The Potential of Soft Sensors for Continuous Emission Monitoring Systems

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Introduction

The growing public environmental awareness and the adoption of more strict environmental regulations are putting a lot of pressure on the operational engineers for operating the production plants in a safer and "greener" way. These are also the reasons for the enforced adoption of continuous emission monitoring systems (CEMS) for the on-line monitoring of the environmental process performance in terms of pollutant emission compliance. Because of the inherently difficulties associated to the use of dedicated analytical equipment (time delay, expensive equipment, high maintenance costs, and so forth), recently, parametric emission monitoring systems (PEMS) have gained more attention for their potential in implementing monitoring programs. The most important advantage of PEMS is the environmental compliance achieved with much less burdensome requirements on the facility (1).
PEMS are based on the use of some sort of simplified parametric model to estimate primary and costly-to-measure process variables (i.e., compositions) from easy-to-measure process variables (i.e., flowrates, temperatures, pressures and so forth). PEMS closely resemble inferential tools (software sensors, SS) that are widely used in the Chemical Process Industry for monitoring and control purposes. In the last few years, the field of software sensors has become enough mature to provide a reliable alternative to conventional analytical techniques (2).
The core of software sensors is constituted of models that are used to describe the functional dependence of the targeted process variable on the secondary (easy-to-measure) process variables. In this regard, neural network modeling provides a powerful modeling environment for developing non-structured process models, as proved by the large number of applications appeared in the recent years (3).
Energy production represents, perhaps, one of the most important sources of air pollution, and could take great advantage from adopting in an efficient way PEMS based on software sensors for improving the operation efficiency of combustion systems (1, 4).
The paper describes the recent results of a project aimed at developing online neural software sensors to monitor the emissions at the centralized chimneys in operation at two Italian refineries (Saras e Raffineria Sannazzaro).

The Case Studies

The centralized chimney operating at the Saras is enslaved to the topping furnace and to three boilers of the thermoelectric power plant. The three boilers are fed with gas-oil or fuel gas and have only one combustion chamber each. They produce high pressure steam (70 bar) at the rate of 70, 70 and 120 ton/h. The topping furnace (nominal power load of 110 Mkcal/h) is operated with gas-oil or fuel gas and has three combustion chambers. The topping feed (oil stream) is preheated before entering the furnace. The furnace is equipped with two chimneys (North and South). Typically, the three boilers and the furnace are operated at full load with fuel gas; the gas-oil is used to integrate the fuel requirements to meet the energy request. When the topping furnace or one of the three boilers goes out of service the combustion air is flowed anyway through the combustion chamber, and the software sensor has to take care of this abnormal event.

The centralized chimney operating at the Raffineria Sannazzaro is used only for the refinery power plant, which is constituted of two turbo-gas units of 25 MW each. Each unit is composed of a compressor, a gas turbine - fueled with fuel gas – and a recovery boiler. The recovery boilers are used to produce medium-low pressure steam (15 bar_g) to meet the refinery steam demand. This is why during the cold months the boilers are also fueled with fuel oil to meet the extra steam needs.

Software Sensors: Generalities

Software sensors are simplified process models that allow the inference of difficult-to-measure process variables or indicators (compositions, conversions, quality indexes, and so forth) starting from easy-to-measure process variables (temperatures, flowrates, pressures and so forth).

The basic structure of a software sensor is constituted of:

- input variables (the process variables that are easy to measure online);
- the process model;
- the output variables (the process variables or performance indexes that we wish to estimate).

The core of a software sensor is the process model and there are several approaches for formulating it. Typically one adopts parametric models (or black box models, in the terminology of process engineers) for their computational ease in on-line applications. The two most popular parametric modeling are based on partial least square models (PLS) (5) and on neural network models (2, 3). The first models rely on linear modeling nevertheless they exhibit good descriptive characteristics. The reason for this behavior may be due to the specific structure of PLS models: they are build-up in terms of latent variables, namely the transformed variables obtained through a PCA analysis. The latent variables are derived so as they are fully uncorrelated to each other, and this could explain the accuracy observed for this sort of linear models. On the other hands, neural network models are nonlinear models that are expected to better describe the nonlinear dependence among the input and the output variables. Indeed, in a recent study (6) on the development of software sensors to estimate the Mooney viscosity of an elastomer (propylene – ethylene – diene) we have compared the performance of SS based on PLS and neural models. The results demonstrate that the latter exhibit better generalization (prediction) characteristics.

