doubles with each 10 °C temperature increase. This matches findings from the literature, where Q10 values between 1.85 and 2.25 have been reported for vegetable oils (Dini et al., 2022). A Q10 of 2.22 suggests moderate sensitivity to temperature, with accelerated oxidation under poor storage or high thermal conditions. Practical implications include strict temperature control during storage and transport and potential use of antioxidants to enhance oil stability.

The mathematical model used to calculate Q10 is expressed as:

$$Q_{10} = 10^{-10 \left( \frac{\text{Log(OSI)} - 5.42}{T} \right)}$$

Where  $T$  is the temperature in °C.

### Reaction Rate Constant ( $k$ ), Activation Energy ( $E_a$ ), and Frequency Factor ( $A$ )

Figure 4 shows the plot of  $\ln(k)$  vs.  $1/T$  from the Arrhenius equation, illustrating how the reaction rate constant ( $k$ ) increases exponentially with temperature. This trend, confirmed by Table 3, aligns with kinetic theory: higher temperatures help overcome the activation barrier, enhancing collision frequency and effectiveness (Ike, 2020). The slope ( $-E_a/R$ ) was used to calculate activation energy ( $E_a$ ), while the intercept  $\ln(A)$  gave the frequency factor ( $A$ ), indicating the probability of effective molecular collisions. The resulting equation describes  $k$  as a function of temperature.

$$k = 2,14 \cdot 10^{12} \cdot e^{\frac{-12290,60}{T}}$$

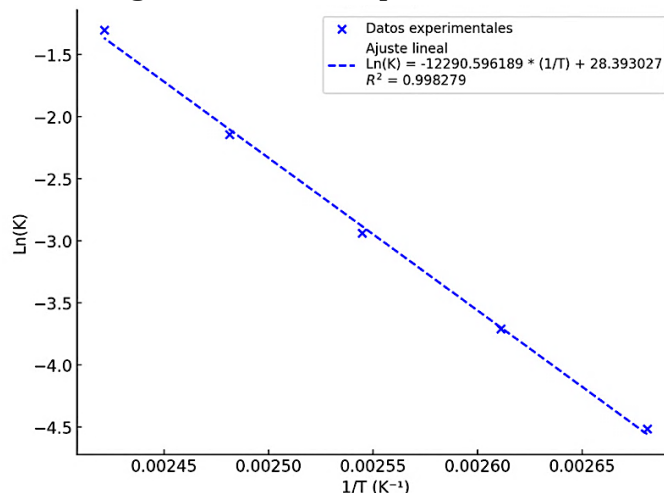
Where  $k$  is in  $\text{h}^{-1}$  and  $T$  in Kelvin.

The results emphasize temperature as a key factor in reaction rates, reinforcing its role in chemical kinetics. The Arrhenius model showed strong agreement with experimental data ( $R^2 = 0.998$ ), validating its use for describing temperature–rate relationships. This study deepens understanding of oxidation mechanisms and



provides a basis for future research on factors like catalysts or reactant concentration.

**Figure 4.** Inverse Temperature vs.  $\ln(k)$



**Source:** Own elaboration.

**Table 3.** Determination of  $E_a$  and  $A$

Temperature (°C)	Temperature (°K)	1/T (°K <sup>-1</sup> )	OSI (h)	K=1/OSI (h <sup>-1</sup> )	Ln(K)	$E_a$ (KJ·mol <sup>-1</sup> )	$A$ (h <sup>-1</sup> )
100	373	0,0027	91,16	0,0110	-4,5127	102,19	$2,14 \cdot 10^{12}$
110	383	0,0026	40,83	0,0245	-3,7094		
120	393	0,0025	18,87	0,0530	-2,9377		
130	403	0,0025	8,53	0,1172	-2,1440		
140	413	0,0024	3,68	0,2717	-1,3029		

**Source:** Own elaboration.

The activation energy ( $E_a$ ) of *L. nepetifolia* oil was 102.19 kJ·mol<sup>-1</sup>, with a frequency factor ( $A$ ) of  $2.14 \times 10^{12}$  h<sup>-1</sup>, indicating moderate oxidative stability. This  $E_a$  aligns with values for monounsaturated oils (Dini et al., 2023), suggesting good resistance at room temperature. The high  $A$  value implies a strong reaction potential once the energy barrier is crossed (Rodríguez et al., 2019). Though stable under moderate conditions, antioxidant addition may enhance heat resistance.

