AMERICAN-EURASIAN JOURNAL OF SUSTAINABLE AGRICULTURE
ISSN: 1995-0748, EISSN: 1998-1074
2016, volume(10), issue(6): pages (52-61)
Published Online 22 February 2016 in http://www.aensiweb.com/AEJSA/

Analysis and prediction of concentration in different dilutions of Pyrimethanil and Iprodione through colorimetry using neural networks

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Received 18 September 2016; Accepted 28 December 2016

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ABSTRACT

The Pyrimethanil and Iprodione are fungicide compounds of broad spectrum used in agriculture in ornamental crops and fruit trees, to increase efficiency and reduce losses. The combination of these compounds affect the development of fungi, preventing the spore germination and the mycelial growth. Due to the intrinsic toxicity of these compounds, if they are in contact with humans, they can produce serious health damage. Reason why was made a nondestructive and fast method of predicting the concentration of Pyrimethanil and Iprodione using neural networks taking as input the measurement by colorimetry of the solutions. Commercial pesticide and distilled water was used to made the dilutions. In colorimetry, the principal parameters were determined as the Hue angle and the Cab chroma with values of -156.69° and 6.3197 respectively for the pure compound. Also, a proportional relationship between the concentration of the dilutions and chroma Cab parameter was found. Correlations characteristics for CIE XYZ color space were determined, obtaining an adjustment greater than 0.99 for all parameters. In prediction of the concentration of the pesticide through neural networks, a maximum accuracy of 0.962 was found in the coefficient of determination. Using as input of the system the reflection spectrum color from 200 to 1000 nm and as output the concentration.

KEY WORDS

Color space, Fungicide, Neural fitting, Spectrophotometry.

INTRODUCTION

Fungi are part of the living beings who have survived for a lot of time on earth, due to his high resistance to contaminants and the ability of spores to survive harsh environments [1]. Because of this, highly toxic pesticides are used to combat these pests [2]–[4]. Most of chemicals used as pesticides are synthetic, ie, they are manufactured through different physicochemical processes in a laboratory. Whereupon, it is unlikely to find these substances in the environment. By increasing the concentration of these compounds increase the probability of adverse effects on humans [5], [6].

3- (3,5-dichlorophenyl) -N-isopropyl-2,4-dioxoimidazolidine-1-carboxamide is commonly known as Iprodione, which comes from urea and glycolic acid, and it is used as nematicidal and fungicidal [7], [8]. This compound is usually used in the agriculture in mixtures with Pyrimethanil, whose IUPAC name is 4,6-dimethyl-N -phenylpyrimidin-2-amine and it is used as a fungicide. Usually it applied on seeds, to inhibit cell division of the fungi. This mixture is used on crops of Rosa, Clavel, Pompon and some fruit trees, in order to prevent the occurrence of pests such as *Botrytis cinerea* and *Sphaerotheca pannosa* [9], [10].

These compounds are classified as moderately toxic, to observe acute toxic effects in rats, the concentration must be greater than 5000 mg/kg in the case of oral and dermal toxicity, whereas, through inhalation, requires a

greater concentration of 1.98 mg/kg. The Iprodione has a half - life of 30 days in the soil 67 days in water and very volatile in air [11], [12]. Reason why, this compound is persistent in water, and with a moderate soil adsorption. For Pyrimethanil, the half - life time is 47 and 76.8 days for the soil and water respectively, this being the compound with longer duration on the applied area [13].

To detect the presence of these compounds, particularly in agricultural areas where ornamental and fruit crops are handled, analytical techniques of measurements performed. Which seek to isolate the compound of interest, this was made by passing the sample through various analytical steps, in which the sample is destroy and the compound of interest is isolate. Currently, the main analytical technique in order to do this just is the chromatography, in which the sample is separate into each of his components, and then is compare against a standard sample to obtain the concentration [14]–[16].

Because the common tests take a long time and spend a lot of resources, recently it being implemented new analytical techniques capable of determining the concentration of the mixtures. One of these techniques, is the colorimetry. In which, is incident a beam of light on the sample, while a spectrophotometer collects the light refracted by the sample an analyze, based on the different colorimetric parameter, such as the Cab chroma, the Hue angle, the color spaces CIE Lab and CIE XYZ [17]–[19].

To obtain a better analysis of the data obtained by colorimetry, in the last decade it begun to implement the use of neural networks, which are algorithms of machine learning, which are based on the operation of nervous system. Where a group of neurons work as a team to find a specific response based on an input [20], [21]. This type of learning has been used for the prediction of solar radiation in different parts of the world, determining physical and chemical properties of new compounds, among others [22], [23]. Este tipo de aprendizaje se ha utilizado para la predicción de irradiación solar en diferentes lugares del mundo, en la determinación de propiedades físicas y químicas de nuevos compuestos, entre otros

Based on the above, in this paper is presented the analysis of Iprodione and Pyrimethanil compounds, the characterization of different dilutions with distilled water and the development of a neural network capable of determining the concentration of pesticides. Based on the reflection spectrum obtained through the spectrophotometer for each sample.

