

Spectral Signature for Quality Assessment of Anchovy Fish meal (*Engraulis Ringens*) using Partial Least Squares

Juan Soto, William Ipanaque, Gerson La-Rosa, Ernesto Paiva

Abstract—Fishmeal is one of the most important foods for the aquaculture, livestock and poultry sectors in Latin America and the world. However, one of the constraints in the fishing industry is to measure online the physicochemical composition of this product and ensure its quality. In this study, the spectral signature of anchovy fish meal (*Engraulis Ringens*) has been obtained in wavelengths from 400 to 900 nm and has been related to its values of Protein, Ash, Moisture, Fat, Free Fatty Acids (FFA), total volatile basic nitrogen (TVB-N), sand, histamine and antioxidant remnant (REM.A/O). To analyze these relationships has been used the regression of Partial Least Squares (PLS) finding the best results to determine the Protein, Fat, Moisture and with some accuracy TVB-N and Histamine. In addition, the most important spectral ranges have been identified for the calculation of the estimates. With these results we have a model to determine the physicochemical composition of anchovy fish meal based on the spectral signature that could be implemented in automatic systems for process control.

Index Terms—Fish meal, Spectral signature, Hyperspectral image.

I. INTRODUCTION

Fishmeal is one of the most important ingredients in the diet of fish and crustaceans [1] and [2], poultry [3], pigs [4][5][6] and other animals, due to its high digestibility, nutritional content and the achievement of better growth yields. According to Hasart and Halwart [7] it is estimated that the distribution of fishmeal consumption is: 56% aquaculture, 12% poultry, 20% pigs and 12% others. In the current context, the demand for fishmeal has exceeded the supply available in the world, influencing price increases and research into new ingredients to replace this product [8].

The fishing industry continues to invest resources to optimize its processes and maintain the competitiveness of fishmeal.

Among the different sources for fishmeal production is the anchovy (*Engraulis Ringens*). If we consider Peru's production and world imports in the period 2013 and 2017 [9], the consumption of anchovy fish meal represents approximately 30% of the world total.

J. Soto, Universidad de Piura, Laboratory of Automatic Control Systems, juan.soto@udep.edu.pe.

G. La-Rosa, Universidad de Piura, Laboratory of Automatic Control Systems, gerson.larosa@udep.edu.pe.

E. Paiva, Universidad de Piura, Laboratory of Automatic Control Systems, ernesto.paiva@udep.edu.pe.

W. Ipanaque, Universidad de Piura, Laboratory of Automatic Control Systems, william.ipanaque@udep.edu.pe.

As shown in Table 1, the quality of fishmeal is determined by levels of Protein, Ash, Moisture, Fat, Free Fatty Acids (FFA), Total Volatile Basic Nitrogen (TVB-N), Sand, Histamine and Antioxidant Remnant (REM.A/O) [10]. For this reason, it is important to know the value of the parameters mentioned during production in order to improve the process and the quality of the final product.

One of the limitations to develop an effective control (100% inspection) of the fish meal quality and other products in the fishing industry has been the lack of objective methods to obtain real time information of the physicochemical parameters.

Techniques based on image analysis are widely used in determining food quality and have great potential for use as a rapid method without require destructive testing [11].

TABLE I
FISH MEAL QUALITY ASSESSMENT

Physical-chemical parameters			P	SP	TW	TH	ST
Protein	%	Min.	70	68	67	67	65/64
Fat	%	Max.	10	10	10	10	10
Moisture	%	Max.	10	10	10	10	10
FFA	%	Max.	7	7.5	10	10	12
Ash	%	Max.	14	14	17	17	–
Sand	%	Max.	4	4	5	5	5
TVBN	100mg g /100g	Max.	85	100	120	150	–
Histamine	ppm	Max.	100	500	–	–	–
REM.A/O	ppm	Min.	150	150	150	150	150

Quality assessment: P= "Premium", SP= "Super Prime", TW= "Taiwan", TH= "Thailand" and ST= "Standard"

