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Soft sensors for product quality monitoring in debutanizer distillation columns

L. Fortuna^a, S. Graziani^a,*, M.G. Xibilia^b

^a Dipartimento Elettrico, Elettronico e Sistemistico, Università degli Studi di Catania, Viale Andrea Doria 6, 95125 Catania, Italy b Dipartimento di Matematica, Università degli Studi di Messina, Contrada Papardo, Salita Sperone 31, 98166 Messina, Italy

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Abstract

The paper deals with the design of neural based soft sensors to improve product quality monitoring and control in a refinery by estimating the stabilized gasoline concentration (C5) in the top flow and the butane (C4) concentration in the bottom flow of a debutanizer column, on the basis of a set of available measurements. Three-step predictive dynamic neural models were implemented in order to evaluate in real time the top and bottom product concentrations in the column. The soft sensors designed overcome the great time delay introduced by the corresponding gas chromatograph, giving on-line estimations that are suitable for monitoring and control purposes.

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1. Introduction

In the last few years ever-growing interest has been shown in production quality standards and pollution phenomena in industrial environments. Government laws enforce hard limits on pollutant and product specifications. Increasingly efficient control policies are therefore required.

The refinery community has recognised the importance of the optimisation of process automation because of the benefits in terms of both profitability and tight control on product quality.

In this scenario the importance of monitoring a large set of process variables by using adequate measuring devices is clear (Arena, Fortuna, Gallo, Nunnari, & Xibilia, 1995; Bozzanca, Licitra, Fortuna, & Xibilia, 1999; Matsumura, Iwahara, Ogata, Fujii, & Susuki, 1998; Park & Han, 2000; Tham, Montague, Morris, & Lant, 1991). A key obstacle to the implementation of monitoring and control policies is the high cost of online measurement devices.

This paper deals with the design of systems, consisting of mathematical algorithms, which produce reliable realtime estimates of unmeasured variables by using their correlation with available data. Such systems are usually known as *soft sensors* (Tham, Morris, & Montague, 1989; Tham et al., 1991; Willings, Montague, Di Massimo, Tham, & Morris, 1992; José de Assis & Maciel Filho, 2000).

The soft sensors used in the described application are designed to take into account the nonlinearities of the processes involved in refineries. Nonlinear autoregressive models, implemented using multilayer perceptron (MLP) neural networks, are proposed (Su, Fan, & Schlup, 1998; Zhang, 1999; James, Legge, & Budmann, 2002; Fortuna et al., 2001).

Soft sensors have a number of attractive properties:

- they offer a lowcost alternative to expensive hardware sensors;
- they can work in parallel with hardware sensors, giving useful information for fault detection tasks (Yang, Chen, & Wang, 2000);
- they can easily be implemented on existing hardware (e.g. microcontrollers) and can easily be retuned when system parameters change;
- they allow realtime estimation of data, overcoming the time delays introduced by slow hardware sensors

^{*}Corresponding author. Tel.: +39-095-738-2327; fax: +39-095-330793.

E-mail addresses: sgraziani@diees.unict.it (S. Graziani), mxibilia@ingegneria.unime.it (M.G. Xibilia).

(e.g. gas chromatographs), thus improving the performance of the control algorithms (Tham et al., 1989; Matsumura et al., 1998).

Soft sensors can be designed either on the basis of an analytical model or by introducing black or grey box identification approaches. In the case of the processes involved in refineries, due to the complexity of the phenomena involved, physical modelling can be very time-consuming and significant parameters are generally unknown. On the contrary, the great amount of historical data, usually acquired for monitoring purposes, allows nonlinear black or grey box process model identification (Park & Han, 2000). Neural Networks can be used to implement the required nonlinear models (Willings et al., 1992; Zhang, 1999).

In this application available process information given by technologists was used to choose both significant input variables and a huge amount of relevant working data, collected in the refinery database over a period lasting more than three years. The set of data was used to tune the parameters of a NARMAX structure implemented by using MLPs with appropriate lagged inputs (Leontaritis & Billings, 1985; Chen & Billings, 1989).

