SOFT SENSOR AS COMPOSITION ESTIMATOR IN MULTICOMPONENT DISTILLATION COLUMN

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Introduction: Physical variables - the most common ones being: temperature, flow and level - are usually those ones which are attractive for chemical processes. To measure physical variables, there is a great variety of very accurate sensors and transducers, that are normally quite affordable for industries that work with short time responses of an order of second decimals or, in the worst case, of few seconds.

When chemical (analytic) variables are concerned, there are cases when measurers also work with short response time and that are sold by relatively low prices as, for example, pH or oxide-reduction potential measurers. However, when the issue is to measure chemical or biochemical variables related to composition, such as the measurement of DO (dissolved oxygen concentration), O_2, CO, CO_2, NH_3 or other variables related to biomass, in terms of measurers the situation is more difficult. There are many cases when the analysis are performed in laboratories, by means of sample collecting and the response time can be minutes or even hours long. Even if an on-line analyser is available, the cost of such instrument and its precision are quite unsatisfactory.

On the other hand, to maintain the quality specifications, it is necessary to know the composition (of the products) to enable the implementation of an efficient control system. In this case, if an on-line analyser with an acceptable response time, of a reasonable accuracy and low price is available, then the implementation of an advanced control strategy is possible to be considered. Unfortunately, such kind of analyser, with all these characteristics and in practical situations, is not usually available in industry. A soft sensor, an inferential measurer or an indirect measurer must be considered as a possible option to estimate the variable(s) of interest in such situations (Chu *et al.*, 1998).

A soft sensor corresponds to an indirect or inferential method of measurement in real time, when a mathematical static model, or preferably a dynamic one, is applied together with one or more measured variables, normally of kind flow, pressure or temperature type (physical variables). For such variables the measurers available in the market are low cost and accurate and they have fast response. The applied dynamic model must have physical variables as inputs and the product of interest composition as output.

According to Zamprogna *et al.* (2001), “although gas chromatographs (GC’s) are available to obtain on-line analysis of product samples, they are seldom used in distillation column applications because they are expensive to buy and to maintain and (most importantly), they provide delayed measurements, due both to sample time and dead time. The delay introduced by a GC can be detrimental therefore, from a process control standpoint. Other measurement techniques such as infrared-based measurements, analysis of refractive index, density, or dielectric constant are not yet reliable or accurate enough for use in distillation applications

For product composition control of distillation columns, it is rarely the case that measurements of product compositions are directly used as controlled variables, because on-line accurate and/or real time measurement of composition is difficult. Most analyzers, like gas chromatographs, suffers from large measurement delays (when realized with the aid of the laboratory), or are difficult to maintenance (when realized on-line) and high investment and maintenance costs. (Kano *et al.*, 2000).

An inferential control is highly advisable to perform an on-line composition control. The product composition estimates employed to control are got starting from other variables measured in the process. Therefore it is essential to obtain a very accurate inferential model.

The phenomenological model, if available, is the ideal one if it is accurate enough for a reasonable computational load. Control has to occur in real time. In practice, however, due to the high amount of the involved differential equations in large columns, there is tendency of an execution delay, which may make the control not feasible.

A faster solution, which generates not an intern model with state variables but an external one only with input and output variables, is to employ an empirical model determined from process data.

To calculate an estimate of an unknown quantity from a set of known quantities, in principle, there should exist a mathematical model to describe quantitatively the relation between the unknown and known quantities. The estimator, which is designed on the basis of the model, should provide a reliable estimate of the unknown quantity even when plant-mode mismatch and unmeasurable disturbances are present, that is, estimation allows estimating unknown quantities, with zero steady state estimation error in the presence of unmeasurable disturbances and model-plant mismatch or when the process varies along time (Soroush, 1998).

This work proposes to employ soft sensors to analyse the composition of the products leaving the distillation column, by measuring the temperature in some trays, the recycle flow and the input and output flows. These inferred variables could be then fed into an inferential control system which aims at maintaining the quality of such products within the specifications or into a supervisory system to follow up the value of these compositions along time.