MATERIALS AND METHODS

A commercial mixture of Pyrimethanil and Iprodione was used for colorimetric samples, which contains the same amount of both components by weight. This version of the product was choose, due to is the most widely used in ornamental crops and fruit trees, as crops rose, pompom, carnation, among others. The initial analysis was performed comparing the data of some physicochemical properties such as density, pH, physical condition, among others. The experimental procedure was performed on the campus of New Granada Military University in Cajicá, Colombia. In an atmosphere at controlled temperature at 19 °C. Preparation of dilutions was made with distilled water. In

Table 1 is shown the relationship between the water and pesticide employed in the colorimetry measurements.

Table 1: Chlorpyrifos solutions.

	Marker	Pesticide volume [mL]	Distilled wáter volume [mL]
Pure	Pure	10	0
Solution 1	S1	10	10
Solution 2	S2	10	20
Solution 3	S3	10	30
Solution 4	S4	10	80
Solution 5	S5	10	180
Solution 6	S6	10	280
Solution 7	S7	10	380
Solution 8	S8	10	580

The initial concentration of each of the compounds was 250 g/L. Which it was applied in equations 1 and 2, to determine the molar concentration and ppm of each solution.

$$C_1\left[\frac{mol}{L}\right] = \frac{C_1\left[\frac{g}{L}\right]}{MW\left[\frac{g}{mol}\right]} \quad (1)$$

$$C_1\left[\frac{mg_A}{kg_{sln}}\right] = \frac{C_1\left[\frac{g_A}{L}\right]}{\rho\left[\frac{g_{sln}}{mL}\right]} * \frac{1\,L}{1000\,mL} * \frac{1000\,mg_A}{1\,g_A} * \frac{1000\,g_{sln}}{1\,kg_{sln}} \quad (2)$$

Where MW was the molecular weight, C was the concentration and ρ was the density. To determine the concentration of other dilutions, it was used the equation 3, in which for solutions, only changes the amount of water, but did not change the solute.

$$C_1 * V_1 = C_2 * V_2 \quad (3)$$

Colorimetry

For colorimetric analysis, a non-contact spectrophotometer Flame-S Ocean Optics was used (Fig. 1, Number 2), with a detector DET2B, with a detection range of 200 to 1100 nm, a light source DH-2000-BAL with Deuterium and tungsten lamp was used (Fig. 1, No. 1). Premium grade fiber of reflectance of 400 microns with solarization-resistant was used, with a range of similar wavelength to the detector employed.

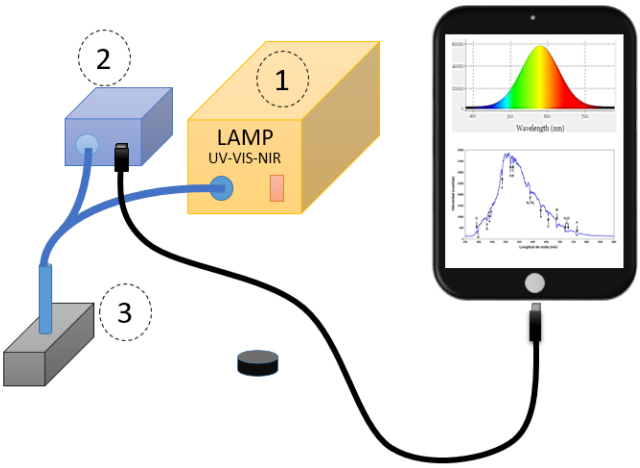


Fig. 1: Mounting handled during experimentation.

A standard diffuse of reflectance from Ocean Optics made of polytetrafluoroethylene (PTFE) was used for calibration of equipment. Colorimetric data such as chroma Cab, the Hue angle, color spaces CIE XYZ and CIE Lab were obtained through the Ocean Optics® software version 1.5.2. Each sample was taken in triplicate, in order to ensure data accuracy.

Hue angle parameter is the color base of the test sample, seen from the spectrum was the wavelength that reflects more light by impinging a standard light on it. The Cab chroma parameter refers to color saturation, where an intense color had higher values, while a dark color had low values. Another parameter obtained was the CIE color space Lab, which consists of the "L", "a *" and "b *" parameters, where the first was the brightness, the second was a color scale between green and magenta colors and the third was a scale between blue and yellow.

Besides the color space CIE XYZ was obtained, where the "X" represents the sensitivity to red and green color, the "Y" indicates brightness and the "Z" was the stimulus to blue color, they seek represent as the human eye perceived colors across different cones that compose it. To determine the parameter of greater weight, normalization of parameters was performed by Equation 4, thereby obtaining the sub-space CIE xyz.

$$x = \frac{X}{X+Y+Z} \qquad y = \frac{Y}{X+Y+Z} \qquad z = \frac{Z}{X+Y+Z} \tag{4}$$

the software Matlab® R2016a was used to obtain the mean and standard deviation of each of the tests of each samples. In addition, a pre-treatment of reflection spectra was done, to obtain then the neural network. In this pretreatment, the spectra were cut to analyze from 200 nm to 1000 nm. Because, outside these limits, it begins to be distorted, due to the margins of the equipment.