In the fishing industry these techniques have been used mainly to estimate the physicochemical characteristics of fresh fish. The species evaluated have been rainbow trout [12] and [13], salmon [14], [15] and [16], coalfish [17], among others in [18], with little research on anchovy. In the research literature can be found of the different techniques application to relate the physicochemical composition of fishery products with the values of reflectance, absorbance and transmittance with the wavelengths of the spectrum. Among the most used techniques we have: Principal Component Analysis (PCA), Multiple Linear Regression (MLR), Principal Component Regression

(PCR), Partial Least Square Regression (PLS), Partial Least Square Regression Discriminant Analysis (PLS-DA), Least Square Support Vector Machine (LS-SVM), Backward Propagation Neural Network (BPNN), Smooth Modelling Independent of Class Analogies (SIMCA), Latent Dirichlet Assignment (LDA) [19][18][20][20][21][22][23].

For this study we used PLS to relate absorbance with the wavelengths between 400nm to 900 nm with quality parameters fish meal: Protein, Ash, Moisture, Fat, Free Fatty Acids (FFA), Total Volatile Basic Nitrogen (TBV-N), Sand, Histamine and Antioxidant Remnant (REM.A/O).

II. MATERIALS AND METHODS

A. Anchovy Fish Meal

Fish meal analysed has made from fresh anchovy, unlike other fish meals residual processes. We analysed the anchovy fish meal produced by the most representative company in Peru.

During this period 122 lots were produced and from each lot samples were taken and sent to a certified laboratory to obtain the values of Protein, Ash, Moisture, Fat, FFA, TBV-N, Sand, Histamine and REM.A/O from standardized methods.

The samples were stored in a temperature and humidity controlled environment. Samples were handled and analysed using different standard measurement techniques for each variable.

Table 2 shows the summary of the values of the selected samples, observing pronounced biases (Skewness greater than ± 2) for Moisture, Sand, TBV-N, Histamine and REM.A/O. Histamine, in addition, has a high standard deviation.

TABLE II
STATICAL SUMMARY OF THE SAMPLES

Physico-chemical parameters	Average	Standard Deviation	Skewness	Kurtosis	
Protein	%	68.11	1.04	0.78	0.37
Fat	%	8.70	0.59	0.67	-0.56
Moisture	%	7.48	0.68	3.25	3.30
FFA	%	6.62	0.75	-0.33	-0.50
Ash	%	15.91	0.44	-0.94	0.00
Sand	%	0.07	0.01	2.10	-2.44
TBV-N	100mg/100gr	115.16	22.62	4.25	1.15
Histamine	ppm	1213.35	1162.78	4.66	0.06
REM.A/O	ppm	642.59	83.23	4.31	3.99

B. Spectral Signature

For the analysis of the spectral signature, samples were taken from 122 batches and prepared in trays to obtain the reflectance (R) with measurements from a hyperspectral camera.

The reflectance have been acquired with a previous calibration of the reference white and the dark current.

The absorbance is obtained from these values.

$$\text{Absorbance} = \log(1/R) \quad (1)$$

To obtain the spectral signature, the hyperspectral camera

Pika II-Resonon was used with halogen illumination and a visible and near-infrared spectral range of 400nm to 900 nm of in-line scanning ("Pushbroom") with a resolution of 2.1nm and 240 spectral bands.

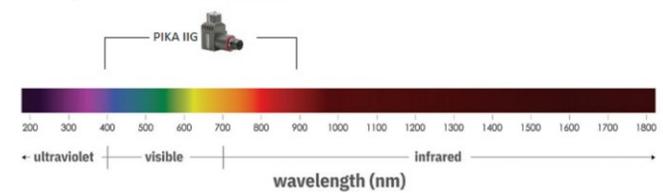


Fig. 1. Hyperspectral Range of the Pika II camera.

C. Partial Least Square (PLS)

It was considered appropriate to use this technique because the number of observations, 122 samples, is much lower than the number of measurements needed for other Machine Learning techniques.

Octave software was used to implement the PLS and the statistics needed for the analysis.