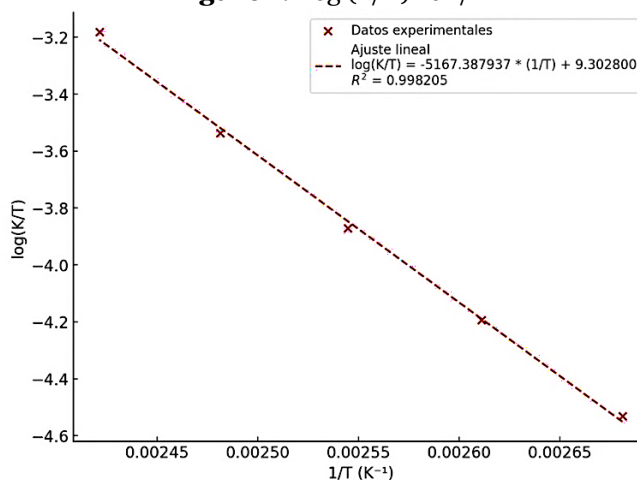
#### Calculation of Enthalpy ( $\Delta H$ ) and Entropy ( $\Delta S$ )

$\Delta H$  and  $\Delta S$  were obtained from the linear plot of  $\log(k/T)$  versus  $1/T$  (Figure 5), based on equation (8). The slope gave the enthalpy ( $\Delta H$ ), while the intercept provided the entropy ( $\Delta S$ ), both key to characterizing the oxidation process. The resulting equation was:

$$\text{Log}\left(\frac{k}{T}\right) = -\frac{5167,39}{T} + 9,30$$

Here,  $k$  is expressed in h<sup>-1</sup> and  $T$  in Kelvin. The data showed a strong fit to the linear model, with a determination coefficient ( $R^2$ ) of 0.998.

Figure 1. Log (k/T) vs 1/T



Source: Own elaboration.

Table 1. Values of  $\Delta H$  y  $\Delta S$ 

1/T (°K)	K=1/OSI (h-1)	log(K/T)	$\Delta H$ KJ	$\Delta S$ J·K-1
0,0027	0,0110	-4,5315		
0,0026	0,0245	-4,1942		
0,0025	0,0530	-3,8702	98,94	-19,53
0,0025	0,1172	-3,5364		
0,0024	0,2717	-3,1818		

Source: Own elaboration.

The thermodynamic parameters of *L. nepetifolia* oil reveal important aspects of its oxidative stability. Activation enthalpy ( $\Delta H$ ) was 98.94 kJ·mol<sup>-1</sup> and activation entropy ( $\Delta S$ ) was -19.53 J·mol<sup>-1</sup>·K<sup>-1</sup>, indicating moderate thermal stability and a more ordered transition state. These values align with oils of similar stability (Hamed et al., 2023; Dini et al., 2022) and suggest slow degradation under standard storage. The oil's oxidative resistance makes it suitable for use in food, cosmetics, and pharmaceuticals. Further research on its fatty acid profile and antioxidant content is recommended to expand its industrial applications.

### Gibbs Free Energy

The Gibbs free energy ( $\Delta G$ ) was calculated using  $\Delta H$  and  $\Delta S$  through equation (9), yielding the following model:

$$\Delta G = 98,94 + 19,53 \cdot 10^{-3}T$$

where  $\Delta G$  is in kJ and T in Kelvin.

Table 5. Gibbs Free Energy Values at Different Temperatures

Temperature (°K)	$\Delta G$ (KJ)
373	106,22
383	106,42
393	106,62
403	106,81
413	107,01

Source: Own elaboration.

