

Soft-Sensor Approach Based on Principal Components Analysis to Improve the Quality of the Application of Pesticides in Agricultural Pest Control

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Abstract—Pesticide application has been an important activity for pest control in agricultural production and in sustaining food security. The quality of an application plays an important role to decrease human and environmental risks, as well as in relation to the costs for food production. To evaluate the quality of the application by sprayers, several quality descriptors are used. Such descriptors are related to the average diameter of drops and the distribution of drops in the application. This paper presents the construction of a soft-sensor, based on Principal Components Analysis (PCA), to infer the quality of application. The soft-sensor has as inputs the operating conditions of agricultural sprayers and offers as output the quality descriptors that serve as a base of information to estimate the level of quality that a pesticide application can meet at a certain time. Hence, the selection of historical data, the exploration and filtering of data, as well as the structure and the validation of the soft-sensor are presented. The results have shown the usefulness of the soft-sensor in the aggregation of value to the process of pesticide application and decision-making in agriculture.

Keywords—Soft-sensor; Inferential sensors; Quality of application; Principal component analysis; Agricultural sprayers.

I. INTRODUCTION

As the population has increased, the need to produce more food has caused the agricultural techniques to constantly evolve. The development of new technologies for the production of inputs, pesticides and agricultural machines such as tractors and sprayers, as well as genetic engineering, have made possible the increase of agricultural production and the reduction of the environmental impacts of agricultural activity. Among the activities of crop management, one of the most expensive is the spraying of pesticides. Spraying is the application of a liquid in the form of small particles on a surface. These particles are called drops or droplets.

An efficient spraying application is based on the following factors: applied chemical efficiency, quality of the product, climatic conditions and biological characteristics of the pest [1] [2]. Among the factors that determine the efficiency of the application, the quality is one of the most important, that is, precision agriculture based on the use of automation and control plays an important role. The knowledge of the size, the distribution and the process of formation of drops are essential factors for the success of the pulverization of pesticides [3]. These factors have an influence on the drift, evaporation of

products, penetration capability inside the canopy of crops and deposition on phytosanitary treatment targets [4].

Since agricultural crops can vary in height as they grow and as the agricultural sprayer is used on different crops on the farm, the sprayer boom height must be accurate to ensure that crops receive the proper application of the liquid being dispensed. A set of sensors have been used to help the operators in such arrangements and also, for calibration of the temperature of the engine, flow and pressure of the pesticides hydraulic pump, among others variables, required in the spraying processes. Furthermore, today advanced sprayers generally include additional sets of sensors which are useful for precision spraying management. However, it is still a challenge to measure and control in the spraying processes all the variables required for spraying quality and a complete characterization of the spraying systems during operation in order to increase precision.

Therefore, regarding this subject and in order to improve the performance of such processes, the concept of soft-sensors can be used to estimate values of important variables that cannot be taken by traditional measurements.

Soft-sensors are computer programs established from models and used for estimating not measurable outputs from production processes. Specifically, they are based on estimation and prediction techniques which use a priori information collected from sensors and mathematical models to describe physical processes. The approach based on soft-sensors is used in cases where sensors (hardware) are not available or their implementation is difficult, have high cost or simply there are no instruments that can do the type of measurement required [5]. In the literature, there are several applications of soft-sensors in production processes and they have achieved good results. In 1995, Luo et al. [6] designed an inference estimator based on fuzzy logic to measure and control the purity of the resulting propylene from the distillation process of a high-purity distillation column. In 1998, Casali et al. [7] used soft-sensors to estimate the size of the particles in a grinding plant where sensors were not available. The authors used an Autoregressive Moving Average Model (ARMAX) as soft-sensor to estimate and test the model predictive capability. Then, in 2007, Lin et al. [8] designed a soft-sensor to detect nitrogen oxide emissions (NOx) produced by a cement kiln system. The authors used robust regression techniques to derive

an inferential model, making possible a basis of estimation with dynamic least squares. Recently, in 2016, Liu et al. [9] used the soft-sensor approach to predict and monitor the indoor air quality in the Seoul metro systems. The authors used a technique of learning Just-In-Time (JIT) to model the nonlinear process based on two local models of prediction, and a linear Partial Least Squares (PLS) method and a nonlinear Least Squares Support Vector Regression (LSSVR) method for the prediction of the indoor air quality were used.