We used the NIPALS algorithm explained by Höskuldsson [25] to find the Principal Components (PC).

The PC will be the directions that maximize the covariance between the mean absorbances obtained in each of the 240 wavelengths (X) and one of the selected physicochemical parameters (Y) (See Figure 2).

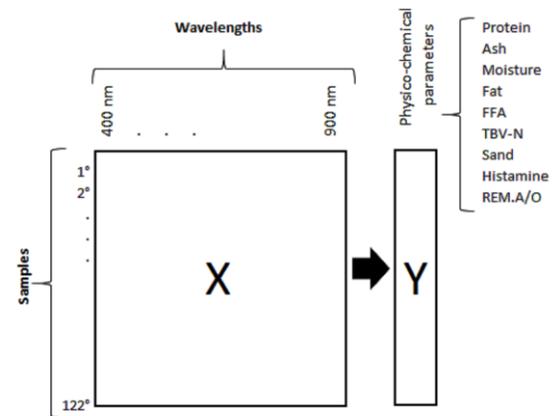


Fig. 2. Data scheme defined for relationship analysis using PLS.

D. PLS Models

PLS models are evaluated for each physicochemical parameter.

In constructing the models, we normalized the dataset and divided the 122 samples into two groups in 3 to 1 ratio, calibration data (92 samples) and validation data (30 samples).

With the calibration data we train the PLS models and select as many PCs as necessary using the following cross validations: 1) cross validation Leaving One Out (LOO), 2) k-fold cross validation using 5 groups (K=5), 3) k-fold cross validation using 10 groups (K=10) and 4) k-fold cross validation using 20 groups (K=20). These validations are explained by Kohavi [26].

In the cross validations we evaluate the Q2 statistic [27] which measures the goodness of prediction for each physicochemical parameter.

$$Q2_{\text{parámetro}} = 1 - \frac{\text{PRESS}}{\text{SCT}} \quad (2)$$

Where: PRESS is the sum of squares of prediction errors of the samples evaluated in the cross validation and SCT is the sum of total squares of the physicochemical parameter.

Once the number of PC is defined, we obtain the coefficients of the PLS model: B_{PLS}

$$B_{pls} = W(P'W)^{-1}C' \quad (3)$$

Where:

"W" is a matrix KxA (K=number of wavelengths, A=Number of components), is the correlation coefficient between the variables of "X" and the score matrix "U".

"P" is a matrix KxA, is the correlation coefficient between the variables of "X" and the score matrix "T".

"C" is a matrix 1xA, is the correlation coefficient between the variable "Y" and the matrix of score "T".

"T" and "U" are the score matrix in the PLS, they are the values of the variables of "X" and "Y" in the new subspace created by the principal components. "T" and "U" are a linear combination of "X" with "W", and "Y" with "C" respectively.

Initialize the value of the vector "U" and through the relationships between the vectors calculates the value of the other vectors in each cycle, until the values of each vector converge.

With the validation data, the difference (error) between the physicochemical parameter value obtained with the standardized methods and the physicochemical parameter value estimated from the PLS model using the spectral signature is evaluated.

To evaluate the quality of the prediction we used the error to calculate: Root Mean Square Error (RMSE), Mean Absolute Error (MAE), Maximum Error (ME) and the determination coefficient (R^2).

To determine the spectral bands with the highest contribution in these estimates of each parameter, we used the Variable Importance in Projection (VIP) static explained by Tahir [28], where bands with $VIP > 1$ value have a higher importance in the estimation of each parameter.

$$VIP_k = \sqrt{N \sum_{a=1}^A [w_{ak}^2 \text{SCEY}(a)] / \text{SCEY}(\text{total})} \quad (4)$$

Where:

SCEY(a) is the total sum of squares of the variable "Y" explained by the a-th component, SCEY(total) is the total sum of squares of the variable "Y" explained by the model with A principal components, "N" is the number of terms in the model (number of wavelengths).

III. RESULTS AND DISCUSSION

Figure 3 shows the spectral signature at wavelengths from 400nm to 900 nm of fish meal.

