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Characterization and Model Tristimulus-Colorimetry of Malathion at Different Solutions

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ABSTRACT

Background: Chemicals such as pesticides, insecticides, pesticides, etc.; currently are the most effective resources in the conservation and crop protection in agriculture. Due to effectiveness, low cost and relative ease in handling these products, are elected by farmers and all other workers. However although their operation is regulated by environmental organizations in their use and exposure as well as in handling and application, it found irregularities with which humans and other biological beings are exposed, gradually affecting their health and quality of life. Therefore, it has been required to develop studies that will contribute to the analysis of the pesticides most used in order to identifying them and characterizing them chemically and biologically. ***Objective***: characterization and model colorimetry of Malathion at different solutions, developed experimentally, in a preliminary study of color spectroscopy. **Conclussions:** Models between the concentration of Malathion and some of the main chromatic parameters were obtained with which it can characterize a physical-chemical behavior of color of this product; with an error of 0.5026 in the multiple regression model. Positive correlations between concentrations of the various solutions and the color parameter of luminosity (L *) also with (b*) were found. It was determined that the luminosity parameter decreases as the concentration of each solution of Malathion decreases.

KEY WORDS
Pesticide Malathion, tristimulus colorimetry, psychometric attributes CIELAB space.

INTRODUCTION

Malathion it's part of the organophosphate pesticides group is used in agriculture for pest management in crop, [1].It is, toxicologically listed in category III in the EPA (Environmental prevention Agency),[2]. Their toxicity depends on factors like the chemical structure, the metabolism of the organism, the concentration, the degree of decomposition and the input mode of the product to the body,[3].

Some studies have identified this chemical as one of the pesticides that cause alterations to the main organic systems [4] (neurological, reproductive, immune, etc.), [5] of various species, such as the anomalies found in the reproductive system male in rats exposed to this pesticide. In similarly it found an alteration in human sperm chromatin by organochlorine and organophosphorus pesticides [6]. Within the latter, they highlight those working with Malathion as agricultural product, [7].

Other studies describe the possibility of malaoxon to induce DNA breaks where the tumor suppressor genes are located so this metabolite of Malathion could be, considered as a potential carcinogen and mutagen, [8].

The effect of pesticides on crops threatens the environment and human health, [9], [10]. This is an issue that has aroused great interest in the characterization of the quantitative relationships between structure / activity and structure / property, [11]as well as studies and experiments that will generate models to characterize the biological and physico-chemical activity of these chemicals developed by pharmaceutical and agrochemical industries, [12].

Some work related to the characterization of physical and chemical pesticides models are, discussed in [13] where the physico-chemical characterization of pineapple fruit was, developed in the analysis of pesticide residues organochlorine and organophosphorus, where they found large concentrations of various highly toxic pesticides.

The present work has as its main objective, the characterization and model colorimetry of Malathion at different solutions, developed experimentally, in a preliminary study of color spectroscopy.

Methods:

Malathion 57% EC, is the product name used in this work, and its main physical and chemical properties are, listed in

Table ***1***.

Table 1: Physical and chemical properties of Malathion.

Physical and chemical properties	
Physical State	Liquid
Color	Colorless to pale yellow.
Odor	Slightly aromatic odor.
Density	1,0707 g/cc
Humidity	0,05 %
Flash Point	>30°C

Experimental development consisted in data acquisition of color analysis by the spectroscopy, initially at 10ml of Malathion in pure state, and then the following pesticide solutions were, developed in distilled water for analysis.

Table ***2***shows the solutions prepared in experimentation. Where V1 is the volume in ml of Malathion and V2 the volume in ml of distilled water.

Table 2: Solutions for experimentation

N° Disolución	V1 (ml)	V2 (ml)
1	10	10
2	10	20
3	10	30
4	10	40
5	10	50
6	10	100
7	10	150
8	10	200
9	10	250
10	10	300
11	10	350
12	10	400
13	10	450
14	10	500
15	10	600
16	10	700

From the volumes of solutions and the concentration of Malathion in pure state (604g / L) for the product used in testing, the molar concentrations (M) were obtained as presented in

Table ***3***.

Table 3: Concentrations of Malathion (Molar) for different dissolutions.