Soft Sensor: In their work on distillation columns, Mejdell and Skogestad (1991b) report one of the major difficulties they have to face to be product composition measurement. Among the existing alternatives for chemical analysers, the most employed one is the gas chromatography, although it also presents some disadvantages like long delays in the measure obtention and high operational costs. Besides, they also point out the economical disadvantage, as this demands high investments in purchasing and installation (including back-up systems) as well as in operation and maintenance.

In another article, Park and Han (2000) conclude that sensors that overcome cost limits, reliability and long response delays enable the implantation of more efficient systems for industrial plant control and monitoring. This allows a reduction of product and energy loss as well as of toxic products and safety problems.

Soft sensors can be widely applied because their operation helps monitoring, controlling and optimising processes in general, supplying measurements that are more reliable, faster and at lower cost not only for development, but also for maintenance. It must me highlighted that these soft sensors can work as substitutes to several physical sensors or they can work together with them as monitoring aid, malfunction control and preventive maintenance.

According to the employed models, there are three distinct classes of techniques for soft sensor development. The first class is composed of sensors that are based on white box modelling, obtained from equations that describe the process physics; the second class is composed of sensors based on black box modelling (or identification); the third class is composed of sensors based on hybrid models, a combination of the first two classes (James *et al.*, 2000).

In practice, the models that have been obtained through empiric approach are the most popular and they will be the favourite ones in this work, when artificial neural networks techniques are to be employed.

Something that cannot be forgotten while developing a soft sensor no matter the approach is to determine the best-input variables for the inferential model. For distillation columns, a fundamental question is to determine the flow, pressure and temperature for measurers (associated to each tray) have to be used to infer output products composition.

The success of an empiric model depends on the quality of the collected data, because it is based on experimental data. Therefore, aspects such as sampling pauses/gaps and noise attenuation must be taken into account.

The process: The distillation column object of this study is based on a model presented by Luyben (1990). Matlab/Simulink® was used for the implementation of the model and it will also be used to generate data of the dynamic simulation.

This non-linear model employs a non-ideal multicomponent column with a non-equimodal overflow and inefficient trays.

The figure 1 presents a schematic draw of the employed distillation column.

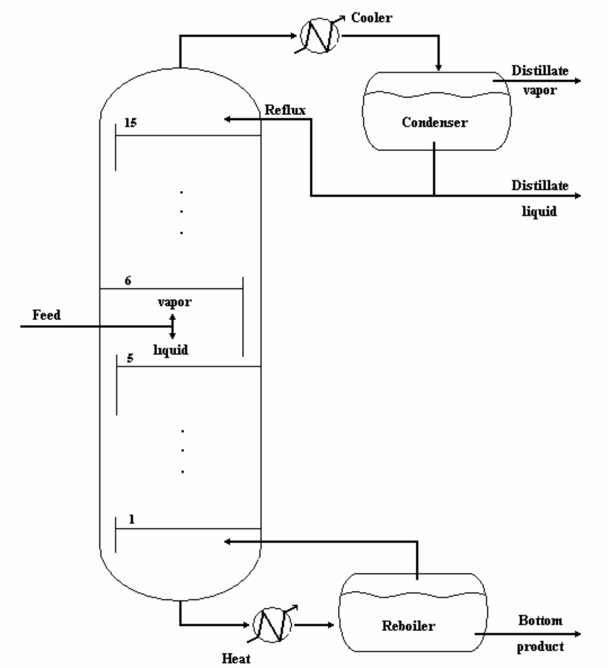

Fig. 1. Scheme of the distillation column

The column is composed of 15 plates (or trays), numbered starting from the bottom, besides the reboiler in the base of the column and a condenser in the top of it, which are modelled as two more/extra stages. The feed/input is done through a unique entrance in the tray 5 of the column.

This unit is divided in two sections: a stripping section which encompasses the stages of the column base to the feed stage and the rectifying section which encompasses the stages of the feed tray up to the top of the column.

The feed/input is composed of 5 hypothetic components (the heaviest, heavy, intermediate, light and the lightest ones) created by the values supplied by Luyben (1990). The feed/input supplied to the distillation unit is a mixture of liquid and vapour /gaseous states; that is the reason why it is said to be mixed and that it is en temperature equilibrium.