With a characteristic curve of a single zone with a high absorbance value between wavelengths 400nm and 450 nm, which is also the zone with the highest variation in the samples (high standard deviation). (See Figure 4). Moreover, along the spectral signature obtained the bias is always negative (Skewness less than -0.05) and the skewness is more negative.

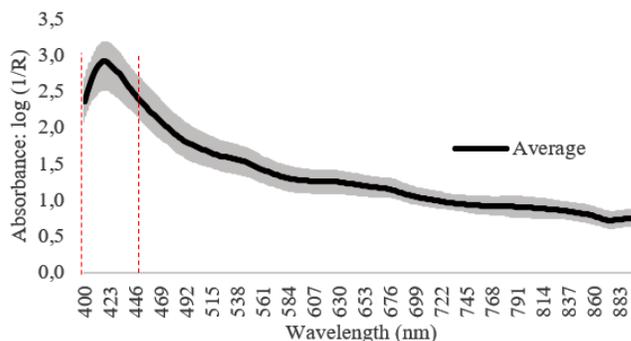


Fig. 3. Fish meals absorbance values.

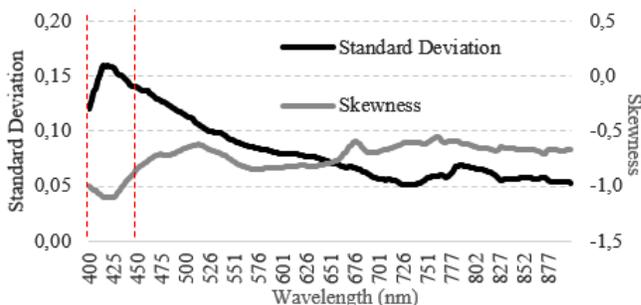


Fig. 4. Standard deviation and Skewness of the absorbance values of fish meal.

Figure 5 to Figure 9 show the Q2 obtained by LOO cross validation and k-fold cross validation using different groups ($k = 5, 10$ y 20) for Protein, Moisture, Fat, TBV-N and Histamine. In the case of Protein, we observed that when we have more than 15 PC, the Q2 curves start scatter from each other and tend to decrease due to over-fitting of the data.

For this reason, we selected the first 15 PC for the Protein model. Under the same criteria we selected for the case of Fat the first 12 PC, for Moisture 16 PC, for Histamine and TBV-N 18 PC.

Table 3 shows the Q2 values using LOO cross-validation for Sand, FFA, Ash, REM.A/O and shows how many PC are necessary to obtain the prediction grade. Q2 (LOO) value < 0.5 indicates that the PLS model does not fit these parameters well.

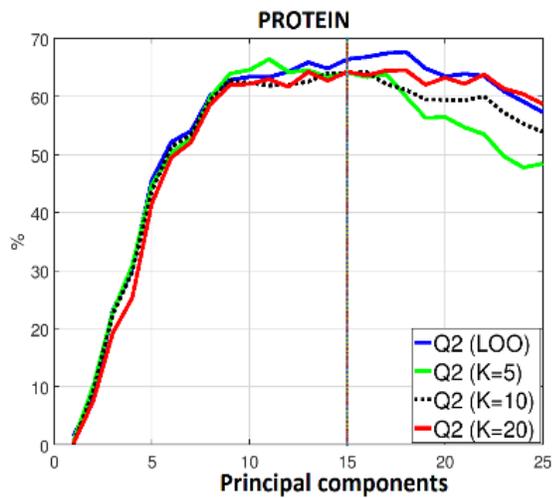


Fig. 5. Predictive goodness according to the number of main components for Protein.