N° Sol	C1 (M)	V1	V2	C2 (M)
1	1.828	10	10	1.82800
2	1.828	10	20	0.91400
3	1.828	10	30	0.60933
4	1.828	10	40	0.45700
5	1.828	10	50	0.36560
6	1.828	10	100	0.18280
7	1.828	10	150	0.12187
8	1.828	10	200	0.09140
9	1.828	10	250	0.07312
10	1.828	10	300	0.06093

11	1.828	10	350	0.05223
12	1.828	10	400	0.04570
13	1.828	10	450	0.04062
14	1.828	10	500	0.03656
15	1.828	10	600	0.03047
16	1.828	10	700	0.02611

The concentrations of the different solutions in (ppm) are illustrated in

Table ***4***.

Table 4: Concentrations of Malathion (ppm) for different dissolutions.

N° Sol	C1 (ppm)	V1	V2	C2 (ppm)
1	604000	10	10	604000.00
2	604000	10	20	302000.00
3	604000	10	30	201333.33
4	604000	10	40	151000.00
5	604000	10	50	120800.00
6	604000	10	100	60400.00
7	604000	10	150	40266.67
8	604000	10	200	30200.00
9	604000	10	250	24160.00
10	604000	10	300	20133.33
11	604000	10	350	17257.14
12	604000	10	400	15100.00
13	604000	10	450	13422.22
14	604000	10	500	12080.00
15	604000	10	600	10066.67
16	604000	10	700	8628.57

In each of dissolutions, three captures of data were performed, with which later they were classified and analyzed, obtaining them the mean and standard deviation for each solution.

Colorimetry:

Color is related to sensory qualities, in such way it have a concept and objective measurement of color through three sensations, which define the color stimulus of three-dimensionality, [14]. Hue, lightness and saturation are the attributes that characterize it.

The luminosity or brightness, allow classify the color as light or dark, this attribute is a relative measure of the light reflected off the absorbed, so this is not, considered as a parameter of the chromaticity.

Saturation versus tone determines the difference from the gray of the same lightness; this describes the reflection to a specific wavelength.

The tone is the main qualitative attribute and classifies a color such as red, yellow green or blue, is related to differences in absorbance / transmittance of radiant energy to different wavelengths [15].

The CIELAB space, is the current system proposed by the International Commission on Illumination (CIE - "Commission Internationale de l'Eclairage"), which allows to set the color. This represents in rectangular coordinates the luminosity, L * and chromaticity a * values from (-a *) to (+ a) and goes from green to red. Chromaticity b * values between (-b *) and (+ b *), and goes from blue to yellow. The color in its three attributes is expressed in CIELAB tristimulus space coordinates, which are related to the psychometric parameters Chroma (C) and tone (hue h), [16].

According to the previous theory chromaticity presented below, the coordinates representative luminosity and chrominance data and psychometric parameters for the first three solutions of the study.

Table ***5***presents the acquired data of the color parameters for the Malathion in pure state.

Table 5: Parameters Dissolution 0 (Pure State).

N° sol	Cn (M)	L*	a*	b*	c	h
0	1.828	103.471	-13.179	-19.428	23.477	-124.151
0	1.828	102.522	-13.227	-18.839	23.019	-125.074
0	1.828	102.461	-13.096	-19.136	23.189	-124.387
Promedio		102.818	-13.167	-19.134	23.228	-124.537
Desviación Estándar		0.566	0.066	0.295	0.232	0.480

Table *6*presents the data acquired of the color parameters for the first solution with a concentration of 0.914 M Malathion.

Table 6: Parameters Solution 1 / Concentration 0.914 M.

N° sol	Cn (M)	L*	a*	b*	c	h
1	0.914	142.415	-8.198	-7.57	11.159	-137.279
1	0.914	143.166	-8.302	-7.794	11.387	-136.807
1	0.914	142.997	-8.3	-7.765	11.366	-136.908
Promedio		142.859	-8.267	-7.708	11.304	-136.998
Desviación Estándar		0.3940	0.0595	0.1218	0.1260	0.2485

Table *7*presents the data acquired from the color parameters for the second solution with a concentration of 0.6093 M Malathion.

Table 7: Parameters Solution 2 / Concentration 0.6093 M.