The input parameter of the neural network were the reflection spectra, while the output was the concentration at which they were taken. The three data of each test by triplicate were used, in order to increase the number of samples and thus increase the accuracy in training. The neural network had the form of the equations 5 and 6, for which H_w and O_w were the weights of the hidden layer H_b and O_b the output layer respectively, while and were the ways.

$$H_L = tansig(H_w * input + H_b) \tag{5}$$

$$output = O_w * H_L + O_b \tag{6}$$

The training of the neural network was performed with 100 neurons in the hidden layer, as shown in Fig. 2, using Bayesian Regularization as training method, to find a relationship capable of predicting the concentration of dilution, based on the reflection spectrum.

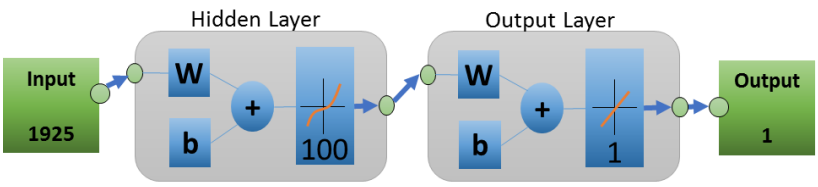


Fig. 2: Diagram of the neural network.

To verify the neural network, it was tested using the average of each sample taken by triplicate, because the concentration values of these samples were known. Furthermore, a second check was performed, in which intermediate spectra between each of the solutions were determined.

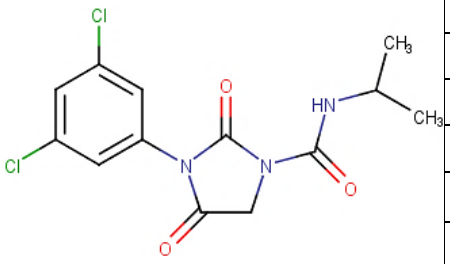
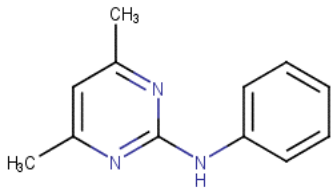
To determine the concentration of these spectra, it approached a linear relationship between each of the tests performed, therefore the average of the two concentrations was noted. This same procedure was performed by normalizing the data, in order to obtain a second response at the output of the neural network.

RESULTS AND DISCUSSION

The mixture of the compounds 3- (3,5-dichlorophenyl) -N-isopropyl-2,4-dioxoimidazolidine-1-carboxamide (Iprodione) and 4,6-dimethyl- N -phenylpyrimidin-2-amine (Pyrimethanil), were used as fungicides for ornamental and fruit crops, the main physicochemical properties were shown in

Table 2.

Table 2: Pesticides data.

Iprodione	Compound / Property	Iprodione	Pyrimethanil	Units
	Concentration	250	250	g/L
	Formula	$C_{13}H_{13}Cl_2N_3O_3$	$C_{12}H_{13}N_3$	
	pH	7.2	7.2	
	CAS	36734-19-7	53112-28-0	
	MW	330.17	199.26	g/mol
	Density	1.08	1.08	g/mL
Pyrimethanil	Chemical group	Dicarboximides	Anilo-pirimidinas	
	Phisical State	Yellow liquid		
	Components of the pesticide			
	Iprodione		0.231	
	Pyrimethanil		0.231	
	Excipients		0.538	

In

Table 2, the identification of pesticide used was shown, it should be noted that the density was slightly higher than the water, whereby this mixture tends to flow toward the ground water areas. The pH of the mixture was 7.2, which will not affect the same when applied on different crops, maintaining the same under neutral conditions. The active compounds were approximately 46% of the total mixture, that was characterized as a yellow liquid. Excipients function, altering the colligative properties of the mixture, ie, increasing the boiling point and decreasing the melting point of the pesticide.

To obtain the initial concentrations of each compound, equations 1 and 2 for the molar concentration and in ppm respectively were used. Equation 3 was also used to obtain the concentration of the dilutions thus to construct the

Table 3. The pesticide manufacturer recommends use 2 mL thereof per liter of water, however, the dose may vary depending the type and severity of the infestation.

Table 3: Molar concentration [mol/L] and ppm[mg/kg] for each solution.