In the following sections we will synthetically describe the results achieved for two industrial refinery chimneys. In particular we will address the most critical issues associated to the development of software sensors:

- acquisition and preprocessing of the raw data;
- selection of the process variables to be used as input to the neural network models;
- selection of the data sets for calibrating and validating the model.

The selection of the input variable is, perhaps, the most critical step in the development of a software sensor and can make the difference between a good and a poor inference model. Often, the novices in software sensor development believe that the use of parametric models, especially the neural ones, does not require any knowledge about the process. This is a gross mistake because in parametric models the knowledge about the process is tightly embedded through the optimal selection of the input variable set. People familiar with process identification well know how critical is to come up with a proper process model with adequate generalization properties.

The calibration of the models requires care to avoid the problem known as overtraing or overfitting. This has to do with fitting the model to tightly to the calibration data in such a way that the model will well perform in fitting data but will miserably fail in prediction (generalization) (8). For this reason we have calibrated the models by adopting the cross-validation approach. The method consists in dividing the data set used for training in two subsets: the training and the cross-validation data sets. The parameter optimizer directly works on the training data set while the cross validation data set is used to control the model error. Doing so, the model generalization characteristics are taken care of already during the parameter estimation.

Since the selection of the input variables represents the key factor on which depends the success or the failure of the project, we typically adopt an hybrid approach that relies both on

the physical knowledge of the process and on computer aided tools (statistical correlation indexes and principal component analysis, PCA).
At this point it is worth spending few words on PCA (7), which represents a powerful tool of the statistical analysis of multivariate processes. The principal component analysis consists of a transformation of the physical measures in scaled process variables that have the following properties:

- they are normalized so as to have zero mean and unitary standard deviation;
- they are fully uncorrelated.

The transformation is linear so as the total variance of the original data is preserved; the new space of the dimensionless variables (Z-scores) is called PC (principal components) space. Because of the uncorrelated nature of the scaled variables, the variance of the process can be described by making use of a reduced number of Z-scores. The principal components (or PC axes) are ordered for descending importance to the contribution to the total variability of the process, which is measured by the eigenvalues of the linear transformation. Consequently, the variability of the process can be described through a reduced number of scaled process variables. Indeed, this represents the most common application of PCA: reduction of the process variables required to monitor a process. This is usually accomplished by analyzing the projection plots in the PC planes. Because of the uncorrelated character of the scaled variables usually it is sufficient to consider the plots in the first planes. The projection plots also provide a powerful tool for detecting “abnormal” conditions (outliers or “non in control” operating conditions). The projection plots are integrated with the confidence volumes constructed by making use of the Hotelling T^2 statistics (7): any points outside the confidence regions (ellipses drawn by specifying a given confidence for identifying outliers) represents an outlier with the prescribed confidence. The most common confidence regions are drawn at the confidence level of 95 or 99% that are equivalent to the region of +/- σ or 2σ for the monovariate case.

Case Study: Centralized Chimney at Saras
This case study offers the opportunity to emphasize how critical is to acquire good data for a proper calibration of parametric models. These models are developed starting from plant data (they are also known as data-driven models), therefore, the “quality” of the data is a critical factor, namely, the data used for the software sensor calibration must be representative of normal (“in control”) operating conditions. Using plant data relative to “out of control” (outlier) conditions may jeopardize the correct calibration of the software sensor. On the other hand, the needs to take a critical look at the plant data can also be valuable to the process engineer who might improve his understanding on the performance of the plant and of the installed instrumentation.
The refinery acquisition system allows the data historicization with a sampling time of 10 min.; the analysis has been pursued on data spanning about six months (October 2003 – March 2004). The chimney was equipped with analytical instrumentation to continuously monitor the concentration levels of CO, O_2, NO_x, and SO_2. A systematic analysis of the analytical data has allowed to detect some problems with the instrumentation:

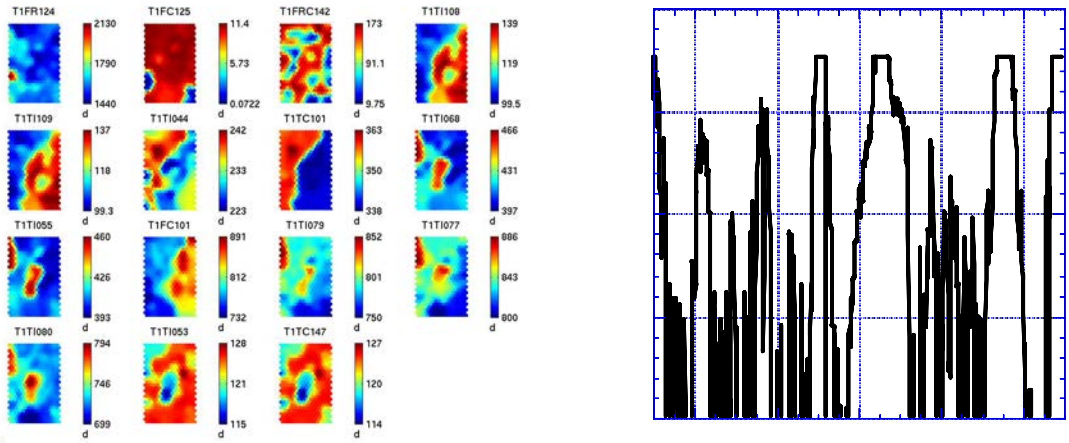
- the CO measure exhibited a strong variability not justifiable in terms of actual plant performance. The observed problems could be due to a deterioration of the measurement cell or to poor calibration;
- the remaining measurements exhibited, on the long term, a drift.

The observed problems with the analytical equipment are mainly due to the recent installation of the instrumentation that was still under the acceptance phase. Even though the quality of the analytical data was considered not adequate for the calibration of software sensors pursued a semi-quantitative analysis with the objective to gain some insights on the plant performance. The analysis was carried out in two phases:

- identification of outliers through the application of PCA;
- identification of correlations among the process variables and various operating conditions through the application of self organizing neural models (also known as self organizing maps, SOM).

The SOM neural networks provide a useful tool to acquire a better understanding of the process by analyzing the correlations among the several process variables. This will be made clear in the following discussion.

Figure 1a shows the maps of the relevant process variables for the topping furnace. At first, the map of the air input flowrate to the topping furnace (T1FRC142) shows a pattern which is completely different from those of the remaining process variables. Indeed a, careful analysis of the chart trends of the variable has highlighted an abnormal behavior shown in Fig. 2b which was due to a wrong reading of the measurement device. The map of the outlet temperature of the topping heated feed (T1TC101) clearly shows that the furnace operates at two different operating conditions, as also verified with the Saras plant engineers.
The inlet and the outlet temperatures of the fuel oil preheating unit (T1TI053 and T1TC147) show similar maps indicating that they carry out the same information content, and thus, that only one of the two temperatures could be selected as input to the software sensors. This reasoning can be applied also to the outlet temperatures from the two furnace chimneys (T1TI068, northern chimney, T1TI055, southern chimney) and to the two temperatures of the inlet air streams to the furnace (T1TI108 and T1TI109).



(a) (b)

Figure 1. (a) SOM maps for the topping furnace; (b) trend chart for air flowrate

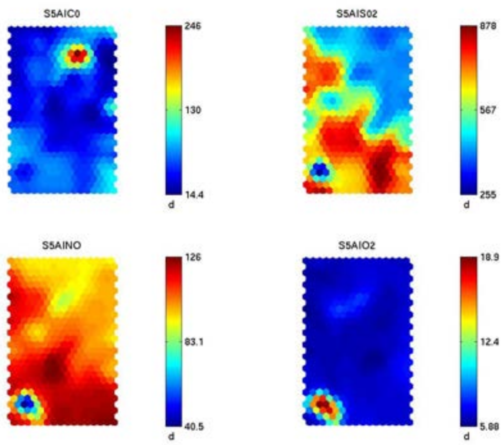


Figure 2. SOM maps for the emission concentrations.