The  $\Delta G$  values of *L. nepetifolia* oil slightly increased with temperature, indicating reduced thermodynamic favorability of oxidation at higher temperatures—suggesting good resistance under moderate storage. These values are comparable to those of palm oil (Velasco & Dobarganes, 2019) and oils rich in unsaturated fats (Dini et al., 2022), highlighting similar oxidative stability. This trend implies lower susceptibility to thermal



degradation, making the oil suitable for food, cosmetic, and pharmaceutical use. Further studies on antioxidant interactions and industrial performance are recommended to confirm its shelf-life potential.

### Shelf-Life Estimation

The shelf life of *L. nepetifolia* oil was estimated using three mathematical models: logarithmic, exponential, and Malthusian. These models were applied to assess oil stability at 20, 25, and 30 °C—common storage and usage temperatures in commercial settings. Each model provided insights into the oxidation kinetics. The logarithmic model best described stability loss under moderate conditions, while the exponential model captured the rapid degradation at higher temperatures. The Malthusian model offered an alternative view, interpreting degradation as a proportional increase over time. This comparative approach enabled a more comprehensive understanding of the oil's oxidative behavior and its practical implications for product preservation.

### Logarithmic Model

To model the relationship between oxidative stability (OSI) of *L. nepetifolia* oil and temperature, a graph of Log(OSI) versus temperature was constructed (Figure 6), based on equation (10). The resulting linear fit provided constants *a*(intercept) and *b* (slope), indicating baseline stability and sensitivity to temperature, respectively.

The derived equation was:

$$\text{Log}(\text{OSI}) = -0,0346T + 5,422$$

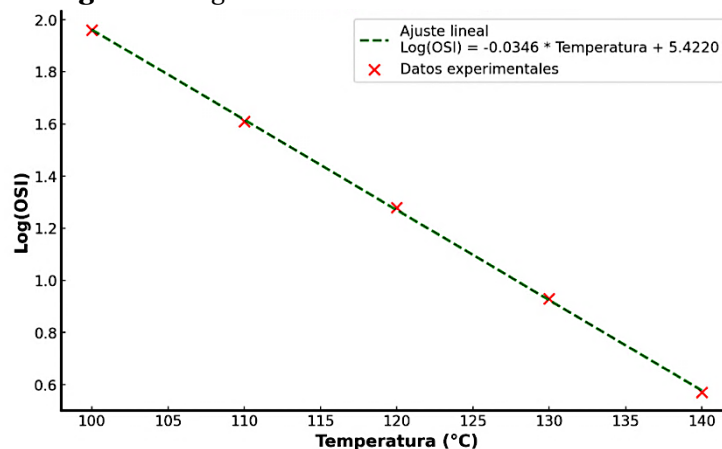
where *T* is in °C and OSI in hours. The model showed strong correlation (*R*<sup>2</sup>), validating its predictive capacity. This model enables shelf-life estimation under different storage temperatures and supports strategies to improve oil stability through antioxidants or protective packaging. It may also be applicable to oils with similar lipid profiles. Shelf-life predictions at 20, 25, and 30 °C are presented in Table 6.

**Table 6.** Shelf-life prediction using the logarithmic model.

Temperature (°C)	Shelf life		
	hours	days	years
20	53703,18	2237,63	6,13
25	36057,86	1502,41	4,12
30	24210,29	1008,76	2,76

**Source:** Own elaboration.

**Figure 6.** Logarithmic model for shelf-life estimation.



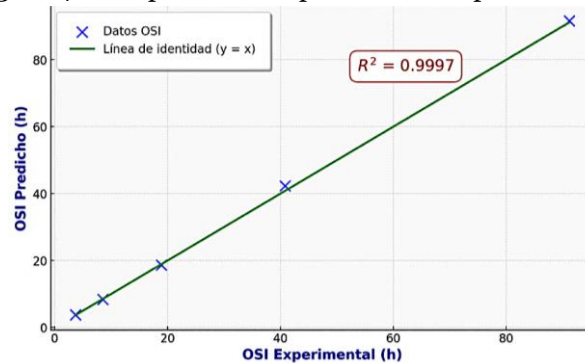
**Source:** Own elaboration.