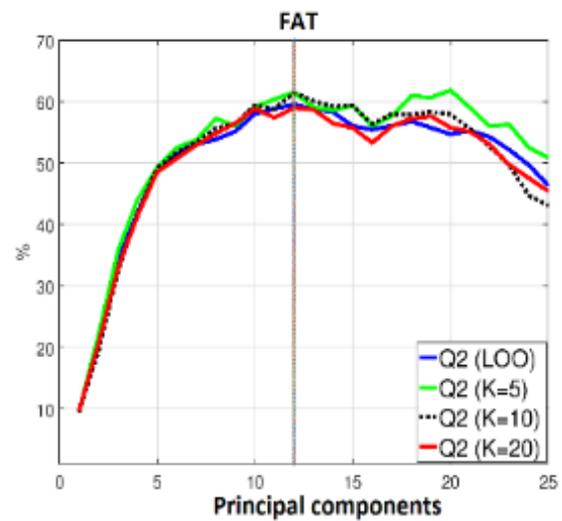


Fig. 8. Predictive goodness according to the number of main components for Fat.

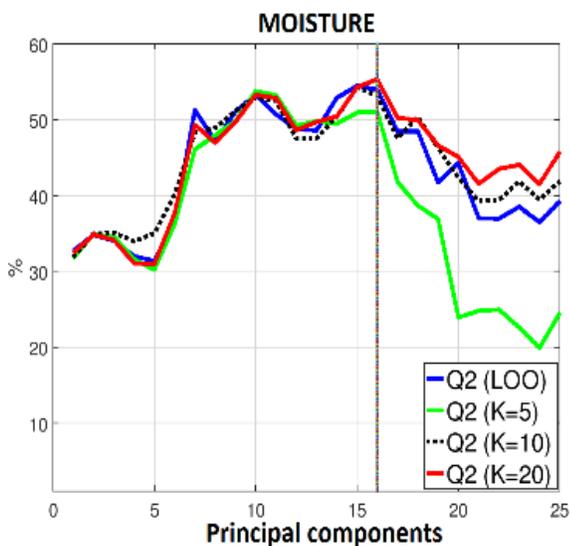


Fig. 6. Predictive goodness according to the number of main components for Moisture.

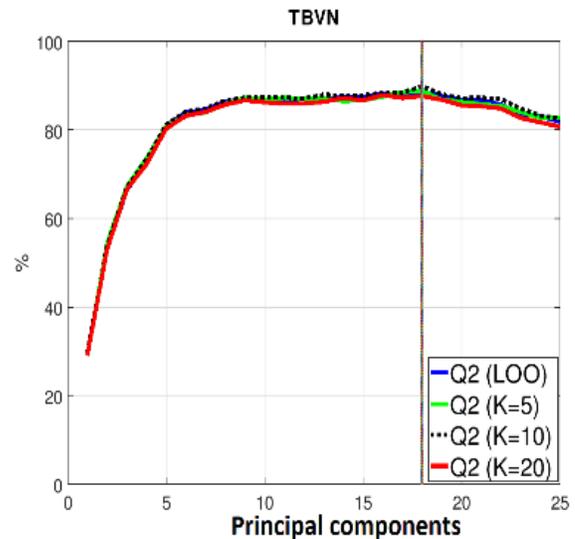


Fig. 9. Predictive goodness according to the number of main components for TBV-N.

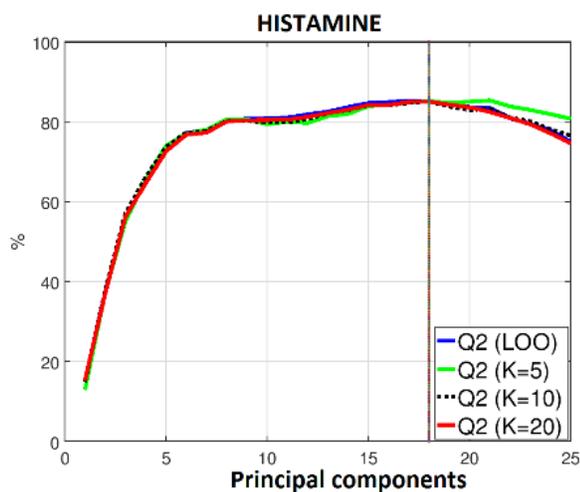


Fig. 7. Predictive goodness according to the number of main components for Histamine.