The maps of the four emission measurements (O_2, NO, SO_2 and CO) are illustrated in Figure 2. A close look at the figure shows a clustering of the operating regions at high oxygen concentrations (left lower most left corner) that correspond to low concentrations of CO, NO and SO_2, as expected.
On the basis of this analysis we have developed a first sensor with 20 inputs, 4 hidden neurons and 4 outputs. As expected, the software sensor could not even describe the trend of CO composition, while for the other composition variables the trend description was satisfactory. We believe that most of the problems could be resolved with the replacement of the air flowrate measurement device and with a better maintenance and calibration of the analytical sensors.

Case Study: Power Plant Chimney (Raffineria Sannazzaro)

For this case study the software sensors were developed by making use of historical data spanning twelve months of operations (March 2002 – February 2003); the data were acquired with a sampling rate of 6 min. The analytical monitoring system measured on-line the concentration levels of CO, O_2, NO, and SO_2. A critical analysis of the analytical data and interviews with instrumentation engineers has allowed to detect some maintenance problems

with the CO sensor, thus, we decided to disregard it from the analysis. In the following we will show the results for the predictions of the emission level of NO, O_2, and SO_2.
At first, we had to estimate the power generated at the two turbo-gas units by combustion and the thermal load at the two boilers. The total power at the turbo-gas units is constituted of various contributions:

- the usable power generated by the turbines (which is continuously monitored);
- the power absorbed by the compressors;
- the sensible heat carry out by the effluent combustion gases.

As a cross check we verified that the power absorbed at the compressors was about 60% of the total power produced by combustion. The thermal load at the boilers was calculated from an energy balance that takes into account the sensible heat loss of the combustion gas coming out from the turbo gas units and the heat required for the production of the steam at 15 bar_g.
In the following we will show the results obtained for two kind of neural software sensors. The first one is based on a neural model that predicts the three compositions; the second is based on three distinct neural models one for each pollutant.
By iteratively applying the PCA analysis we were capable to detect several outliers corresponding to the calibration periods of the analytical equipment that, unfortunately, could not be identified through a status-flag. The pre-processing analysis of the plant data has allowed to select a first set of 20 variables (10 for each unit) to be used as inputs to the neural models. The data set used to calibrate the neural models is based on two sets: the calibration and the cross validation data sets. The first one was constituted of 1370 data for training and the second 709. Figure 3 shows the projection plots – in the PC1-PC2 and PC1-PC3 planes - for the calibration data sets; the projection plots also show the control volumes constructed at the 95% of confidence. The results clearly indicate that the calibration data are representative of three operating conditions. Indeed, the data set was build up by taking data from the following periods: 6/4/2002 – 11/4/2002, 31/7/2002 – 12/8/2002, 15/11/2002 – 18/11/2002, and 28/12/2002 – 1/1/2003.