To validate the model, experimental and predicted OSI values were compared (Figure 7, Table 7), showing excellent agreement with an *R*<sup>2</sup> of 0.999.

This confirms the model's reliability for predicting shelf life based on temperature in *L. nepetifolia* oil. Its precision supports industrial use and suggests potential for application to similar vegetable oils. Future

research should test the model under varying storage, light, and antioxidant conditions to expand its predictive scope.

**Figure 7.** Comparison of experimental vs. predicted OSI.



**Source:** Own elaboration.

**Table 7.** OSI values predicted by the logarithmic model.

Temperature (°C)	OSI (Experimental) (h)	OSI (Predicted) (h)
100	91,16	91,62
110	40,83	41,3
120	18,87	18,62
130	8,53	8,39
140	3,68	3,78

**Source:** Own elaboration.

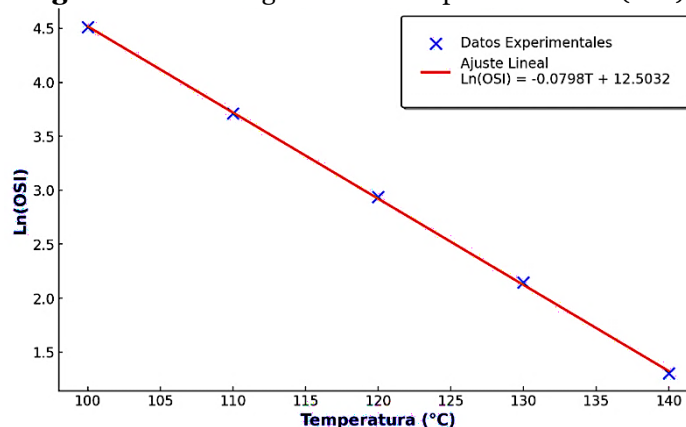
### Exponential Model (translated and reduced)

The exponential model was derived from the  $\ln(\text{OSI})$  vs. temperature plot (Figure 8), allowing prediction of *L. nepetifolia* oil stability under different temperatures. The slope (B) shows temperature sensitivity, while the intercept ( $\ln(t_0)$ ) reflects baseline OSI. Equation (22) describes the exponential decrease in OSI as temperature rises:

$$t_{\text{OSI}} = 269143,51 \cdot e^{-0,0798T}$$

The model showed strong correlation with experimental data, validating its use for shelf life prediction. Its alignment with previous studies on vegetable oils suggests applicability to other lipid systems. Practically, this model helps estimate the time the oil remains stable at specific temperatures, aiding in decisions on storage, packaging, and formulation. Future work could integrate factors like antioxidants, light exposure, and packaging materials to enhance predictive accuracy.

**Figure 8.** Linear regression of temperature vs.  $\ln(\text{OSI})$



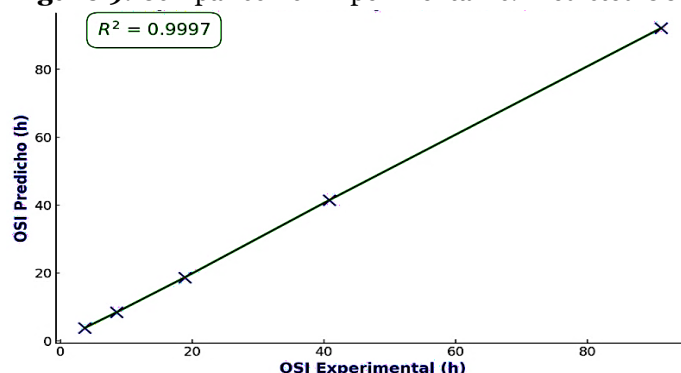
**Source:** Own elaboration.