The conception and construction of a data-driven soft-sensor have five main pillars: collection and selection of historical data of the process, detection of outliers and data filtering, selection of the model structure, estimates of the model and validation of the model [5]. Therefore, these five pillars or steps must be executed sequentially to obtain a soft-sensor with a high degree of accuracy. The main focus of this work is the improvement in the quality of pesticide application. For this, a soft-sensor based on Principal Components (PC) was built in order to predict the quality descriptors of the application as a function of operating conditions of the agricultural sprayers.

The next sections of the paper are organized as follows. In Section II, the main concepts and the theoretical foundation of the analysis of principal components are given. In Section III, the electrohydraulic devices and the experimental configuration used for data collection are shown. Also, in this section the setup of the soft-sensor in the control loop of the pesticides spraying system is studied. Subsequently, in Section IV, the simulated results of the application of the soft-sensor in the control loop are shown. Finally, some concluding remarks and future works are presented in Section V.

II. PRINCIPAL COMPONENT ANALYSIS

The main idea of PCA is to reduce the dimension of the data set by keeping the variation of the original data set as much as possible. To achieve this goal, this technique transforms the data set into a new set of principal components. The PCs are ordered so that the first components keep most of the variation present in the original data or variables [10]. To start with the formulation, the simplest one-dimensional space case ($M = 1$) is used, that is the projection of the data is in an one-dimensional space. The mean of the set of samples is calculated with the following expression:

$$\bar{x} = \frac{1}{N} \sum_{n=1}^N x_n \quad (1)$$

where x_n is the sample vector, with $n = 1, \dots, N$. The covariance matrix S is defined by the following expression:

$$S = \frac{1}{N} \sum_{n=1}^N (x_n - \bar{x})(x_n - \bar{x})^T. \quad (2)$$

Define a D -dimensional vector u_1 as the direction of this space which is chosen in such a way that $u_1^T u_1 = 1$. Each data point x_n is then projected onto a scalar value $u_1^T x_n$ and the idea is to maximize the variance of the projected data in relation to the vector u_1 . The variance of the projected data is given by:

$$\frac{1}{N} \sum_{n=1}^N \{u_1^T x_n - u_1^T \bar{x}\}^2 = u_1^T S u_1. \quad (3)$$

To prevent that $\|u_1\| \rightarrow \infty$, the maximization of the projected variance must have a constraint. Thus, the constraint comes from the normalization condition $u_1^T u_1 = 1$. To comply with the constraint, a Lagrange multiplier λ_1 is introduced [11]:

$$u_1^T S u_1 + \lambda_1 (1 - u_1^T u_1). \quad (4)$$

Thus, deriving (4) in function of u_1 and equating to zero, the following expression is obtained:

$$u_1^T S u_1 = \lambda_1. \quad (5)$$

Therefore, u_1 is an eigenvector of the covariance matrix S and the variance is maximized when the set u_1 is equal to the eigenvector having the largest eigenvalue λ_1 . This eigenvector is known as the first principal component [11]. Considering the case of a projection of M -dimensional space, the optimal linear projection for which the variance of the projected data is maximized is defined by the m eigenvectors u_1, \dots, u_m of the covariance matrix S that corresponds to the largest m eigenvalues $\lambda_1, \dots, \lambda_m$. To establish the principal components as a basis for regression, first define an X ($n \times p$) matrix which consists of n observations of the p predictor variables whose (i, j) th element is the value of the j th predictor (or regressor) variable for the i th observation. Accordingly, the corresponding standard regression model is defined as:

$$y = X\beta + \epsilon. \quad (6)$$

where y is the vector of n observations of the dependent variable, measured about their mean, β is a vector of p regression coefficients and ϵ is a vector of error terms; the elements of ϵ are independent, each with the same variance σ^2 . Also, in matrix form, one can define the PC values for each observation as $Z = XA$, where the (i, k) th element of Z is the value (score) of the k th PC for the i th observation, and A is a $(p \times p)$ matrix whose k th column is the k th eigenvector of $X^T X$. The idea is to use the PC to replace the original predictor variables. For this purpose, the orthogonality concept of the eigenvector matrix is used. Since matrix A is orthogonal, then $X\beta$ can be rewritten as $Z\gamma = XAA^T\beta$, in which $\gamma = A^T\beta$. Then, (6) can be rewritten as [10]:

$$y = Z\gamma + \epsilon \quad (7)$$

Thus, in (6) the predictor variables were replaced by their PCs in the regression model. In addition to the PCA regression model in (1), the following reduced model is also used:

$$y = Z_m \gamma_m + \epsilon_m \quad (8)$$

where γ_m is a vector of m elements that are a subset of elements of γ , Z_m is an $(n \times m)$ matrix whose columns are the corresponding subset of columns of Z , and ϵ_m is the appropriate error term. An estimate of β can be found using $\hat{\beta} = A\hat{\gamma}$. The vector $\hat{\gamma}$ can be calculated as $\hat{\gamma} = (Z^T Z)^{-1} Z^T y$.

III. EXPERIMENTAL ARRANGEMENT

To validate the developed soft-sensor, the platform that was developed at the Brazilian Agricultural Research Corporation (Embrapa Instrumentation) in partnership with the School of Engineering of São Carlos University of So Paulo (EESC-USP), both from Brazil, was used. This platform for sprayers development and analyzes operates as an Agricultural Sprayer Development System (ASDS) and uses a National

Instruments® embedded controller, known as NI-cRIO.

A. Main Electronics and Mechanics used in the ASDS

The ASDS was designed and developed taking into account the concept of an advanced platform based on the use of sensors and actuators, controllers circuits, and intelligent electronics to enable the project and development of sprayer systems [12]–[14].

This laboratory infrastructure has an advanced development system that enables the design of architectures involving the connections of hydraulic components and devices, mechanical pumps, electronic and computer algorithms, as illustrated by Figure 1. On the other hand, the system also has the hydraulic devices that are used to make any configuration of commercial agricultural sprays and new prototypes of sprayers, the user interface for system monitoring and control, as well as an electromechanical structure which emulates the movement of the agricultural sprayer in the field, as shown in Figure 2.

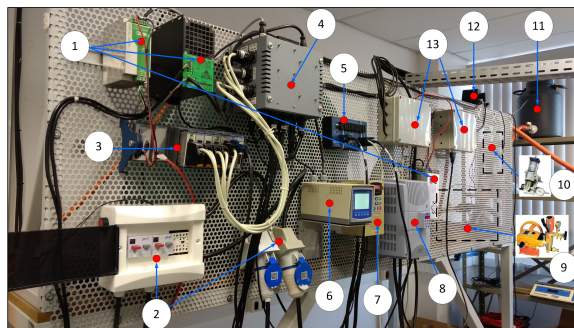


Figure 1. Front view of ASDS electro-hydraulic devices: (1) power supplies, (2) electrical protection circuits, (3) modules for automation and control of the inputs and outputs variables, (4) box with electronic circuits for signal conditioning, (5) CAN network bus, (6) transmitter for analog sensors, (7) frequency inverter for control of the spray pump, (8) frequency inverter for control of the Industrial belt that simulates the tractor movement in relation to the sprayers, (9) spray pump, (10) two piston pumps for injection of pesticides, (11) pesticide reservoir tank, (12) proportional valve for pressure and flow control, (13) valve actuation circuits via CAN network.



Figure 2. Development system for projects dedicated to the application of liquid agricultural inputs: (1) spray nozzle, (2) system that emulates the movement of the sprayer, (3) pesticide disposal tank, (4) user interface of the development system, (5) spray booms.

B. Data Collection

Water-sensitive papers were used to collect the drop size distribution pattern. This type of paper collects the watermarks produced by the drops which can be analyzed by a pattern recognition program to obtain the average diameters. A detailed diagram of the experimental setup is shown in Figure 3. The water-sensitive papers were displayed in an aluminum bar, with an impermeable paint coating, positioned transversely to the movement of the application and spaced so as to collect all the information from the drop distribution of all the nozzles.

The spraying was performed at a height of 51 cm. The distance between each nozzle was 50 cm (Figure 3) [15].