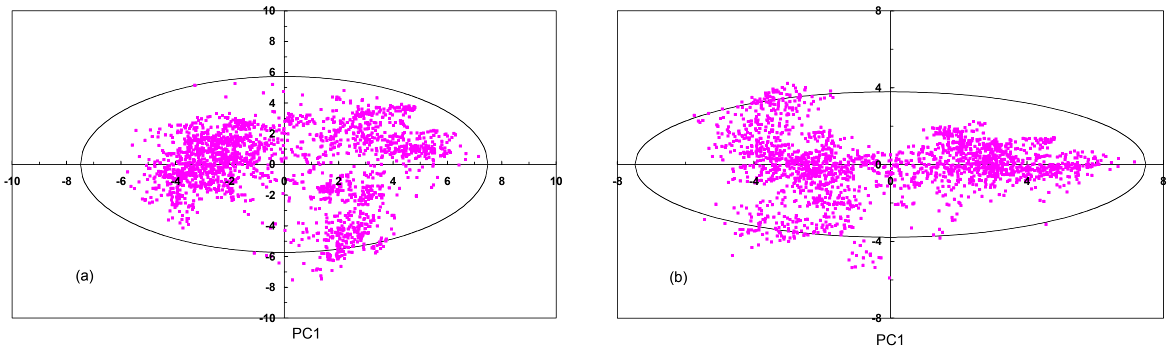


Figure 3. Projection plots of the data set used to calibrate the neural models

It is worth mentioning that for the data of Figure 3 the first three principal components are able to recover about 75% of the original data variance, as shown in Figure 4. This gives an idea of the variable reduction that can be achieved through the principal component analysis.

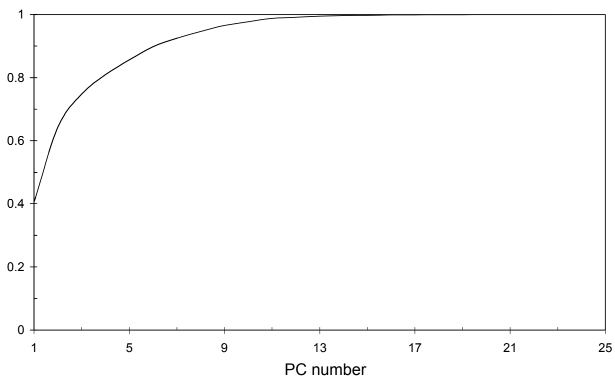


Figure 4. Described percentage variance by the PC's

For the cross validation data set, the comparison between the predicted and the experimental measurements of the pollutants emission is shown in Figure 5, where, in the inserts, are also reported the average percentage error (APE). The results refer to a neural model constituted of 20 input neurons, 5 hidden neurons and 3 output neurons, which can be simply indicated as (20,5,3).

In calibration (training and cross validation) good agreement between the predictions and the experimental measurements are attained for O_2 and SO_2. For NO there are some problems: as shown by the group of points of Fig. 5 that are off the diagonal. These are the points that were extracted from the operating conditions spanning the period of time 13/01/2003 – 28/02/2003. During the latter part of this period of time the SS exhibited a systematic offset from the experimental measurements that could not be explained in terms of changes in the operating conditions. The observed discrepancy could be explained in terms of drift in the measures themselves. This is something we are looking at more thoroughly.