**Table 8.** Shelf-life prediction using the logarithmic model.

Temperature (°C)	Shelf Life		
	hours	days	Years
20	54556,93	2273,21	6,23
25	36607,19	1525,30	4,18
30	24563,09	1023,46	2,80

**Source:** Own elaboration.

A detailed comparison was made between experimental OSI values and those predicted by the exponential model to assess its accuracy and predictive capacity. The coefficient of determination ( $R^2$ ) was calculated, showing a near-perfect fit ( $R^2 = 0.999$ ), confirming the model's reliability in estimating OSI as a function of temperature. As shown in Figure 9 and detailed in Table 9, the small differences between observed and predicted values validate the model's precision. This confirms its applicability for shelf-life prediction of *L. nepetifolia* oil and potentially other oils with similar characteristics. The model's high accuracy also supports its use in food, pharmaceutical, and cosmetic industries. Future studies may enhance its predictive power by incorporating factors like antioxidants, light exposure, and packaging interactions.

**Figure 9.** Comparison of Experimental vs. Predicted OSI.

**Source:** Own elaboration.

**Table 9.** OSI Values Predicted by the Exponential Model

Temperature (°C)	OSI (Experimental) (h)	OSI (Predicted) (h)
100	91,16	92,11
110	40,83	41,47
120	18,87	18,67
130	8,53	8,41
140	3,68	3,78

**Source:** Own elaboration.

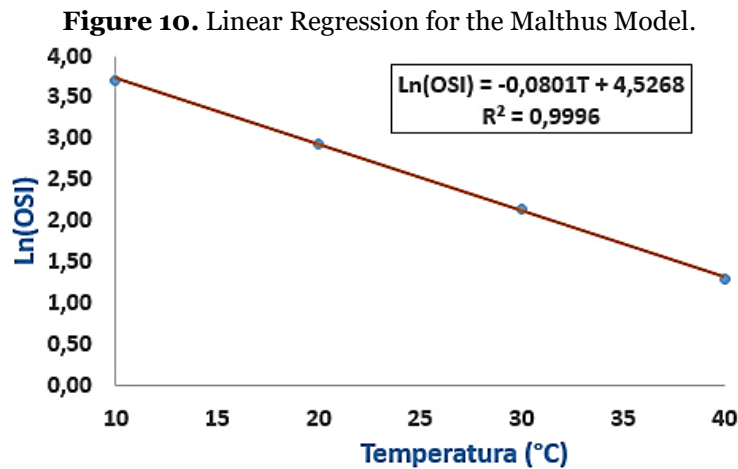
### Malthus Model

A mathematical model relating the oxidative stability index (OSI) to temperature was developed by analyzing the linear relationship of  $\ln(\text{OSI})$  versus temperature, as shown in Equation (23) and Figure 10. This approach yielded a predictive equation capable of accurately describing OSI variations under different thermal conditions, serving as a valuable tool to estimate the oxidative stability of *L. nepetifolia* oil. The slope of the fitted line, denoted as constant  $k$ , reflects the OSI's sensitivity to temperature changes and the oil's oxidation rate. The intercept,  $\ln(\text{OSI}_0)$ , represents the initial OSI under standard conditions. The final model is expressed as:

$$\text{OSI} = 91,16 \cdot e^{-0,0801(T-100)}$$

Table 10 presents the model's predicted OSI values, showing strong agreement with experimental data, confirming the model's reliability. This equation helps estimate shelf life based on temperature, supporting

optimized storage strategies. The model proves useful for the food, cosmetic, and pharmaceutical industries, where predicting oil stability is essential for product quality and safety.



**Source:** Own elaboration.

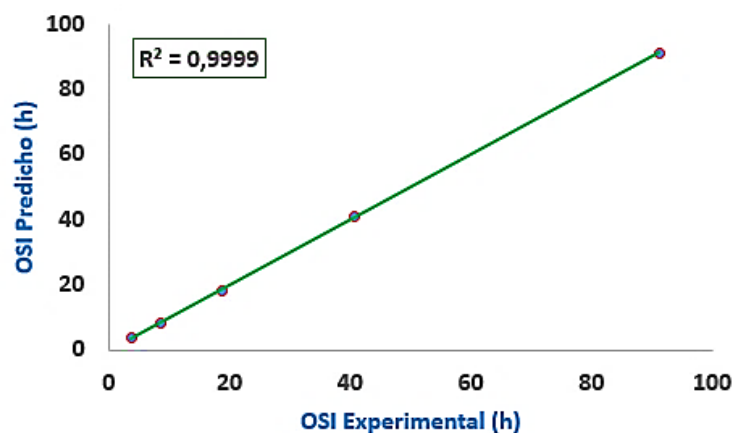
**Table 10.** Shelf-Life Prediction Using the Malthus Model