Products outputs happen in just two places: in the condenser and in the reboiler. The softest components that reached the top of the column are cooled by heat transfer and stored in the condenser. There are three output flows: one part of the liquid, which has a constant flow, returns to the column (reflux); another part, which also has constant flow, is taken out from the distillate in vapour/steam/gaseous state and, finally, the third output of the distillate, in liquid state, whose flow is controlled by an ideal valve which maintains a constant level in the reservatory (takes instantaneously output all exceeding liquid).

The heaviest component that got to the base of the column are stored in the reboiler, were they are heated. Then, a flow, in vapour state, leaves the reboiler, returning to the column below the first tray; next, a withdrawal of liquid occurs from the base of the column whose flow is controlled by an ideal valve which maintains a constant level in the reservatory (takes instantaneously output all exceeding liquid).

Table 1 Column specification

Column diameter	
Rectifying section	1,829 m
Stripping section	1,829 m
Weir length in the tray	
Rectifying section	1,219 m
Stripping section	1,219 m
Height of weir in the tray	
Rectifying section	0,032 m
Stripping section	0,019 m

Besides, the efficiency of trays is modelled according to the Murphree formula, employing a coefficient of 0.5. It considers that the column having a pressure gradient between the top and its base. The liquid accumulation (holdup) in the condenser and in the boiler is also supplied. The dynamic flows in each tray are expressed by Francis formula, which considers rectangular weirs.

Table 2 Operation conditions of the column

Reflux	181.44 kg_mol/h
Distillate vapour	90.72 kg_mol/h
Heat duty in reboiler	$5.280 \cdot 10^9$J
Feed/Input	
Temperature	322.04 ºC
Liquid flow	362.84 kg_mol/h
Flow of vapour	90.72 kg_mol/h
Liquid composition	[0,05 0,60 0,01 0,30 0,04]
Vapour composition	[0,40 0,53 0,02 0,05 0]
Pressure	
Reflux drum	135,83 kPa
Reboiler	146,17 kPa
Holdup	
Reflux drum	0,2832 m^3
Reboiler	0,2832 m^3

4. RESULTS

As it has already been mentioned above, this work aims at developing a soft sensor that could estimate the instantaneous composition of component no. 2 at the top of the column, employing physical measures supplied to a neural network. The first step to develop this sensor is to determine the data set to be used and then train the neural net.

4.1 *Data set*

The data set comprises the values measured in the variables that are used as input for the neural network. This set has been divided into two sub-sets – one for the neural network training and the other one for soft sensor testing.
The input variables of the soft sensor are divided in two classes: *internal* and *external* The internal ones are not directly subject to manipulation, whereas the external ones can be manipulated.

The external variables are excited by a random signal with variations of ±5% around their nominal steady state values, with a different seed for each one. The external variables are as following:

- Heat duty in reboiler - QR
- Reflux flow in the column - R
- Feed temperature (liquid and vapor) – TF
- Liquid feed flow - FL
- Vapor feed flow - FV

Among the internal variables, the temperature in 6 trays of the column (chosen so as to reduce the number of inputs of the neural net according to correlation analysis of the values) will also compose the input vector of the sensor. The temperatures in the following trays were selected: *1, 3, 5, 7, 11* and *17.* Those temperatures are measured with a sampling time of 9 seconds, defined as 1/10 of the minor time constant of the system.

The random signal used to excite the external variables is maintained constant for 3 sampling times, that is equivalent to a period of 27 seconds.

4.2 *RNA training*

The ability to efficiently represent non-linear systems is one of the most attractive aspects of using artificial nets in soft sensing systems (Fileti *et al.*,1999).

Matlab® toolbox has been used to implement and train the neural net. The net employed had a feedforward architecture, due to their better results, comparing to those of Elman type, that were initially also considered.

