Abstract—Soft sensor is a mathematical model which used to estimate variables of interest when secondary variables measure is easy to obtain. This technique arises from an operational difficulty or high cost of obtaining the desired variable. This paper proposes a strategy for a soft sensor construction, that involves data acquisition, sensitivity analysis of input variables, inferential black model box construction that uses neuro-fuzzy technique, and model validation. The strategy was developed using data from an experimental methanol–water distillation column with 10 trays. The distillation process was found interesting for the present study, since it presents difficulties in obtaining the composition of the product. The computational strategy used produced good results for estimating composition.

Index Terms—Soft sensor, distillation column, neuro-fuzzy, estimating composition

I. INTRODUCTION

SOFT sensor is a mathematical model which is used to estimate variables of interest when secondary variables measure is easy to obtain. This technique arises from an operational difficulty or high cost of obtaining the desired variable.

Industries are increasingly using this mathematical tool, mainly to improve the product specifications and to control the rates of emissions of volatile pollutants [1].

Several applications for a soft sensor could be named: inference variables, fault detection, performance prediction, nonlinear functions approximation, and process standards identification.

The soft sensor can be a good alternative to the traditional methods, since the usual measured variables can be used without problems in the simulation model for generating the sensor to estimate the desired variable.

The inputs for the soft sensor model can be, for example, temperatures, pressures and flows, the secondary variables easily measured online. Due to the nature of the chemical processes, the states of these secondary variables reflect the state of complex variables.

II. DEVELOPMENT OF SOFT SENSOR

Due to the inherent characteristics and operational restrictions in any typical chemical process, distillation columns have some restrictions: hydraulic, separation and heat transfer.

The motivation for this work rises from the difficulty to obtain products compositions in the distillation column. Traditional methods for measuring compositions, such as gas chromatography have a major delay measurement when performed in the laboratory. Online systems have highly acquisition costs and maintenance [1].

A. Methodology

This paper proposes a strategy for a soft sensor construction, that involve data acquisition, sensitivity analysis of input variables, inferential black model box construction that uses neuro-fuzzy technique, and model validation. The goal of this work is to build a soft sensor model for online final methanol composition estimation for the top of the distillation column. This was achieved using the methodology described in Figure 1.

Fig. 1. Methodology Employed in the construction of Soft Sensor.

III. DATA ACQUISITION

All data used to build a soft sensor model were obtained from the dynamic model of a continuous distillation column designed to separate a binary mixture of methanol water. The dynamic model used was validated experimentally by [2]. The pilot plant scheme is shown in Figure 2.
The distillation column has 10 trays, each containing two bubble cups, except the feed tray which has four bubble cups. The column is also equipped with samples points, rotameters and thermocouples for temperature measurements and base and top temperature control. The column has a single feed point in the sixth tray. It also has a total condenser, a reflux drum and reboiler. The column has a thermical insulation.

A. Model and Simulation Process

The dynamic model used to generate the data and to train data for the neuro-fuzzy network is obtained so that the total mass balances and component balance is solved for each tray, all equations in the model were obtained in [2].

Vapour-liquid equilibrium relationships were used, and a Francis formula relation was used to describe the retained liquid in reboiler (M_{12}) and the retained liquid on each tray (M_n). The column has ten real trays and the Murphree efficiency was 85% at each stage. The feed stream (F_L) is liquid in its bubble point. The pressure is constant through the column, constant molar overflow and non-linear equilibrium liquid-vapor. The model was developed in ForTran/Matlab® language and validated against experimental data.

To estimate the behavior of the column at different operational condition some disturbance were introduced in the column and the responses were record and analyzed. The disturbances were limited to the real column operating conditions of the pilot plant.