Marker	Concentration Iprodione [M]	[ppm]	Concentration Pyrimethanil [M]
Pure	0.7572	231481	1.2546
S1	0.3786	115741	0.6273
S2	0.2524	77160	0.4182
S3	0.1893	57870	0.3137
S4	0.0832	25438	0.1379
S5	0.0399	12183	0.0660
S6	0.0261	7982	0.0433
S7	0.0194	5935	0.0322
S8	0.0128	3923	0.0213

The concentration in ppm for both pesticides were the same, because they have the same initial concentration. Inside the measures of the dilutions made, were some of the recommended concentrations to treat pests doses. To made the dilutions, it was used as solvent water, to simulate the way as farmers prepare the fungicide in the field. In Fig. 3, the average of Cab chroma parameter was shown for each sample analyzed.

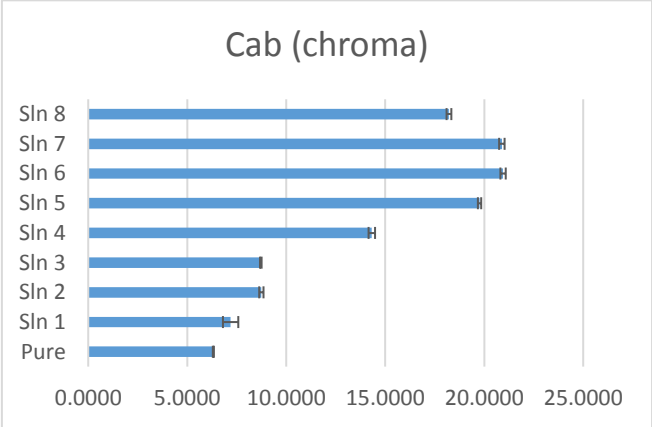


Fig. 3: Cab chroma for solutions of the pesticide employed.

For the Cab chroma parameter, an inverse tendency with the concentration of the solutions was observed, however, this value decreases in the last solution. The gradual increase in value was due to the addition of distilled water. In each test the standard deviation of the samples was indicated with a black line. This parameter was related with the Hue angle and the space color CIELAB in

Table 4. In each point of the data the standard deviation was shown.

Table 4: Hue angle and CIE Lab color space.

StD	Hue angle	L	a*	b*
Pure	-156.690 ± 0.887	157.736 ± 0.156	-5.803 ± 0.020	-2.500 ± 0.099
Sln 1	-162.779 ± 2.791	157.442 ± 0.227	-6.866 ± 0.461	-2.111 ± 0.235
Sln 2	-145.768 ± 0.944	157.985 ± 0.043	-7.227 ± 0.009	-4.919 ± 0.179
Sln 3	-160.737 ± 0.046	156.691 ± 0.094	-8.226 ± 0.036	-2.874 ± 0.019
Sln 4	-150.076 ± 0.277	151.212 ± 0.110	-12.416 ± 0.118	-7.140 ± 0.126
Sln 5	-125.013 ± 1.100	130.372 ± 0.261	-11.336 ± 0.265	-16.185 ± 0.283
Sln 6	-152.526 ± 0.571	122.915 ± 0.765	-18.588 ± 0.215	-9.664 ± 0.124
Sln 7	-154.600 ± 0.192	117.729 ± 0.563	-18.871 ± 0.152	-8.960 ± 0.026
Sln 8	-146.368 ± 0.456	99.532 ± 0.921	-15.170 ± 0.177	-10.089 ± 0.062

Hue angle parameter didn´t show connection with the concentration, however, it was found that the average of all solutions containing the pesticide had a value of -150 °. The CIE Lab color space had a proportional trend between parameters and concentration, however, the same phenomenon in the above parameters was observed at low concentrations. To apply the CIE XYZ color space, the parameter with the highest weight was determined, for which the sub space CIE xyz determined in

Table 5, by Equation 4.

Table 5: CIE xyz color space.

	x	y	z
Pure	0.440 ± 4.71 E-05	0.410 ± 8.16 E-05	0.149 ± 1.25 E-04
Sln 1	0.439 ± 3.74 E-04	0.411 ± 4.32 E-04	0.149 ± 2.36 E-04
Sln 2	0.437 ± 1.41 E-04	0.409 ± 1.25 E-04	0.153 ± 2.16 E-04
Sln 3	0.437 ± 4.71 E-05	0.411 ± 4.71 E-05	0.150 ± 0.00 E-00
Sln 4	0.429 ± 2.05 E-04	0.412 ± 4.71 E-05	0.157 ± 2.16 E-04
Sln 5	0.421 ± 9.43 E-05	0.405 ± 4.24 E-04	0.173 ± 3.86 E-04
Sln 6	0.416 ± 5.55 E-17	0.416 ± 2.49 E-04	0.166 ± 2.87 E-04
Sln 7	0.415 ± 8.16 E-05	0.417 ± 9.43 E-05	0.166 ± 8.16 E-05
Sln 8	0.414 ± 4.64 E-04	0.414 ± 2.87 E-04	0.170 ± 1.89 E-04

For samples analyzed, it was found that the variables with most weight were the parameters "x" and "y", i.e. the main color components of the pesticide were the brightness and sensitivity to green and red color, the cones L and M of the human eye. The deviation of the data was sufficiently low as to be statistically insignificant. Because, this sub space comes from CIE XYZ color space, the color space deviation was not significant too.