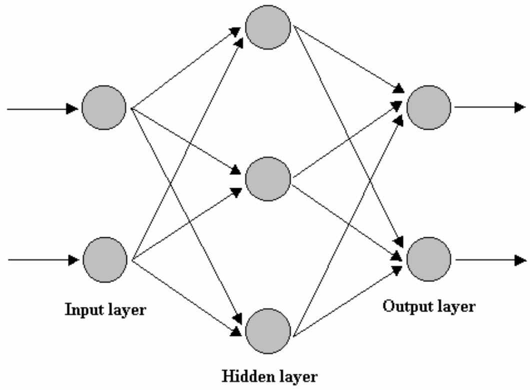

Fig. 2. Architecture of a feedforward neural network with one hidden layer

The four–layer topology of the neural net has 2 hidden layers. The first one (of input) is composed of 11 neurons. The hidden layers have 50 and 25 neurons, respectively, as observed in several tests performed so as to combine good results and an acceptable usage of computational resources. Finally, the output layer has just one neuron, which supplies the estimate result for the composition of component 2 in the column top product.

Hyperbolic sigmoid tangents were used as transference functions in the hidden layer neurons. The training algorithm was the Levenberg-Maquardt one, as available in Matlab®, because it presents faster convergence.

To be sure that the soft sensor is sufficiently reliable, the proposal is to train it initially with a determined amount of points and then put it into operation in a plant, in parallel with a hard sensor (probably NIR). After a certain period of time of operation, when more data are available from the hard sensor and from the secondary variables of the soft sensor, it is possible to compare the results presented by the two sensors. If the results are sufficiently close, the soft sensor could be considered ready to assume its role as a supervisor of the hard sensor and work by itself. If not, a new training period can be performed. These tasks can continue until the sensor performance is considered satisfactory for the application. The idea is to use the soft sensor as a redundant sensor, which takes care of the hard sensor. In case of a discrepancy between them, it would sound an alarm to alert the plant operator that one of the sensors has problems.

Next it is analysed two different ways to train the neural network, that is, partial training and full training.

Partial training consists of starting the network training with a small data set, until it converges (error below a stipulated value). After that, this same net is retrained with a set twice as big (two times the initial one) and so on, and so forth. The objective is to discover the influence of this kind of training compared to the one employing all data at the same time.

The main errors have been calculated and compared, based on an evaluation criterion for each one of the nets. Thus, the obtained errors are: *SSE error*, the somatory of the square error and the *Max error*, which is the major pick of errors presented for cross validation. The equations defining those errors are presented next.

$$SSE = \sum_{i=1}^{N} \left| Z(i) - \hat{Z}(i) \right|^2 \tag{1}$$

$$Máx = \max\left(\left| Z(i) - \hat{Z}(i) \right| \right).100\,[\%] \tag{2}$$

The following table sums up, after several evaluations, the sensor results obtained along 20 hours. Each group of points was obtained through 3 different training options, that is, 2 partial and 1 full.

Table 3 Comparison of different training

	SSE Error	Max Error
1.000 data		
4 times of 250	$11{,}2240.10^{-5}$	0,5426
2 times of 500	$1{,}7697.10^{-5}$	0,1050
1 time of 1.000	$1{,}4863.10^{-5}$	0,1060
2.000 data		
4 times of 500	$0{,}2071.10^{-5}$	0,0265
2 times of 1.000	$0{,}1802.10^{-5}$	0,0243
1 time of 2.000	$0{,}0575.10^{-5}$	0,0047
3.000 data		
6 times of 500	$0{,}1712.10^{-5}$	0,0210
3 times of 1.000	$0{,}1220.10^{-5}$	0,0229
1 time of 3.000	$0{,}0584.10^{-5}$	0,0089
4.000 data		
4 times of 1.000	$0{,}1220.10^{-5}$	0,0229
2 times of 2.000	$0{,}0575.10^{-5}$	0,0047
1 time of 4.000	$0{,}0954.10^{-5}$	0,0087

According to the above mentioned data, the way of training affects the results for the same data set. So, the lower the amount of retrainings, the better the obtained results. This happens because when the trainings are performed with smaller data sets, the net converges to a situation that is not the best when more points are added to the set.

Another characteristic that can also be observed is that there is an optimum data value for the training set, with a minimum error. So, the trainings performed with few points (for instance, 1000) generate small errors, but those performed with large sets (3000 or 4000 points) also generate large errors. Therefore, the best result was obtained with a training of 2000 points.

Error correction: After the evaluation of the previous neural nets, it has been observed that the best option is to perform directly a net training with 2000 points.