Two cases were studied: the first case was made a step change (+) 10% in Reflux Flow (R) and in steam entering the reboiler (V_3), waiting to reach a new steady state and step change back of (-) 10% R and V_3 was made, bringing back the old initial conditions, as is show in Figure 3; the second case was a step change on (+) 10% in liquid flow (F_L) and in feed composition (X_f), waiting to reach a new steady state and step change back of (-) 10% in F_L and X_f was made, bringing back the old initial conditions, as is show in Figure 4.

IV. SELECTION OF VARIABLES

In this work we used the technique of secondary variable selection through sensitivity analysis. This technique provides information on the process responses in the face due changes in the manipulated variables.

According [3], the seeking of mathematical model that relates a dynamically two variables of a system, starts from the assumption that there is a significant correlation between these variables to justify the model. Thus, intuitively the cross-covariance function (FCC) in (1), presented as a tool to determine if there is a significant correlation between these two candidates variables to compose a model.

\[ Cov(x, y) = \frac{1}{N} \sum_{k=1}^{N} [(x(k) - \bar{x})(y(k) - \bar{y})] \]  

(1)

Where: \(N\) is number of elements (vectors of same size \(x, y\)); \(x\) and \(y\) are respectively the input and output vectors; \(\bar{x}\) and \(\bar{y}\) are the average of \(x\) and \(y\); and \(\xi\) is the lag (number of delays for the signal analysis).

This relationship can be used, for example, to choose which temperature is used in the model inference for composition avoiding the use of all redundant temperature trays.

Sensitivity Study is described in steps. The first step is to describe the possible input and output variables for the soft sensor; the second step is to select the input variables and check if they are highly correlated with the composition of the product.

First Step: the input variables of a virtual analyzer can be
In this study the following manipulated variables were selected to the model inferential input: liquid flow (F_l) in the feed, the reflux flow (R), feed composition (X_f) and the reboiler of the heat (Q_R). The steam flow (V_s) that comes into the reboiler was used to determine the amount of the reboiler heat (Q_R) to promote the separation. The product composition is sensitive to variation in liquid flow (F_L) and vapor (F_v) in the feed, once the decrease or increase of these variables determines the separation efficiency. However, in this work the steam flow rate (V_s) variable was not used, because the column feed is liquid on the bubble point. The feed temperature (T_m) was not used as an input variable because it showed very little variation.

The non-directly manipulated variables selected for the sensitivity study were the following temperatures of the column T_1, T_2, T_3, ..., T_n, and the temperature of the reboiler, totaling 11 temperatures in the system. All these temperature will be tested to see which have more influence in the composition. The internal pressure of the column may not be selected, because the model assumes a constant pressure in the system. The output of the inferential model was the methanol top composition of the column (X_1).

Second Step: In this step, the secondary variables were selected. This selection was based on the perturbations and sampling time responses. A step change of (±) 5% was performed on the following manipulated variables: liquid flow (F_l), heat of the reboiler (Q_R), the discharge flow (R) and feed composition (X_f). The step change either (+) or (-) was performed in order to obtain lower temperatures on the plates, an increase of the composition. Figure 5 shows the top composition responses. In Figure 5 can be seen that the composition response to the reflux flow is faster and higher than the others responses.

The sampling time (T) was calculated, time between two samples. In order to have the fundamental characteristics of the original signal, the sampling time should be shorter enough to retain the characteristics. In this work, the calculation of the sampling time was done using three methods, based on [3] and [4]. Then, the method selected was the one that gave the lowest sampling time.

The constant time method (t_cons) consist in gives perturbations in the system and verify which disturbance gives the quickest and highest response, in this case, the reflux flow (R). For this response, composition response for a step change in the reflux flow, calculates the time constant, 63.2% of the final value, and take 10% of this value. The result is the sampling time. The time constant calculated was 0.35 h or 1260 s that corresponds to 63.2% of delta between the two steady states. Taking 10% of this value gives 126 s and this will be the sampling time.

The soft senor should represent the system for giving compositions in the real range. Thus, it is necessary to introduce a noise in the manipulated variables of the system, disturbing the operation point of the column. The disturbances introduced were the (+) or (-) 5%, in the frequency time of 3 sampling times, or 378 s or 0.105h for 18 hours column operating. Figure 6 shows the response.