For CIE XYZ color space, the characteristic equations that describe each of the parameters depending on the concentration of the solution were determined in Fig. 4, the relationships were shown using as an "x" axis the concentration of Iprodione.

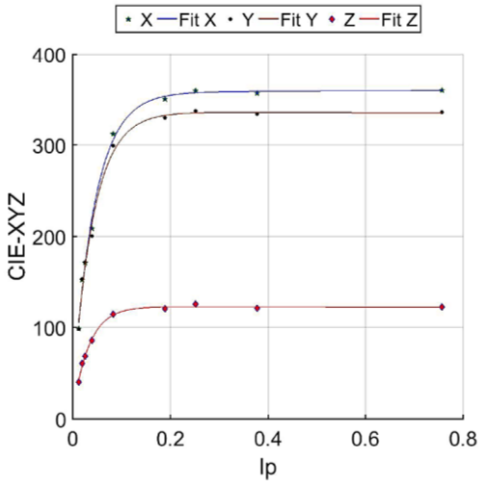


Fig. 4: Relationships of the CIE XYZ parameters.

In Fig. 4, it was shown the appropriate relationship between the actual values and the exponential curve, the curves with the fungicide Pyrimethanil were not shown, due to they had the same tendency. In

Table 6, the characteristic equations were shown, where the first three were for the pesticide Iprodione and the following three were for Pyrimethanil.

Table 6: Characteristics equations for the CIE XYZ parameters.

Equation form	f(x) = a*exp(b*x) + c*exp(d*x)		
Coefficients (with 95% confidence bounds):			
Parameter	X Ip R^2 = 0.9957	Y Ip R^2 = 0.9928	Z Ip R^2 = 0.9955
a	358.1 (332.7, 383.6)	336.8 (307.7, 365.9)	123.5 (116.4, 130.6)
b	0.00689 (-0.1433, 0.1571)	-0.00564 (-0.1905, 0.1792)	-0.01226 (-0.1404, 0.1159)
c	-336.3 (-376.4, -296.3)	-310.3 (-358.6, -262)	-118.9 (-135.1, -102.8)
d	-22.34 (-28.61, -16.06)	-23.41 (-31.74, -15.07)	-30.26 (-38.17, -22.34)
Parameter	X Py R^2 = 0.9957	Y Py R^2 = 0.9929	Z Py R^2 = 0.9955
a	358.1 (332.8, 383.3)	336.8 (307.8, 365.7)	123.5 (116.4, 130.6)
b	0.00435 (-0.0856, 0.0943)	-0.00323 (-0.1141, 0.1076)	-0.0072 (-0.0843, 0.0699)
c	-336.9 (-376.9, -296.9)	-310.9 (-359.1, -262.6)	-119.3 (-135.5, -103)
d	-13.52 (-17.29, -9.745)	-14.17 (-19.18, -9.149)	-18.32 (-23.1, -13.54)

For all parameters, the characteristic equation was determined exponentially, with a coefficient of determination (R^2) greater than 0.99 for all cases. In addition to this, the coefficients were shown with a confidence limit of 95%.

Another way to analyze the color was through reflection spectra (Fig. 5), they were treated, how was described in the section of methods and materials, to be used for training a neural network capable of predict the concentration of the fungicide based on the spectrum.