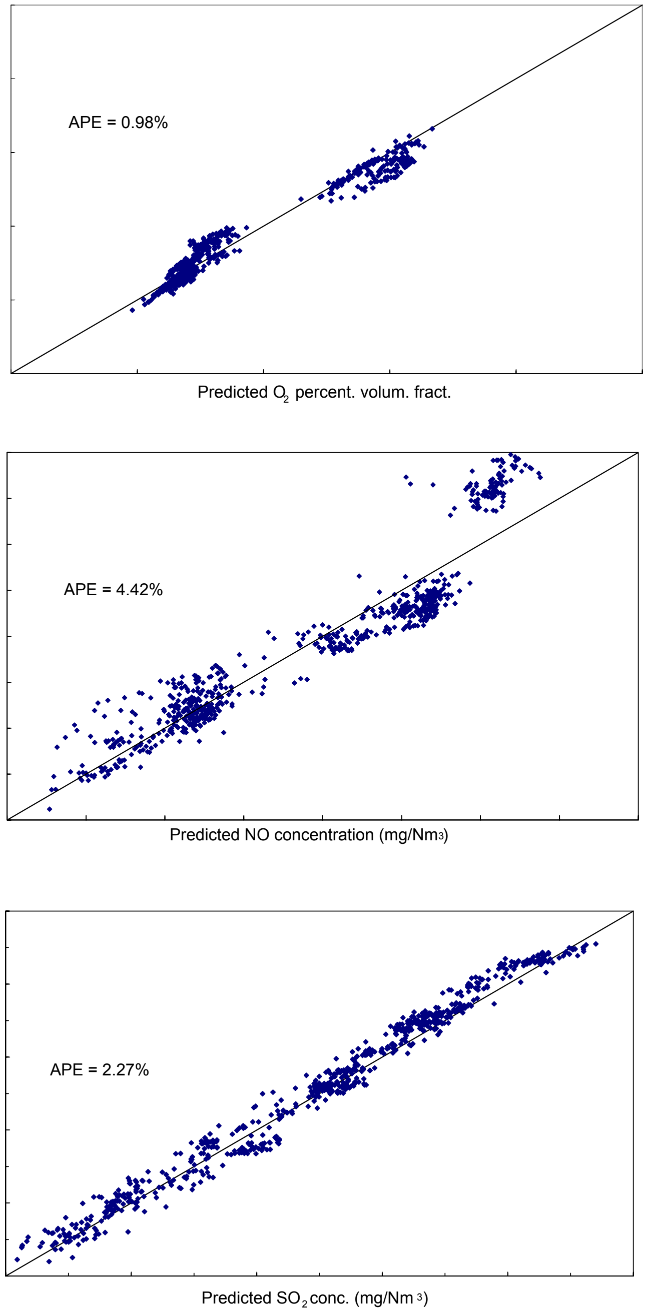


Figure 5. Comparison between the predicted and the experimental emission measurements for a SS based on a (20,5,3) neural network (cross-validation).

The predictions of the software sensor for the most critical period of operations (time 13/01/2003 – 28/02/2003) are shown in Figure 6. The results are rather good for the predictions of oxygen and sulfurous anhydride emission levels,; the software sensor appears to be less performing with respect to the emission level of nitrous oxide. It is worth mentioning that the prediction errors observed for the other periods of operations do not exceed the value of 5%.With the same 20 input variables we have also developed software sensors to estimate the emission levels through software sensors capable to estimate the concentration of one pollutant at the time. The results indicate that the best standard deviation error is obtained with the following single output SS structures:

- O_2: (20,3,1);
- NO: (20,5,1);
- SO_2: (20,4,1).

For the data set of Figure 6, with the single software sensor the accuracy of the NO predictions slightly improved (APE= 7.21%) while the predictions of the oxygen and SO_2 deteriorated a little (APE= 1.06 and 6.8%, respectively). This might be due to the fact the 20 variables could not be the best selection for all the three single output SS.
This is made more clear if we look at the contribution plots for the first three PC's (Fig.7) that gives the correlation between the *i*-th physical process variable and the generic PC.
In Figure 7 we have reported the results for the first three PC's. The last three variables (21, 22, and 23) are the emission levels of oxygen, nitrous anhydride, and sulfurous oxide, respectively. The results indicate that the NO concentration is strongly correlated (aligned) to the PC1, and thus, we might expect a strong dependence on the process variables that exhibit the same sort of correlation. In this regard, the NO concentration behaves differently from O2 and SO2 concentrations. The latter appear to be strongly correlated to both the first and the second PC. From the analysis of Figure 7 we could conclude that the input variables n. 11 and 12 could be eliminated from the model used to predict the NO emission; work is underway in order to optimize the single output software sensors.