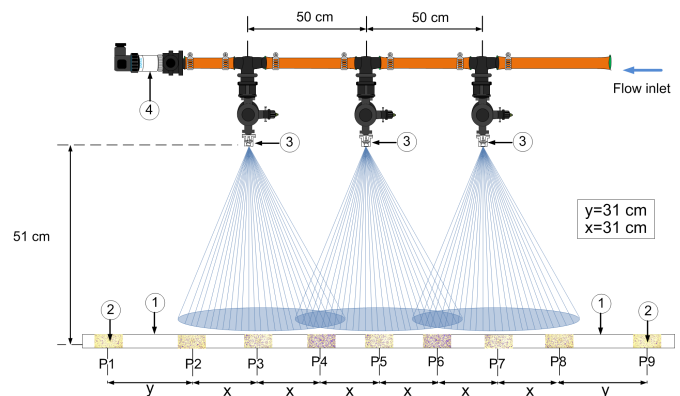


Figure 3. A zoom of the spray boom with the nozzles used for data collection containing: 1) aluminum bar with an impermeable paint coating; 2) water-sensitive papers; 3) set of nozzles; 4) pressure sensor.

The position of the water-sensitive papers, in the aluminum bar, obeys the critical points which are to be considered in the distribution of mean diameters, that is, the papers placed outside of the aluminum bar (P1 and P9 in Figure 3) in order to collect the data of the drops with potential of drifting. Two other papers were placed at the external nozzles to collect the application pattern without overlapping (P2 and P8 in Figure 3). A pair of papers was placed in the center of the overlapping of the nozzle cones (P4 and P6 in Figure 3) and three more papers were placed in the center of the cones, perpendicular to the nozzle (P3, P5 and P7 in Figure 3).

Table I shows the operating conditions used to collect data for each tested nozzle where Q_p [m^3/s] is the nozzle flow, D_p [l/ha] is the application rate, V_p [m/s] is the speed of application and d_0 [mm] is the discharge orifice of the nozzle. Four conditions were tested, one per nozzle with different discharge orifice diameters of the models CH0.5, CH 1, CH 3 and CH 6 of the Magnojet® company. These four types of nozzles were selected with the help of a specialist in the area of agricultural application in order to have a wide range of drop sizes within the database.

TABLE I. OPERATING CONDITIONS FOR THE ASDS USING FULL CONE NOZZLES (magnojet®).

	Nozzle	P [bar]	Q_p [L/min]	D_p [L/ha]	Temp [°C]	Humid [%]	V_p [km/h]	d_0 [mm]
1 st	CH0.5	3.4	0.53	67	23.6	51	10	0.5
2 nd	CH1	3.4	1.02	85	23.4	61	14	1.0
3 rd	CH3	3.4	1.46	100	24.0	49	18	1.5
4 th	CH6	2.4	1.90	120	23.7	58	20	2.0

Four conditions named full cone nozzles CH05, CH1, CH3 and CH6 were considered. For each condition, there were 5 replicates of which the first 3 had the same operating conditions (S in Table III). The fourth repetition was performed by lowering the sprayer boom pressure by 10% and the fifth repetition was done by increasing the sprayer boom pressure by 10%. For each paper positioned in the metal bar there are two samples and thus, the total of the samples per repetition are 18, so the total samples for each condition, which is composed of 5 repetitions, are 90 samples. Accounting for all four conditions, 360 samples were collected. The information collected experimentally, from each water-sensitive paper, was

for the following quality descriptors: $D_{0.1}$, SMD, VMD, $D_{0.9}$, as well as the relative amplitude (RA) and the application rate (AR).

TABLE II. ARRANGEMENT OF SAMPLES, FOR EACH CONDITION, WHICH MAKE UP THE DATABASE.

	Nozzle	N° repetition		Total	N° papers	N° samples	Total samples
		S	-10% +10%				
1 st	CH0.5	3	1 1	5	9	18	90
2 nd	CH1	3	1 1	5	9	18	90
3 rd	CH3	3	1 1	5	9	18	90
4 th	CH6	3	1 1	5	9	18	90
Total collected samples							360

To obtain the average diameters in the papers sensitive to the water, the tool DropScope® of the Ablevision® company was used. The data exploration, the analysis of results and the construction of the soft-sensors were performed with the MATLAB® and Simulink® software.

C. Soft-sensor

The applications of the soft-sensors can be divided into three large items: monitoring of processes, process control and off-line assistance of operations [16]. In this work, the soft-sensors were used in the monitoring of the spraying process, specifically as a predictor of the quality of the variables (PPQV), as well as in control to plan the operations (OPP). The soft-sensor used as PPQV applied to the agricultural spraying process is shown in Figure 4.