N° sol	Cn (M)	L*	a*	b*	c	h
2	0.60933	137.923	-9.983	-15.369	18.327	-123.005
2	0.60933	137.851	-9.914	-15.365	18.286	-122.832
2	0.60933	137.622	-9.903	-15.429	18.334	-122.696
Promedio		137.799	-9.933	-15.388	18.316	-122.844
Desviación Estándar		0.157	0.043	0.036	0.026	0.155

The average data obtained for the luminosity and chromaticity in all solutions are presented in

Table ***8***.

Table 8: Average and Standard Deviation of the parameters L, a, and b.

Cn (M)	L*	a*	b*
1.82800	102.818 ± 0.566	-13.167 ± 0.066	-19.134 ± 0.295
0.91400	142.859 ± 0.394	-8.267 ± 0.059	-7.710 ± 0.122
0.60933	137.799 ± 0.157	-9.933 ± 0.043	-15.388 ± 0.036
0.45700	145.251 ± 0.165	-10.162 ± 0.064	-15.435 ± 0.190
0.36560	141.955 ± 5.912	-8.251 ± 0.554	-15.377 ± 1.335
0.18280	125.646 ± 0.526	-10.572 ± 0.403	-19.218 ± 0.482
0.12187	122.377 ± 0.991	-12.290 ± 0.144	-19.004 ± 0.262
0.09140	115.877 ± 1.368	-11.962 ± 0.464	-18.941 ± 1.286
0.07312	102.651 ± 9.149	-11.873 ± 0.103	-18.251 ± 3.159
0.06093	107.348 ± 0.134	-12.400 ± 0.025	-18.351 ± 0.021
0.05223	104.724 ± 0.108	-10.300 ± 0.013	-20.055 ± 0.137
0.04570	99.073 ± 0.439	-9.596 ± 0.047	-20.423 ± 0.068
0.04062	93.263 ± 0.444	-9.466 ± 0.088	-18.640 ± 0.101
0.03656	94.093 ± 0.177	-9.198 ± 0.060	-19.247 ± 0.093
0.03047	82.665 ± 0.572	-8.633 ± 0.115	-17.861 ± 0.053
0.02611	93.852 ±0.061	-17.456 ± 0.061	-8.968 ± 0.132

The average data obtained in psychometric parameters in all solutions are presented in

Table ***9***.

Table 9: Average and Standard Deviation of the parameters c and h.

Cn (M)	c	h
1.82800	23.228 ± 0.232	-124.537 ± 0.480
0.91400	11.304 ± 0.126	-136.998 ± 0.248
0.60933	18.316 ± 0.026	-122.844 ± 0.155
0.45700	18.480 ± 0.183	-123.366 ± 0.252
0.36560	17.455 ± 1.366	-118.259 ± 1.567
0.18280	21.938 ± 0.290	-118.825 ± 1.458
0.12187	22.813 ± 0.234	-122.892 ± 0.162
0.09140	22.403 ± 1.333	-122.303 ± 0.759
0.07312	21.819 ± 2.637	-123.433 ± 4.770
0.06093	22.147 ± 0.020	-124.048 ± 0.066
0.05223	22.545 ± 0.116	-117.185 ± 0.188
0.04570	22.557 ± 0.084	-115.177 ± 0.091
0.04062	20.906 ± 0.122	-116.924 ± 0.155
0.03656	21.332 ± 0.108	-115.542 ± 0.068
0.03047	19.838 ± 0.012	-115.797 ± 0.365

0.02611	19.625 ± 0.075	-152.807 ± 0.370

From the above data, it proceeded to evaluate the factors of correlation between the concentration and the different chromatic variables.

Table ***10***presents the correlation coefficients between concentration and the other parameters.

Table 10: Correlation Coefficients.

	L*	a*	b*	c	h
Cn (M)	*0.3183*	-0.0222	*0.2089*	-0.2433	-0.1701

A positive correlation coefficient only between concentration and luminosity (L*) was found and between concentration and the chromaticity (b *).

Analysis of Results:

The results of experimentation and analysis of data and models derived from mathematical approximations performed with the Matlab software are presented below.

The scatterplot between concentration and brightness L * coordinate shown in Figure 1.