Neural based modelling is a consolidated strategy, often used in a large number of industrial applications, when real-time estimation of plant variables is required for monitoring and/or control purposes and on-line sensors may give variable measurements with long delays. This is often the case of petrochemical plants (Tham et al., 1991; Willings et al., 1992).

In this paper two soft sensors are proposed to estimate both the stabilized gasoline content in the overheads and the butane content in the bottom flow of a debutanizer column. The sensors designed provide a realtime estimate of the relevant variables, thus overcoming the problem of the delay introduced by the gas chromatograph.

The paper is organized as follows. In Section 2 the plant is described, together with the relevant variables and available measuring devices. In Section 3 the design of the proposed soft sensors is described and their performance is discussed. In Section 4 the on-line performance of the sensors is illustrated.

2. Description of the plant

The column is located in the ERG Raffineria Mediterranea s.r.l (ERGMED), in Syracuse (Italy) and it is part of a desulfuring and naphtha splitter plant, shown in Fig. 1.

In the debutanizer column C3 (propane) and C4 (butane) are removed as overheads from the naphtha stream.

The debutanizer column is required to:

- ensure sufficient fractionation in the debutanizer:
- maximize the C5 (stabilized gasoline) content in the debutanizer overheads (LP gas splitter feed), while respecting the limit enforced by law;
- minimize the C4 (butane) content in the debutanizer bottoms (Naptha splitter feed).

A detailed scheme of the debutanizer column is shown in Fig. 2.

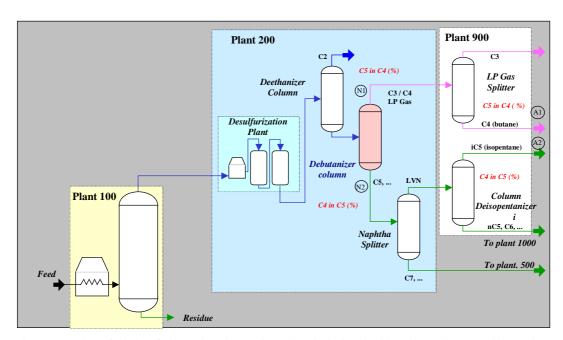


Fig. 1. Schematic representation of the desulfuring and naphtha splitter plant, including the debutanizer column, working at the ERG Raffineria Mediterranea s.r.l (ERGMED). The location of the two gas chromatographs is shown.

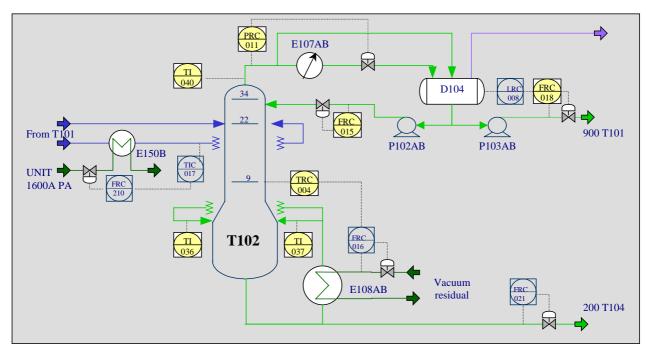


Fig. 2. Schematic representation of the debutanizer column with indication of the location of the measuring devices.

Table 1 Sensors relevant to the described application and corresponding characteristics

Tag	Description	Units	Working range	Accuracy
P011RC	Top pressure T102	kg/cm ²	0–15	< 0.2%
F015RC	Reflux flow T102	m^3/h	0-350	< 0.5%
F018RC	Flow to 900-T101	m ³ /h	0–70	< 0.5%
T040I	Top temperature T102	$^{\circ}\mathbf{C}^{'}$	0-750	< 0.2%
T004RC	VI° tray temperature $T102$	$^{\circ}\mathrm{C}$	0-200	< 0.2%
T036I	Bottom temperature E108A	$^{\circ}\mathrm{C}$	0-750	< 0.2%
T037I	Bottom temperature E108B	$^{\circ}\mathrm{C}$	0-750	< 0.2%
A002BR	C4 content in IC5	_	0-15%	< 1.0%
F012RC	IC5 flow to stock	m^3/h	0–28	< 0.5%
A001DR	C5 content in C4	<u> </u>	0-5%	< 1.0%
F006R	C4 flow to stock	m^3/h	0–60	< 0.05%

^a Accuracy values are intended to be one half of the amplitude of a rectangular PDF distribution.