TABLE III
CROSS VALIDATION LOO WITH PLS

Variables	Q2 (LOO)	PC
REM.A/O	34.45%	7
FFA	33.79%	9
Ash	31.29%	8
Sand	9.81%	2

A. Obtained Partial Least Square PLS Models

With the PC defined for parameter we obtained the PLS coefficients (B_{pls}) and used them for parameter estimation with the validation data.

Determination coefficients higher than 70% were obtained with the validation data, indicating a good linear fit of the constructed models.

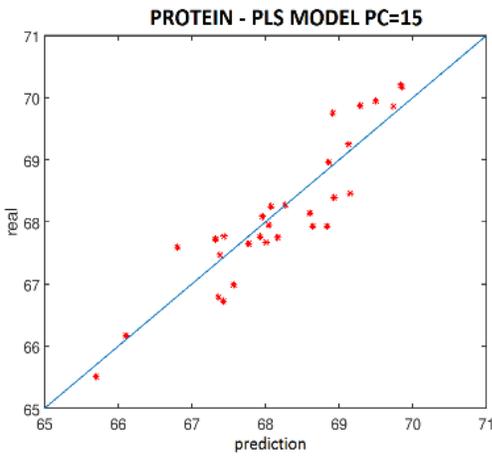


Fig. 10. Actual and predicted values with validation data for protein.

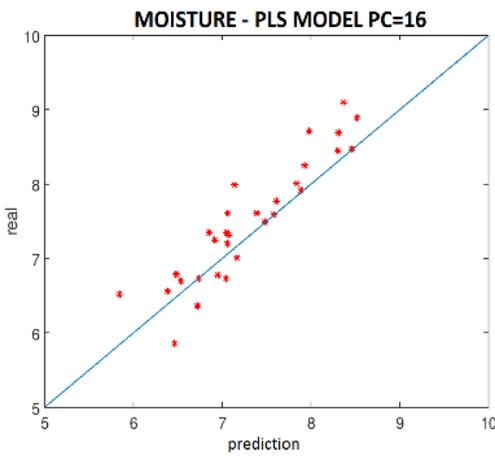


Fig. 11. Actual and predicted values with validation data for moisture.

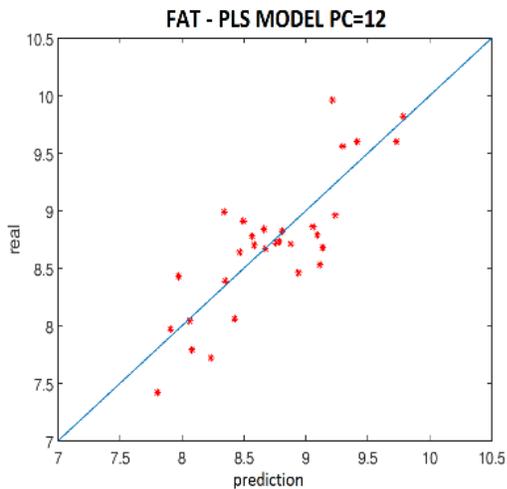


Fig. 12. Actual and predicted values with validation data for fat.

Considering the measurement scale of the parameters measured, low values of Maximum Error (ME), Mean Absolute Error (MAE) and Root Mean Square Error (RMSE) were obtained, with the exception of Histamine.

For Protein, Fat and Moisture the maximum measurement

error per spectral signature does not exceed 1%, for TBV-N the Maximum Error found was less than 3g in 100g of sample. For Histamine the Maximum Error is very high (1000ppm error).

Figure 10 to Figure 14 shows the dispersion of the actual values (standardized methods) and the predicted values (with spectral signature) of the validation data for Protein, Moisture, Fat, TBV-N and Histamine.