As previously mentioned in A section III, it is necessary to select the inputs for the inferential model. The cross covariance method was used to choose which temperatures should be select as an input to a soft sensor. As can be seen in the graph in Figure 7, the temperatures of the early stages have a higher covariance and shorter delay.

In this work was decided to use the five temperatures that were more sensitive to composition, based on the work of [5]. Finally, the data acquisition from the model was performed using 442 points relating to 18 hours of operation of the pilot plant, the 9 input variables values were collected for training and validation of the neuro-fuzzy network, which are; T_1, T_2, T_3, T_4, Q_R, R, X_f and F_l and the output variable X_1 (Composition of methanol at the top of column).
These data were saved in Matlab® file for use in the next step.

V. INFERENTIAL MODEL (RESULTS AND DISCUSSION)

Most chemical processes such as distillation have nonlinear behavior providing a complex modeling when classical estimation techniques are used. Of the usual methodology employed in the inferential model construction (soft sensor), highlight the white-box models, gray-box models and also the black-box models. The black-box model applies the intelligent techniques in generating the soft sensor and it requires no knowledge of the physics and chemical laws of the process.

Recently appears the hybrid systems technique concept, the term hybrid means crossing different species. This technique uses two modeling techniques, which provides a heterogeneous system with smart features. The basic idea of a neuro-fuzzy system is to implement a Fuzzy Inference System, a distributed parallel architecture in the way that paradigms of learning common to the ANN can be used in this hybrid architecture, which allows to integrate the advantages of each technique, approach and minimize the weaknesses of both.

The Neuro-Fuzzy system is the technique employed in this work because it is the easiest way to insert a priori knowledge into a soft sensor. Among the adaptive models more used in the soft sensor construction the model the ANFIS (System Adaptive Neuro Fuzzy Inference) is in highlighted by [6]. The ANFIS model can be constructed by the anfisedit command in Matlab®.

A. Validation of the Model

The ANFIS neuro-fuzzy inference adaptive system was used in the construction of the soft sensor. After the study of the selection of variables in section IV, nine input variables were selected for the soft sensor. To obtain a better performance of the neuro-fuzzy network, and to represents the dynamic behavior of the process it was used a regression of one sampling time in selected variables, changing the number of entries from 9 to 18 variables, 9 variables at the present time and 9 variables at the previous sampling time. In the neuro-fuzzy network training stage, 440 points were used. These were divided into two groups: training group with 286 points and the validation group with 154 points. A neuro-fuzzy system with 18 inputs and one output was built with 42 fuzzy rules. Figure 8 represents the soft sensor and shows the ANFIS network architecture.

In the Figure 8, the 1st layer calculates the degree of pertinence of the inputs, based on pertinences functions, $A_i = \text{high}$ and $B_i = \text{low}$, this stage is known as fuzzification; the 2nd layer, each node is related to a rule and calculates what pertinence degree the consequent of the rule is being served (known as firing rules) in the 3rd layer is performed a normalization in the levels of firing rules; the 4th layer calculates the neurons outputs. The final layer is known as defuzzification, which calculates the output of the system. Figure 9 shows the top compositions inferred values by the soft sensor versus the real value of the compositions.

According to this graphic, Figure 9, the soft sensor presents very good results for estimating the top composition of the column. The Soft sensor response is closer to the real composition value giving an absolute error around $10^{-3}$.

VI. CONCLUSION

This paper proposed a soft sensor construction strategy. This strategy was developed in five stages. The soft sensor built showed good results to infer the composition of the top distillation process. The soft sensor is a very powerful tool to replace the traditional methods of measurement, allowing to infer the composition from the available measurements from the column in real time. The application of soft sensor is feasible to overcome the operational difficulties found in industrial processes. For further work, others clustering technique can be use.

REFERENCES