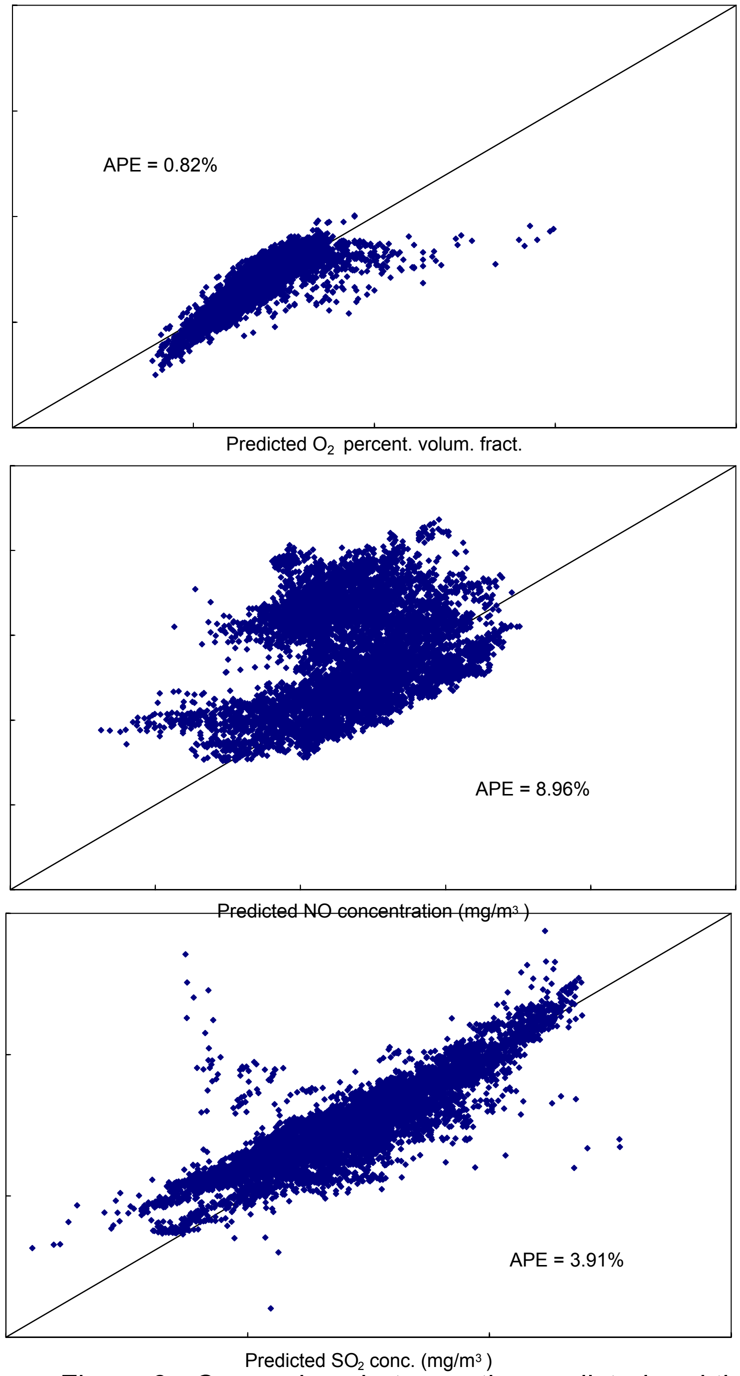


Figure 6. Comparison between the predicted and the experimental emission measurements for a SS based on a (20,5,3) neural network (predict. data).

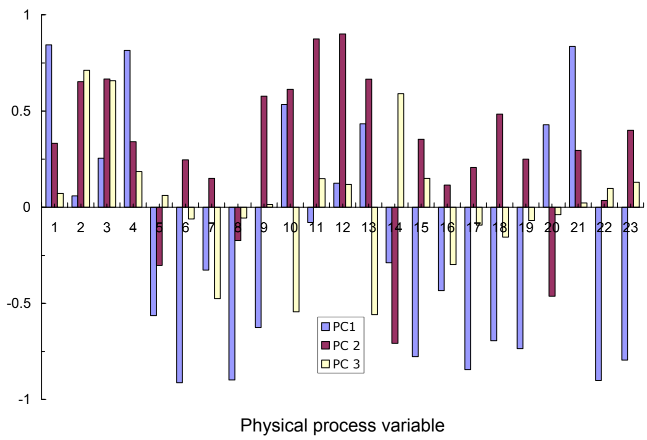


Figure 7. Contribution plots for the first three PC's.

Conclusions

The paper discusses the results obtained for the development of software sensors capable to monitor the emission concentration of pollutants from combustion units. The results are shown for two industrial case studies.

The first case study (Saras Refinery) shows the importance of having good data for the calibration of software sensors. We have discussed the use of SOM neural network to extract process information from plant data.

For the second case study we show the results for software sensors with single and multiple outputs. The accuracy of the developed SS are satisfactory and work is underway in order to optimize the single output SS.

The illustrated results prove the potential of neural-based software sensors as continuous emission monitoring systems.

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