The obtained sensor can be put into operation in parallel with the hard sensor to perform evaluations of its behaviour. However, after a period of several hours of work, it can happen that a relatively large error appears.

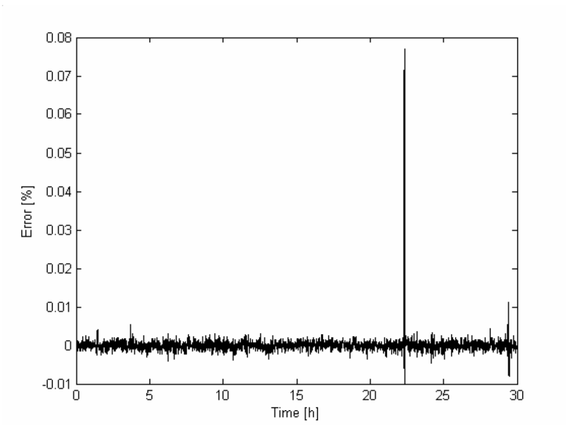

Fig. 3. Example of spurious error

This kind of error, as the one that can be observed in figure 3, was called spurious error. It is punctual and it affects the sensor behaviour in just a small region of points.

It occurs because the net has been trained with a number of points not so large (2000). This way, some data combinations may have not been presented in the training or, at least, they may be quite different from those in training. To solve this problem, it is necessary to perform a retraining of the net, now employing the values expected for a range of points around this error.

After retraining for a range of 100 points (15 minutes) the error in this region was eliminated, as shown in figure 4.

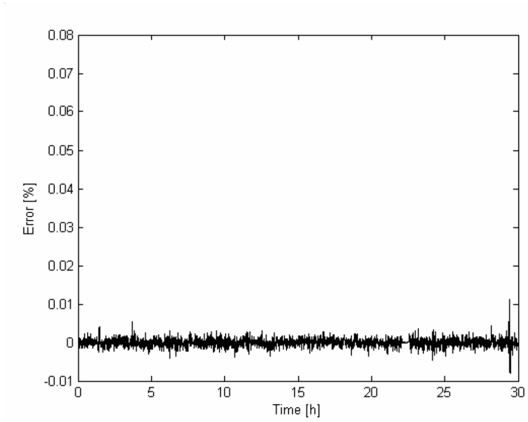

Fig. 4. After error correction (retraining)

To ensure the sensor to produce just adequate/good results, a longer simulation of 60 hours was performed. No new spurious error occurred, as can be seen in figure 5.

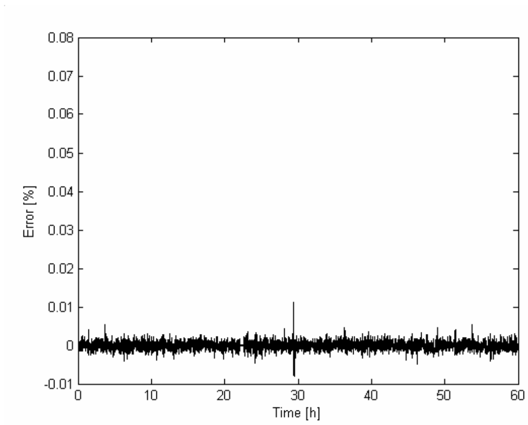

Fig. 5. Sensor results after a period of 60h

Conclusions: Multicomponent distillation columns are difficult to control not only for their non-linear and transient behaviour, but also because the product quality cannot be measured rapidly and with reliability. The present work developed an inferential estimate system of the distillate composition based on the application of artificial neural networks.

This system proved to be quite accurate (error lower than 10^{-3}) and fast, two of the main problems previously presented. This solution has a low cost if compared to the alternative measuring systems of the market.

Nevertheless, it is important to highlight the importance of the data set training for this kind of analyser. As it was observed, small sets can be not large enough for major variations in the plant operation, when local retraining procedures are needed.

The obtained system can be implemented to supply data for a more modern and powerful system operating in the plant.

NOMENCLATURE

FL – Liquid input flow
FV – Flow of input gas
QR – Heat duty ratio in the reboiler
R – Intern reflux rate
TF – Input flow temperature
Z – Estimate value supplied by the soft sensor

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