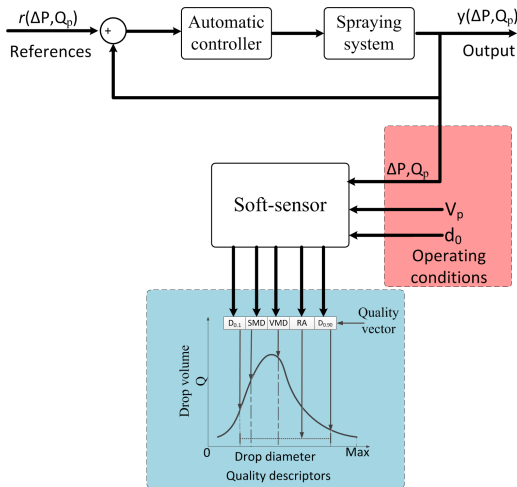


Figure 4. Block diagram of the soft-sensor used as predictor of process quality variables (PPQV) in the agricultural spraying process.

In the block diagram, the control loop of the spraying system is shown. In this loop, the inputs are the pressure and flow references $r(\Delta P_{ref}, Q_{pref})$. The outputs of this loop are the pressure ΔP and flow measured in the system by the sensors Q_p , which are the actual value that the spraying system has at a given time. In the case of the soft-sensor as PPQV (Figure 4), the operating conditions (red square with dotted lines) are the inputs to the soft-sensor. The operating conditions are the pressure and flow, which come directly from the spraying system, the speed of application V_p and the diameter of the discharge orifice of the nozzle d_0 . In the configuration as a predictor of quality variables, the soft-sensor

offers as output the prediction of the quality descriptors, that is, the mean diameters: $D_{0.1}$, SMD, VMD, $D_{0.9}$.

On the other hand, the application of the soft-sensor, in process control, as an operations planner in the process, is shown in Fig 5. For this configuration, the soft-sensor receives as input the quality descriptors of the spraying and delivers as output the required operating conditions in the spraying system to obtain the given quality values.

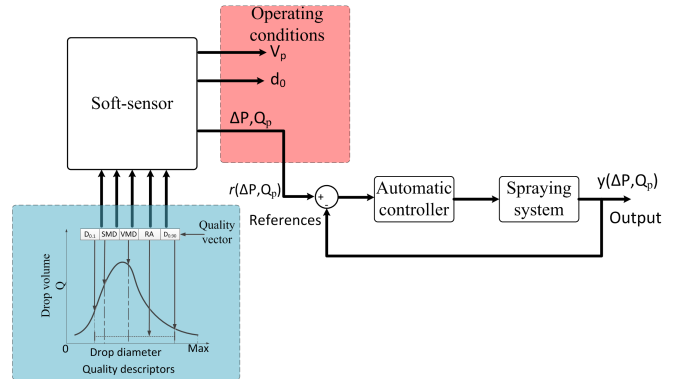


Figure 5. Block diagram of the soft-sensor used as an operations planner in the process (OPP) in the agricultural spraying process.

In the block diagram of Fig. 5, it is shown that the soft-sensor delivers the pressure and flow reference values for the control loop. The soft-sensor also delivers the model of the nozzle represented by the diameter d_0 and the speed V_p that the sprayer must have at the time of making the application.

IV. RESULTS AND DISCUSSION

First, an exploration of the data was made. To apply techniques that work with maximization of variances, such as PCA, or reduction of errors, it is important that the data of the random observations fit a normal curve. Thus, a quantile-quantile graph (Q-Q plot) was used to determine the adjustment that the data can have to a normal distribution. Then, a Grubbs test to all the collected observations in order to detect possible outliers was carried out. The Q-Q plots and the Grubbs test are explained in more detail in [15].

The model chosen to build the soft-sensors was the PCA regression. The steps for the construction of the model are presented in Algorithm 1. The algorithm is divided into two procedures, the first procedure (REGRESSION) is the construction of the principal component regression model. This procedure has as entries the data matrix X , the matrix of eigenvectors A , the matrix of scores of the PC's Z and the vector of data required for the model y . Also, this procedure returns the value of the regression coefficients $\hat{\gamma}$ and the prediction value \hat{y} . Therefore, the regression model is delivered based on the principal components. The second procedure in the Algorithm 1, has as its main function to estimate output values for new observed data (NEWOBSERV). Then, the procedure receives a vector containing new observations x_{new} , as well as receives the regression coefficients based on the PCs $\hat{\gamma}$ and the eigenvalue matrix A . In the procedure, a new score matrix Z_{new} , a new vector of values \hat{x}_{new} and a new observed data \hat{y}_{new} are estimated.