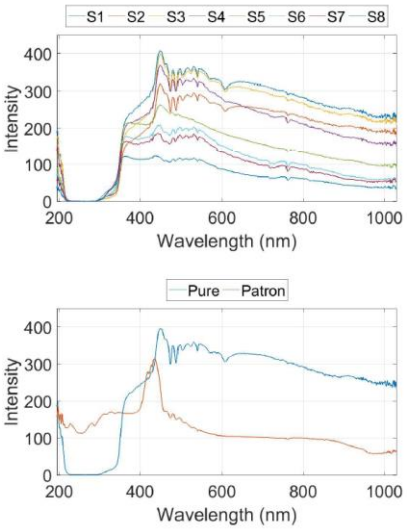
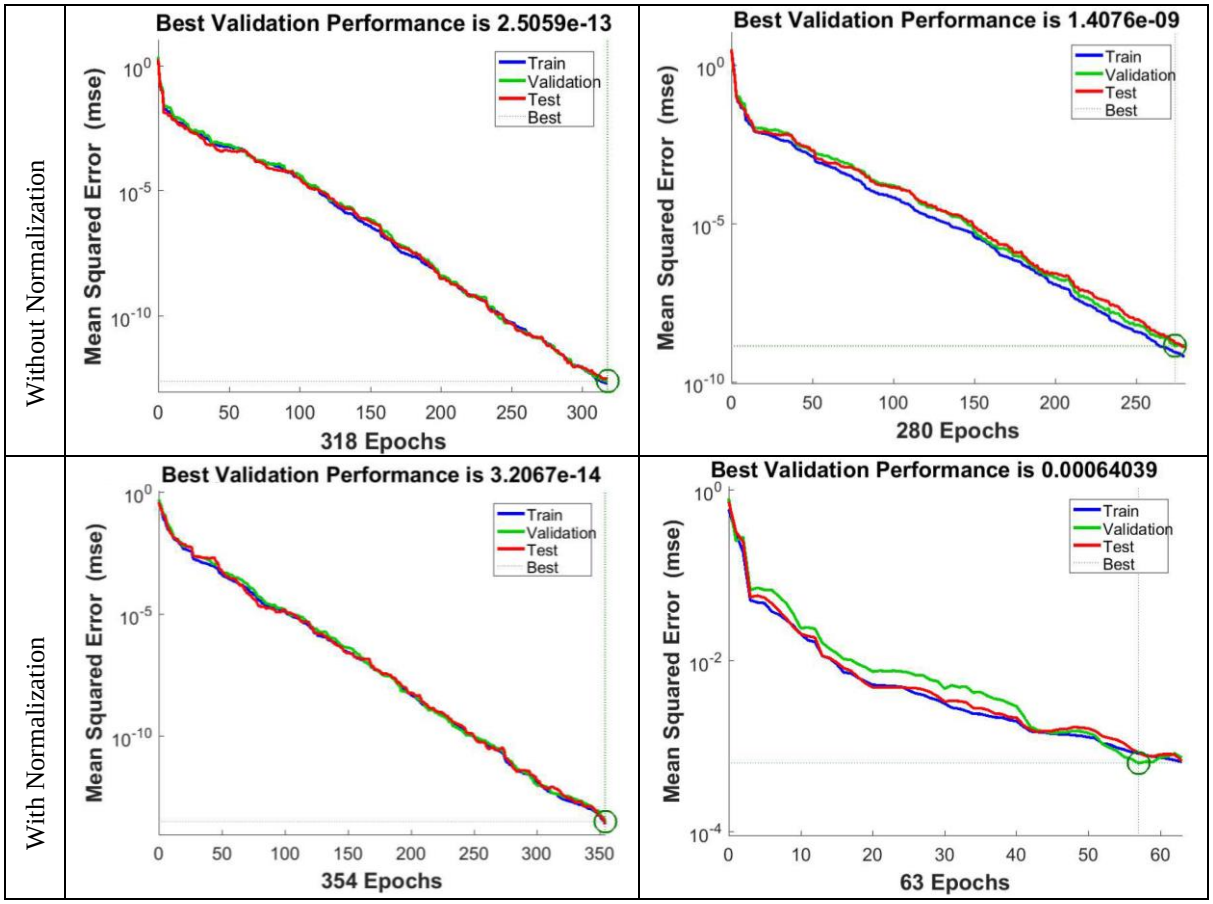


Fig. 5: Average color spectrums for each pesticide solution.

In part A of Fig. 5, a proportional relationship between the intensity of the sample and the concentration of the analyzed sample was shown. While in Part B, was the standard solution for calibration of equipment, which in this case was distilled water. It was noted, that water did not interfere with the characteristic peaks and characteristic shape of the pesticide spectrum, therefore, the measure was not affected.

In the training of the neural networks, spectra values were taken from 200 nm to 1000 nm, due to as seen in Fig. 5, these values had a lot of dispersion due to the equipment limits. In addition, the training was performed with the neural fitting module of Matlab R2016a®. The development of the neural network was proposed in section methods and materials, thus obtaining the

Fig. 6. It should be noted that this process was repeated until obtain a network that could accurately predict the concentration.



	Iprodione	Pyrimethanil

Fig. 6: Training of the neural networks.

In the trainings, very small values for the mse were reached, however, for Pyrimethanil with normalization, this value was relatively higher. To verify the neural networks, two tests were implemented, on the first the average data were taken by triplicate as input and the output was verified with known solutions of concentration, while in the second a linear relationship was used to predict concentrations and an intermediate spectrum. Each of these tests were conducted with and without the standard for each pesticide data.