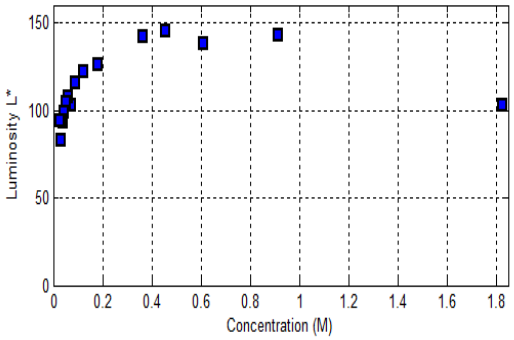

Fig. 1: Scatterplot of Concentration and luminosity L*.

(1) Describes linear approximation found for the relationship between concentration and luminosity.

$$y = 13.49x + 109.1 \quad (1)$$

In Figure 2, the scatter plot between the concentration and chromaticity a * is shown.

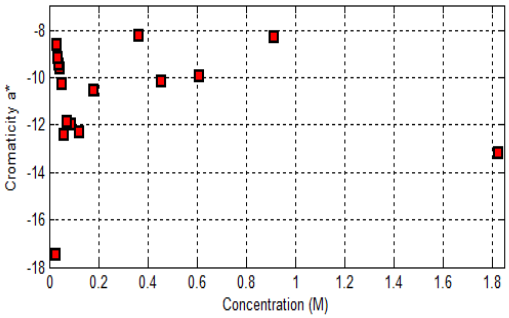

Fig. 2: Scatterplot of Concentration and a*.

Linear approximation found for the relationship between concentration and a * is described, by (2).

$$y = -0.11x - 11 \quad (2)$$

The scatterplot between concentration and b *, is shown in Figure 3.

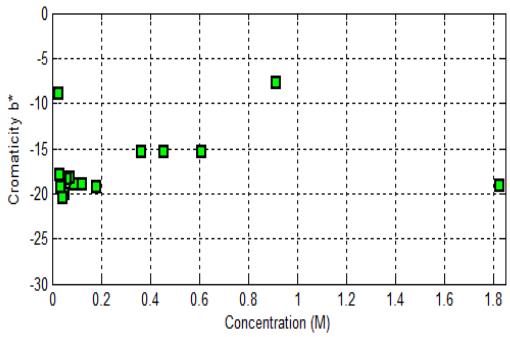

Fig. 3: Scatterplot of Concentration and b *.

Linear approximation found for the relationship between concentration and a * is described by (3).

$$y = -1.6x - 17.5 \quad (3)$$

The scatter plot between the concentration c and the parameter is presented in Figure 4.

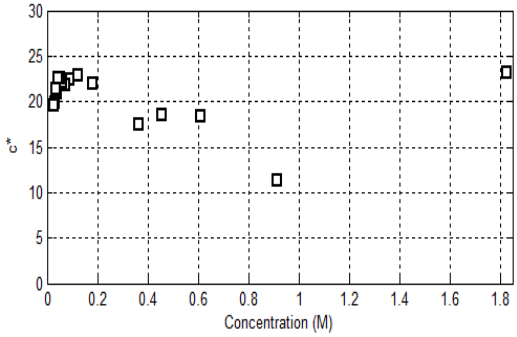

Fig. 4: Scatterplot of Concentration and c.

Linear approximation found for the relationship between concentration and a * is described by (4).

$$y = -1.53x + 20.89 \quad (4)$$

In Figure 5, the scatter plot between the concentration parameter and h is, presented.

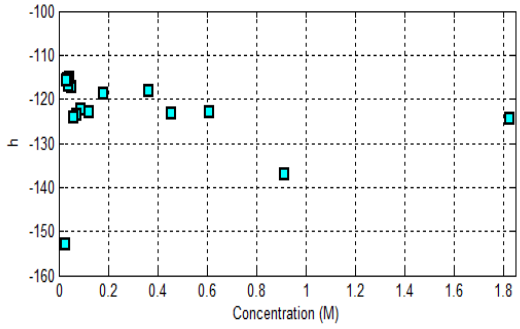

Fig. 5: Scatterplot of Concentration and h.

Linear approximation found for the relationship between concentration and a * is described by (5).

$$y = -3.39x - 122.14 \quad (5)$$

According to the results of the correlation, the approximation model among main parameters was obtained. The corresponding model between the concentration and the luminosity with a correlation index 0.3183 is shown in Figure 6.