Algorithm 1 PCA regression

Require: X consists of n observations of p predictor variables;
 A Matrix of eigenvectors;
 Z Matrix of scores of the PC's;
 y Vector of data required for the model;
procedure REGRESSION(X, A, Z, y)
 $Z = XA$ \triangleright Calculate the matrix Z of the scores PC
 $\hat{\gamma} = (Z'Z)^{-1} Z'y$ \triangleright Returns the $\hat{\gamma}$ value
 $\hat{y} = Z\hat{\gamma}$ \triangleright Returns the prediction \hat{y} value
end procedure
procedure NEWOBSERV($x_{new}, A, \hat{\gamma}$)
 $z'_{new} = x'_{new}A$ \triangleright Calculate the x_{new} scores value
 $\hat{x}_{new} = z'_{new}A'$ \triangleright Find the predicted value
 $\hat{y}_{new} = z_{new}\hat{\gamma}$ \triangleright Returns the predicted value
end procedure

Figure 6. Model construction algorithm.

To validate the model, four new repetitions were made, one for each operating condition (Table I), each repetition had 14 samples of water sensitive paper totaling 56 new observations. Figures 7b, 8d, 9f, 10h show the xbar charts and error bars which describe the behavior of the PCA-based models in the presence of new observations. It is important to emphasize that the spraying process is highly random and therefore there are several values which are above the maximum (UCL) and minimum (LCL) values allowed. For the first three conditions (samples: 1-14 (first condition CH05), 15-28 (second condition CH1), 29-42 (second condition CH3)), the estimation errors are low, which showed that the models provide adequate estimates for the spraying quality descriptors. Observing the responses of the models, Figures 7a, 8c, 9e, 10g, one can consider that the best regression responses are for the descriptors SMD, VMD and $D_{0.9}$.

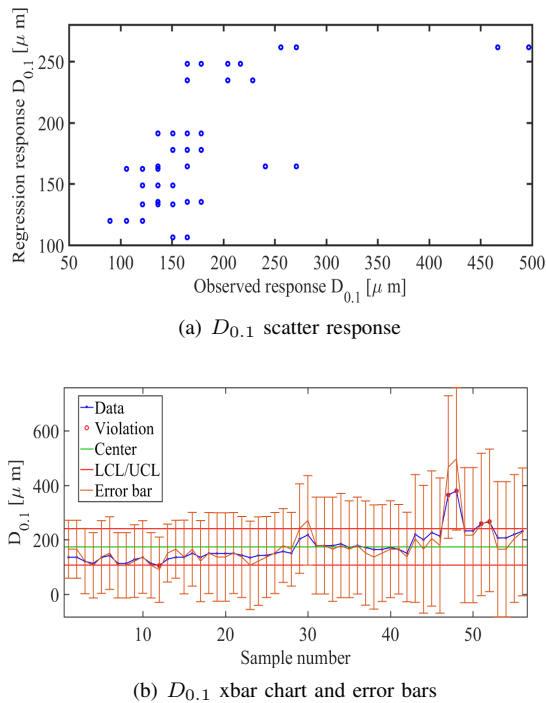


Figure 7. Results of the soft-sensor for the $D_{0.1}$ descriptor.

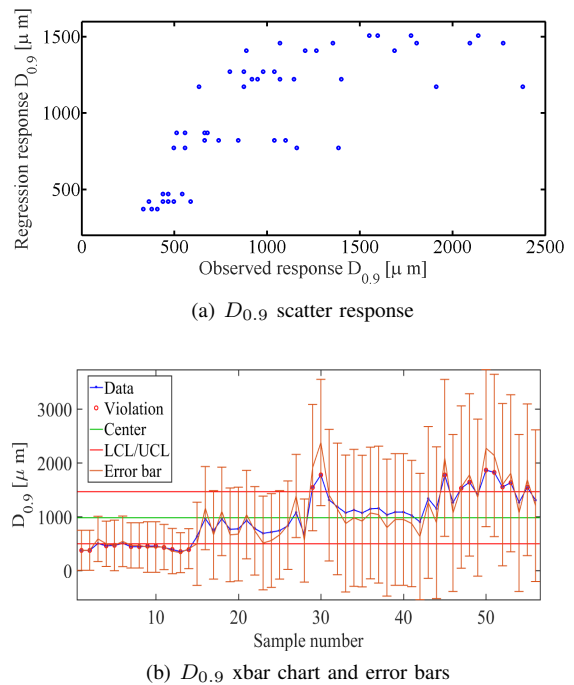


Figure 8. Results of the soft-sensor for the $D_{0.9}$ descriptor.