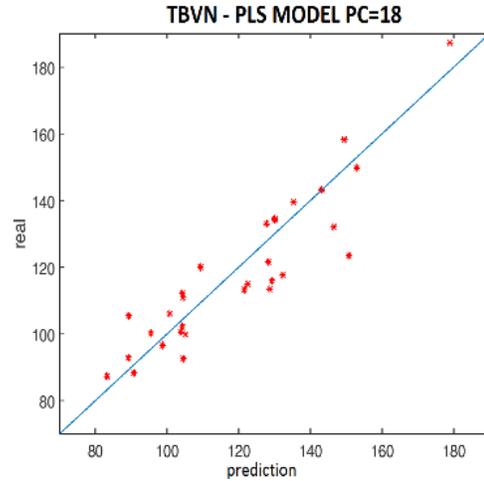


Fig. 13. Actual and predicted values with validation data for TBV-N.

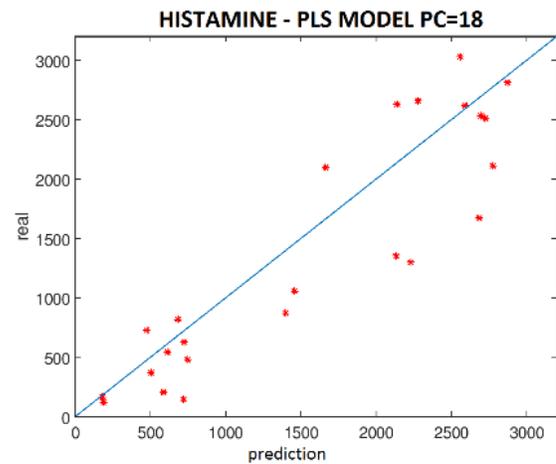


Fig. 14. Actual and predicted values with validation data for Histamine.

B. Obtained Variable Importance in Projection VIP

The most important wavelengths for estimating Protein, Fat, Histamine and TBV-N can be seen in Figure 15 with a VIP value greater than 1.

Some wavelengths overlap in their importance for estimating Protein, Fat, TBV-N and Histamine, and we have grouped them by Zone 1 between 400nm to 450nm come in the blue spectral range, Zone 2 between 620nm to 690nm come in the green spectral range, Zone 3 between 750nm to 805nm come in the red spectral range and Zone 4 between 865nm to 900nm come in the near infrared spectral range.

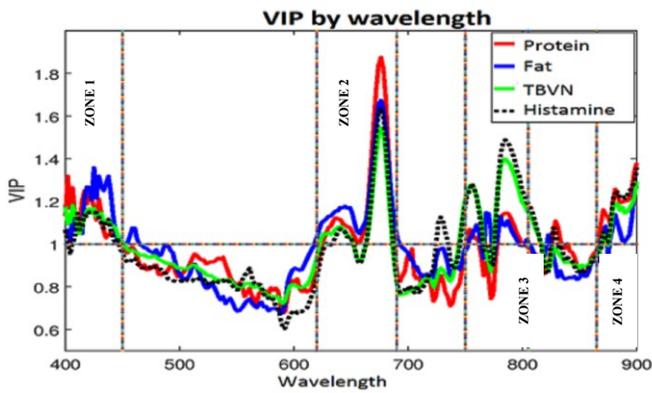


Fig. 15. VIP of the spectral band (nm) for Protein, Fat, TBVN and Histamine.

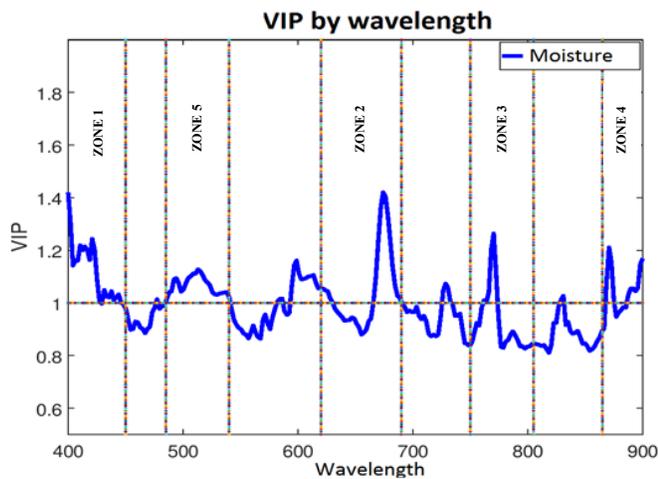


Fig. 16. VIP of the spectral bands for Moisture.