The main devices shown in Fig. 2 are:

- E150B heat exchanger;
- E107AB overhead condenser;
- E108AB bottom reboiler;
- P102AB head reflux pump;
- P103AB feed pump to the LPG splitter;
- D104 reflux accumulator.

A number of sensors are installed on the plant to monitor product quality. The subset of sensors relevant to the described application are listed in Table 1, together with the corresponding description, working range and accuracy.

The C5 content in C4 (overheads of the debutanizer column) is indirectly measured by an analyser located at the bottom of the LPG splitter column of Plant 900 (indicated by the encircled symbol A1 in Fig. 1). The device has a measuring cycle lasting for 10 min.

The C5 content in the butane flowing to stock is totally due to the overhead of the debutanizer column. The location of the measuring device causes a delay which is not well known, but constant, but is likely to lie in the 20–60 min range.

In the same way, the C4 content in the debutanizer bottoms is not detected on the bottom flow, but on the overheads of the deisopentanizer column, as can be observed in Fig. 1, where the location of the gas chromatograph is indicated by the encircled symbol A2. It measures the content of C4 in the *i*C5 flow to stock. The C4 content in *i*C5 depends exclusively on the debutanizer operating conditions: the C4 detected in the *i*C5 flow can be assumed to be that coming out of the debutanizer bottoms. In this case the device has a measuring cycle lasting 15 min. Because of the analyser location, concentration values are obtained with a great

delay which is not well known, but constant, and is likely to lie in the 30–75 min range.

In order to improve the control quality of the debutanizer column, real-time estimation of both the C5 content in C4 and the C4 content in C5 is required. To this end, two virtual sensors based on neural networks (NNs) have been designed, as will be described in the following sections. The location of the abovementioned virtual sensors is shown in Fig. 1. The circled symbol N1 refers to the NN that estimates, in real time, the percentage (F_C5) of C5 in C4, while the circled symbol N2 refers to the NN that estimates, in real time, the percentage (F_C4) of C4 in C5.

3. Soft sensor design

Nonlinear autoregressive moving average models (Leontaritis & Billings, 1985; Chen & Billings, 1989) are used to fit real input/output data. The model output can be expressed as

$$y(k) = f(y(k-n), ..., y(k-1), u_1(k-n_1), ..., u_1(k), ..., u_m(k-n_m), ..., u_m(k)),$$
(1)

where y(k) is the current system output estimation, y(k-i) is a generic lagged sample of the system output, and $u_i(k-j)$ is a lagged sample of the *i*th system input. The maximum output delay is assumed to be n, while n_i represents the maximum delay for the *i*th input.

The number of lagged samples to be used are obtained by using a trial and error approach, guided by expert knowledge and physical insight.

The unknown function f(.) is implemented by a multilayer perceptron neural network with one hidden layer and a sigmoidal activation function. It is known, in fact, that such computing structures are universal approximators for generally continuous functions in the unity hypercube (Cybenko, 1989), assuming that a suitable number of hidden neurons are used. The number of neurons is obtained by a trial and error approach.

Of course the approximation capability of the neural model depends on the set of variables chosen to be used in (1). Moreover, the examples processed by the neural network during the learning phase must fully represent the system dynamic.

Data analysis and expert plant knowledge was largely used in this phase of the work.

The input data were pre-processed in order to correct for anomalies in the recorded data. Lack of data was corrected, when possible, by an interpolating algorithm; elsewhere data were eliminated from the learning set. Outliers were truncated and both the input and output data ranges were normalised.

3.1. Estimation of C5 concentration in the top flow

Data representing both input and output variables in Eq. (1) are collected at a sampling rate of 10 min.