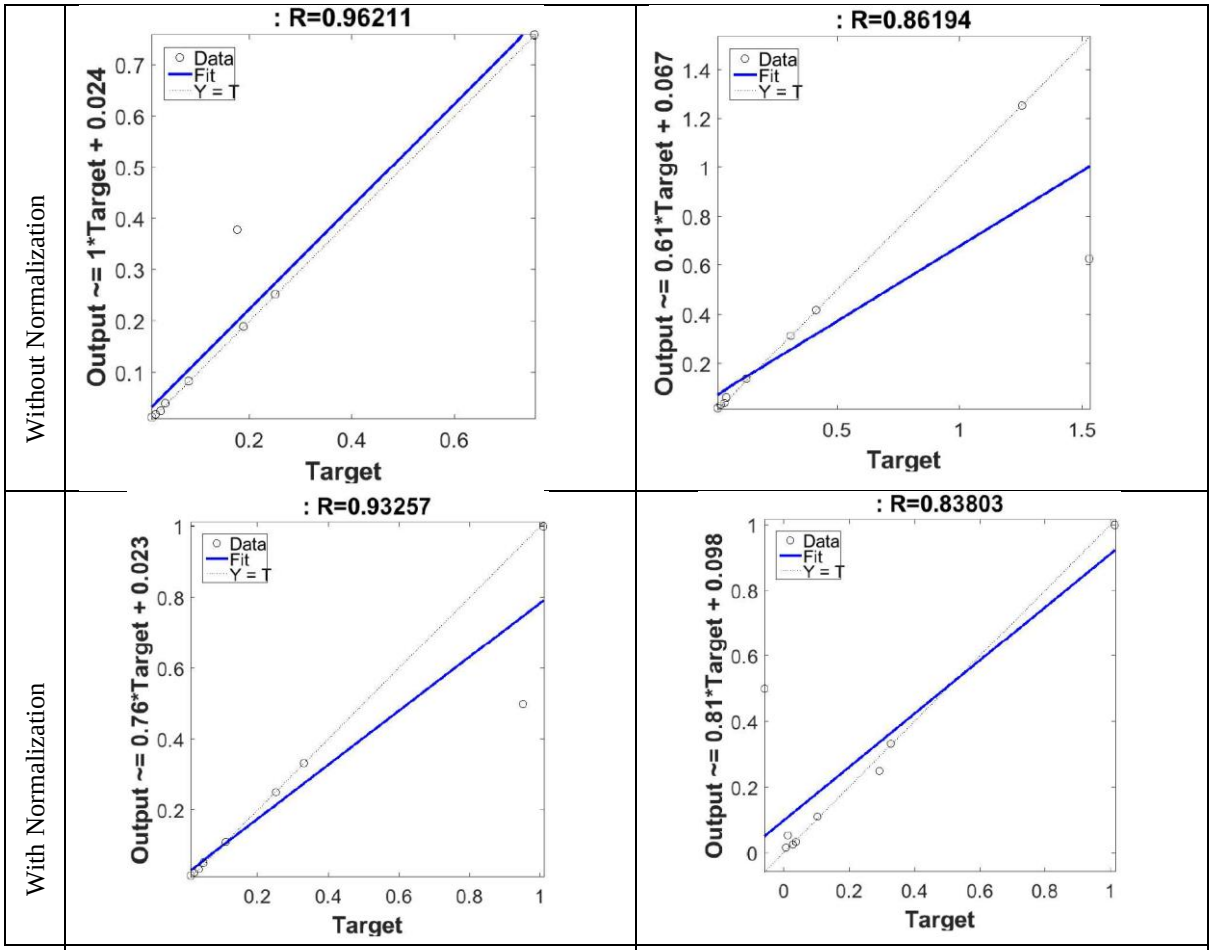


Fig. 7: Test 1 for neural networks.

As indicated in section of methods and materials, test 1 had the greatest weight in the results, due to the source of data with which they were taken. Tests with the fungicide Iprodione had better result than with the other fungicide, this was because the values of concentration handled, due to for the first, these values were in the range between 0 and 1, whereas, for Pyrimethanil these values exceed 1, thus training the neural network is more complex, generating poor results.

The network behavior with linearly interpolated values was the Test 2, shown in Fig. 8. This test was performed as indicated in materials and methods section.