For the moisture parameter, the most important wavelengths are found in zone 1 and zone 4 previously identified. In addition, for moisture it is observed that in zones 2 and zone 3 identified there are wavelengths that do not contribute to the estimation of moisture and also appears a 5th zone between 485nm to 540nm with importance for this parameter. See Figure 16.

IV. CONCLUSIONS

The knowledge obtained in this work is a key step to implement an automatic control system in fishing companies, measuring the quality of fishmeal in real time to optimize processes and maintain the competitiveness of the product.

We have obtained three models based Partial Least Square (PLS) techniques with good accuracy for on-line measurement of these parameters during the production of fish meal.

Based on the analysis of PLS statistical models, the best estimate of quality parameters, based on the absorbance measured between 400nm to 900nm, was obtained for Protein, Moisture and Fat with a Maximum Error of less than 1%.

The most important wavelengths for estimating Protein, Fat, Histamine and TBV-N have a VIP value greater than 1.

For estimating Protein, Fat, TBV-N and Histamine we have grouped them by Zone 1 between 400nm and 450nm, Zone 2 between 620nm and 690nm, Zone 3 between 750nm and 805nm

and Zone 4 between 865nm and 900nm.

We have identified the characteristic spectral signature for anchovy fishmeal in which the wavelengths with the highest absorbance occur for the zone we have identified with VIP>1.

For moisture an interesting zone to analyse for future work is between 400nm to 450nm to simplify the estimation of quality parameters in order to reduce costs in the implementation of automatic control systems.

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Juan Soto Mechanical – Electrical Engineer from the University of Piura, in 2013; he has completed a Master with mention in Energy Efficiency at the University of Piura, 2014. He is currently a researcher at the University of Piura; author of papers on Embedded Systems, Automatic Control of Industrial Processes, Image Processing, Development of models based on Machine Learning and Deep Learning, Algorithms for parameter estimation based on hyperspectral images and their spectral signature. Participates in I + D + i projects with funds from INNOVATE PERÚ and CONCYTEC programs; has intellectual property registers (Copyright and Invention Patent).



William Ipanaque Ph.D. in Computer and Automatic Engineering from the Polytechnic of Milan (Italy). His research fields are automatic control, optimization and automation of emerging processes and technologies. Founder and director of the Mechanical/Electrical Master with mention in Automation and Optimization from UDEP. He has worked as a member of the Advisory Council of the Congress of the Republic of the commission of Science, Innovation and Technology. For his work in technological research, in 2015 he was recognized with the order of merit Santiago Antúnez de Mayolo Gamero and in 2014 he received recognition from Concytec for the working group of automatic control systems that he directs at the UDEP.



Gerson La Rosa is an industrial and systems engineer from the University of Piura (UDEP) with an M.Sc in Data Analysis Engineering, Process Improvement and Decision Making from the Department of Statistics of the Polytechnic University of Valencia (UPV). He currently works in the Research Department of the UDEP and supports the laboratory of Automatic and Control Systems (SAC) of the same university. He is currently pursuing a PhD in Engineering with mention in Automation, Control and Process Optimization at UDEP. His areas of interest are the identification and validation of models based on statistical and Machine Learning techniques to estimate characteristic parameters in fishing, agricultural and hydrological processes.



Ernesto Paiva received the degree of Mechanical-Electrical Engineer from the University of Piura, Peru, in 2013; he has completed a Master's degree in Mechanical-Electrical Engineering with mention in Automatics and Optimization at the University of Piura funded by CONCYTEC 2016. He is currently a research assistant at the Department of Technology and Innovation (DTI) - SUPSI, in charge of the development of Deep Learning algorithms ANN, CNN, LSTM, Conv LSTM.