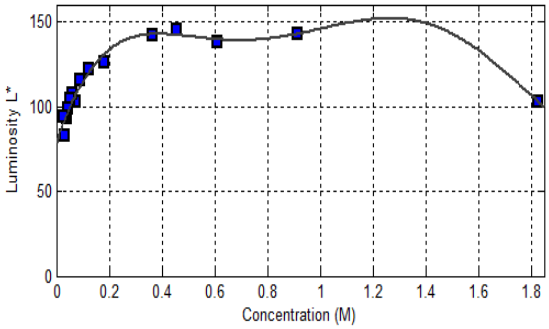

Fig. 6: Model of Concentration and Luminosity.

The best model adjusted for this relationship was approximated to a polynomial function of degree 5, described in equation (6).

$$y = 137.2x^5 - 752.3x^4 + 1468x^3 - 1259x^2 + 473.8x + 78.47 \quad (6)$$

The corresponding model between concentration and b *, with a correlation index of 0.2089, it is shown in Figure 7.

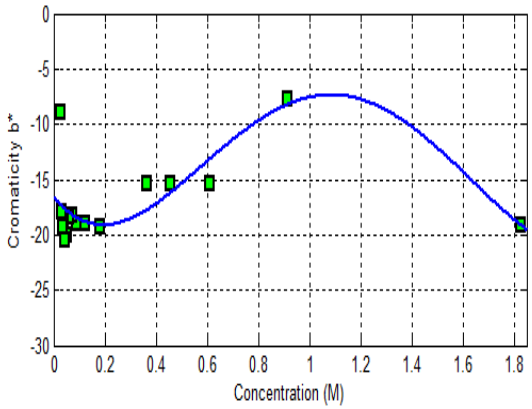

Fig. 7: Model of Concentration and b*.

The best model adjusted for the relationship it was approximated to a polynomial function of degree 4, and it described in equation (7).

$$y = 18x^4 - 78x^3 + 99x^2 - 30x - 17 \quad (7)$$

The corresponding model between the concentration and the parameter c, with a correlation index of -0.2433 it is, shown in Figure 8.

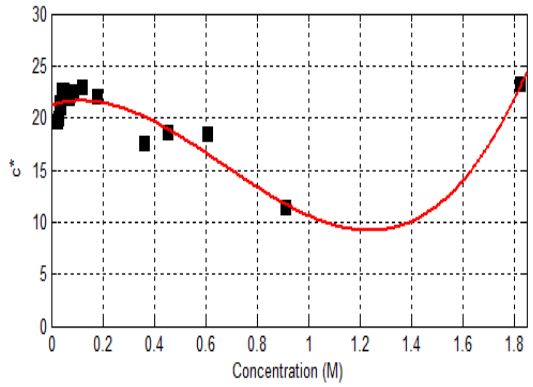

Fig. 8: Model of Concentration and c.

The best model adjusted for the relationship it was approximated to a cubic function, and it described in equation (8).

$$y = 18x^3 - 36x^2 + 7.6x + 21 \quad (8)$$

Finally, a general multiple regression model was obtained between Concentration, Luminosity and coordinates a*, b*.

The main parameters of the multiple regression are presented, in Table 11.

Table 11: Multiple regression model.

	coefficients
Interception	-0.6265
L*	0.0076
a	-0.0210
b	0.0090
Error	0.5026
Model $y(M) = L * (0.0076) - a(0.0210) + b(0.0090) - 0.6265$	

Conclusions:

In the development of this work, positive correlations between concentrations of the various solutions and the color parameter of luminosity (L *) was found, describing the gray scale between black and white; and the chromaticity coordinate (b *), which describes the range of colors between blue and yellow.

From the data obtained in the experiments, it was determined that the luminosity parameter decreases as the concentration of each solution of Malathion decreases, while a clear behavior was not found, between concentration and the other chromatic parameters.

Models between the concentration of Malathion and some of the main chromatic parameters were obtained with which it can characterize a physical-chemical behavior of color of this product; with an error of 0.5026 in the multiple regression model for the characterization of tristimulus color of Malathion at different solutions proposed.

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