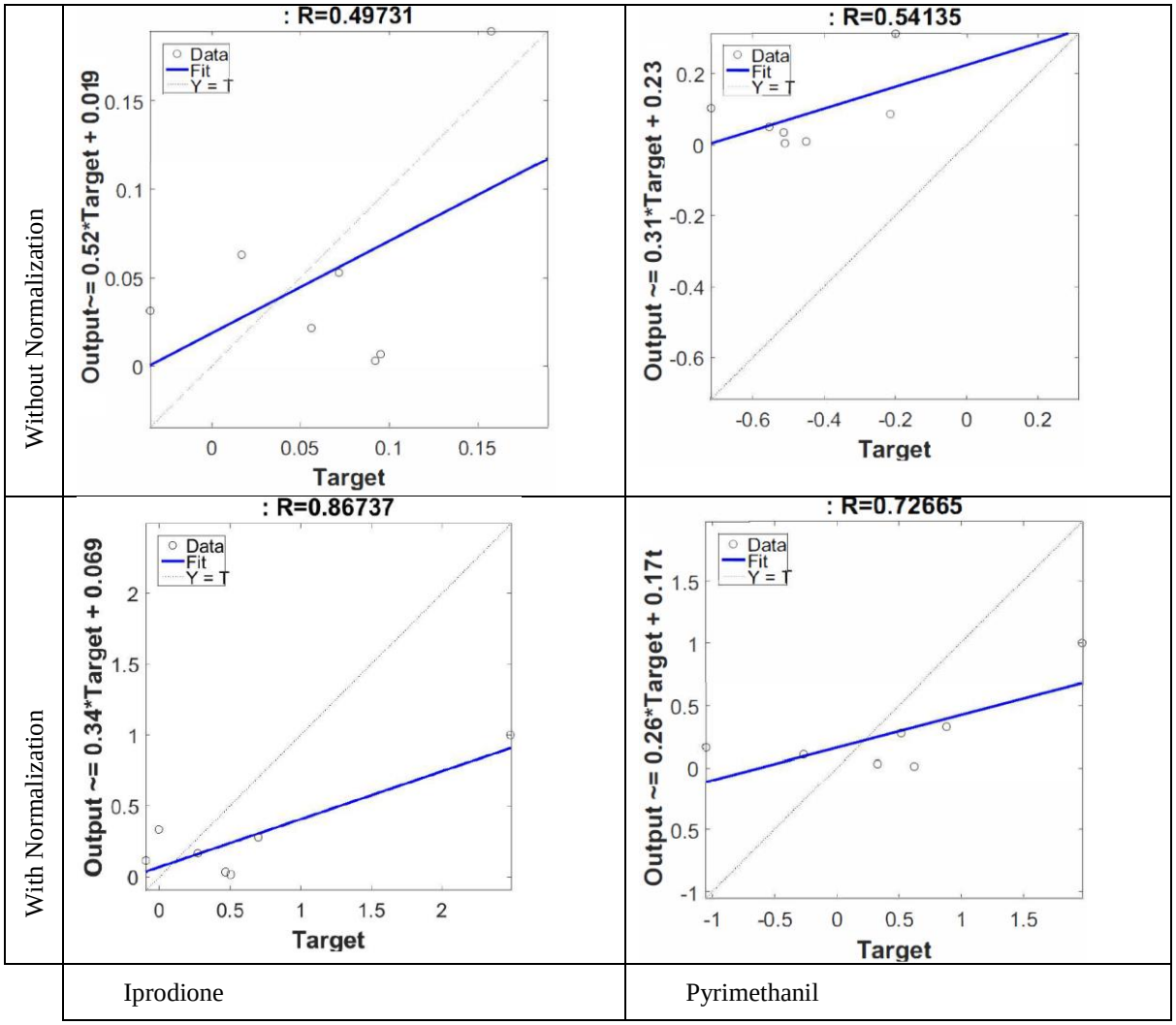


Fig. 8: Test 2 for neural networks.

For test 2, the data training was insufficient to develop a neural network capable of predicting the data with a determination coefficient greater than 0.9. However, in the normalized data the coefficient increase about 158% on average. In pesticide Iprodione was found that for most data prediction value was close to the real value, except for one case. Reason why, this network was suitable for the prediction of data at low concentrations of the fungicide.

Conclusions:

The amount of chemical pesticide used on crops, has increased due to the need to produce more food per hectare. Reason why the intrinsic toxicity of these compounds used as pesticides is an alarming issue. Because of this, it became necessary to develop a method capable of determining the concentration of the fungicides Iprodione and Pyrimethanil, through reflection spectrum, whereby this technique was characterized by being nondestructive, easy to obtain data and easily implemented in rural areas.

The mixture of Pyrimethanil and Iprodione was widely used in ornamental crops and fruit, because of its power fungicide. However, they also were characterized by being toxic compounds that affect human health when were ingested. This mixture was characterized with a Hue angle of -156.69 ° and a Cab chroma of 6.3197, the initial concentration, for which the characterization was carried out were 0.7572 and 1.2546 for Pyrimethanil and Iprodione respectively.

Colorimetric properties for the dilutions with distilled water were evaluated, obtaining an inverse relationship to the Cab chroma parameter with the concentration of solutions. As for the parameters of CIE Lab color space, the relationship was directly proportional. However, for very low values of concentration, an inflection point was found in the trend curve. Due to this, we worked with the color space CIE XYZ, for which the characteristic equations able to predict the concentration of a solution based on parameters "X", "Y" and "Z" were determined, with coefficients greater than 0.99.

Furthermore, neural networks were used to predict the concentration of the dilutions, based on the reflection spectrum. The procedure was performed for the two fungicides with and without normalization of the data. In test 1, a coefficient of determination higher than 0.83 was found for all cases, while for the test 2 any value exceeds 0.86. It was found, the best form prediction of the data was to use the Iprodione with normalized data as indicator.

ACKNOWLEDGMENT

The authors would like to offer their special gratitude to the Research Vice-chancellorship of Nueva Granada Military University for financing the research project IMP_ING 1777 titled: "Análisis de residuos de plaguicidas en frutas tropicales en Colombia para la predicción de posibles efectos en la salud humana", 2016.

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