Temperature (°C)	Shelf Life		
	hours	days	Years
20	55304,87	2304,37	6,31
25	37053,43	1543,89	4,23
30	24825,24	1034,39	2,83

**Source:** Own elaboration.

Experimental OSI values were compared with those predicted by the model to assess accuracy. As shown in Figure 11 and Table 11, results were highly consistent. The model showed excellent correlation ( $R^2 = 0.999$ ), confirming its strong predictive capacity for the oxidative stability of *L. nepetifolia* oil. This supports its use in estimating shelf life under various conditions. Future improvements may include factors like antioxidants, packaging, and environment to enhance its applicability.

**Figure 11.** Experimental vs. Predicted OSI Values (Malthus Model).



**Source:** Own elaboration.

**Table 11.** OSI Values Predicted by the Malthus Model.

Temperature (°C)	OSI (Experimental) (h)	OSI (Predicted) (h)
100	91,16	91,16
110	40,83	40,92
120	18,87	18,37
130	8,53	8,25
140	3,68	3,7

**Source:** Own elaboration.

All three mathematical models (logarithmic, exponential, and Malthus) showed excellent fit to the experimental data, each with a correlation coefficient of 0.999, confirming their reliability for predicting oil shelf life based on temperature. Despite structural differences, all models produced similar shelf life estimates, particularly at lower temperatures. At 20°C, predicted shelf lives ranged from 6.13 to 6.31 years. At higher temperatures (25°C and 30°C), the Malthus model slightly overestimated values, but differences remained minimal, and all models followed the same decreasing trend with temperature, ensuring consistent and practical predictions.

Compared to other oils, *L. nepetifolia* showed superior oxidative stability. At 25°C, its shelf life exceeded 4 years, significantly higher than values reported by Moreira et al. (2020) for sunflower, sesame, and grape seed oils (0.2–0.39 years), and by Hashim et al. (2023) for flaxseed oil (0.18 years at 20°C). This stability may be due to natural antioxidants in *L. nepetifolia* oil.

Similarly, when compared to *Physalis peruviana* oil (120 days at 25°C; Ugarte-Espinoza et al., 2021), *L. nepetifolia* oil again demonstrated superior shelf life, likely due to lower polyunsaturated fat content and higher antioxidant levels like tocopherols and phenols.

## 5. CONCLUSION:

It can be concluded that there is an inverse relationship between temperature and the oxidative stability of *L. nepetifolia* oil. As temperature increased, OSI values significantly decreased, reflecting greater susceptibility of the oil to oxidation under higher thermal conditions. This behavior suggests that the oil undergoes accelerated degradation at elevated temperatures, which can be explained by the increased rate of oxidation reactions as the activation energy barrier is surpassed.

*L. nepetifolia* oil showed moderate oxidative stability, with a  $Q_{10}$  value of 2.22 and an activation energy of 102.19 kJ·mol<sup>-1</sup>, indicating that oxidation accelerates at higher temperatures. While the oil maintains acceptable resistance to oxidation under normal storage conditions, its heat sensitivity suggests that stability could be improved through the addition of natural antioxidants. These results provide a foundation for optimizing its shelf life in commercial and high-temperature storage applications.

The three mathematical models developed to predict the shelf life of *L. nepetifolia* oil showed excellent fit, with a determination coefficient ( $R^2$ ) of 0.999. These results demonstrate that the models accurately predict the reduction in shelf life as temperature increases, highlighting the importance of thermal control to preserve oil quality. The models offer a useful tool for optimizing oil preservation and extending its shelf life in commercial applications.

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