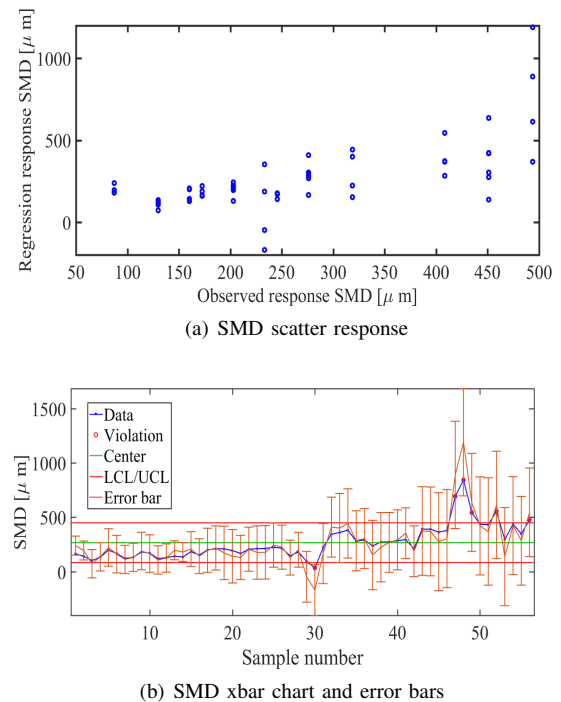
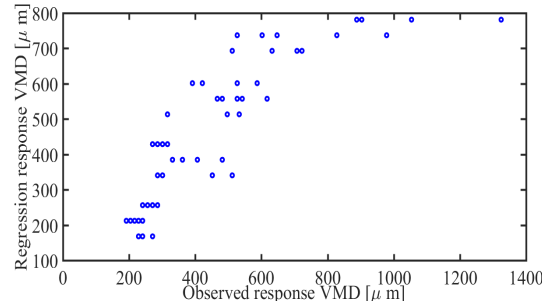


Figure 9. Results of the soft-sensor for the SMD descriptor.

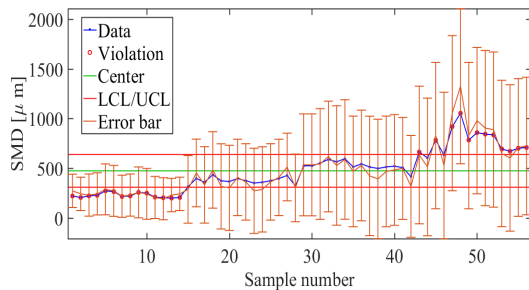
The regression coefficients estimated with the scores of the principal components are shown in Table III. The coefficients β relate the quality descriptors with the operating conditions.

TABLE III. ESTIMATED REGRESSION COEFFICIENTS $\hat{\beta}$.

	$D_{0.1}$	SMD	VMD	$D_{0.9}$
P	0.41	0.36	0.50	0.45
V_p	0.14	0.16	0.14	0.07
d_0	0.00	-0.03	0.21	0.33



(a) VMD scatter response



(b) VMD xbar chart and error bars

Figure 10. Results of the soft-sensor for the VMD descriptor.

V. CONCLUSION AND FUTURE WORK

This work presented the development of customized soft-sensors for agriculture. The soft-sensors have shown the possibility to aggregate value in the processes, that is, improve the quality in the agricultural pesticide application. In addition, they serve as versatile tools to help agricultural producers to improve the application based on knowledge and the systems control, providing support for decision making in agricultural spraying for pest control. Furthermore, the models based on PCA regression proved to be useful and have allowed finding good estimators for spraying quality descriptors, as well as the adjustment of the operating conditions and calibration of the agricultural machinery. In future works, the soft-sensor will be embedded in a circuit, and prepared to operate with a CAN network, making it possible the actual sprayer operate in agricultural field conditions.

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nozzles for the practical experiments, respectively. The authors also acknowledge the relevant discussions with Heitor V. Mercaldi.

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