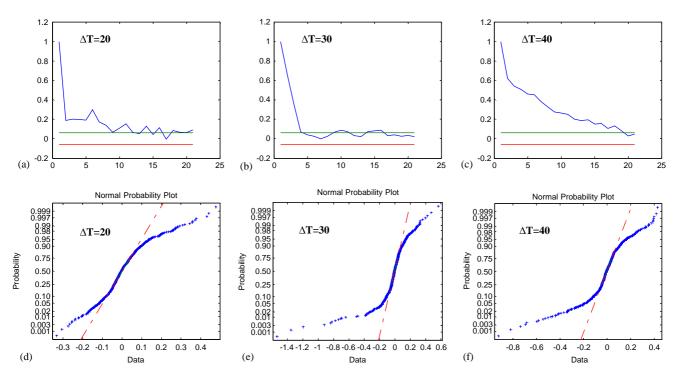


Fig. 3. Performance of network models with different values for the time lag Δt . (a) and (d) normalized autocorrelation and normal plot of the residual for $\Delta t = 20$ min; (b) and (e) normalized autocorrelation and normal plot of the residual for $\Delta t = 30$ min; (c) and (f) normalized autocorrelation and normal plot of the residual for $\Delta t = 40$ min. Plots corresponding to $\Delta t = 30$ min show that the corresponding residual is close to being uncorrelated and normally distributed.

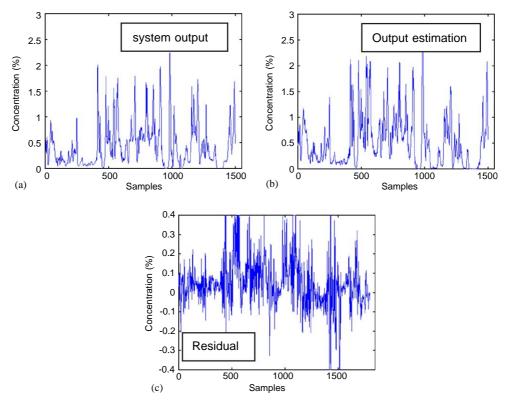


Fig. 4. Comparison between the concentration of C5 in the top flow of the debutanizer and the corresponding neural network estimation on a set of validation data. (a) actual data; (b) neural network estimation; (c) residual.

In order to indirectly measure the C5 concentration of the top output flow of the column, a gas chromatograph installed on a different plant at quite a distance from the column of interest, is used (see Fig. 1). There is, therefore, an unknown, yet constant, time delay, between the time scale used in (1) and the time at which the flux is sampled by the measuring device. Also, the measuring cycle is time-consuming and a further delay should be considered. The total time Δt elapsing between the time scale considered in (1) for both input and output representation, and the time at which the concentration of C5 in the top flow of the debutanizer column is available at the measuring device output should be estimated (plant experts hypothesized a delay in the range of 20–60 min).

The quantities to be determined can be summarised as follows:

- time delay Δt ;
- number of regressors for each input variable n_i where i = 1, ..., m;
- number of regressors of the system output, i.e. the system order, *n*;
- number, n_h , of hidden neurons.

The search for the quantities mentioned above introduces a combinatorial problem and a trial and error procedure was used. A large number of different

neural structures were trained with different values for n_i , n, and n_h and reorganizing the pattern structure, assuming Δt to be in the set $\{20, 30, 40, 50, 60\}$ min.

Only one-layer MLPs were taken into account and they were trained using the Levemberg–Marquardt algorithm. To avoid overlearning phenomena, learning data were organized into two sets and cross-validation with an early stopping approach was used.

Expert knowledge guided the choice of the number of regressors to be used for each input variable. After input structure selection, a growing strategy was used to fix the optimal number of hidden neurons.

The performance of the models obtained was tested on a new set of validation data. The following criteria were used to test model performance (Billings & Voon, 1986a,b):

- normal plot of the model error;
- covariance tests

$$\begin{cases} \phi_{\hat{\imath}\hat{\imath}}(\tau) = \delta(\tau), \\ \phi_{u_i\hat{\imath}}(\tau) = 0 \quad \forall \tau, \ i = 1, ..., 7, \\ \phi_{\hat{\imath}(\hat{\imath}u_i)}(\tau) = 0 \quad \forall \tau, \ i = 1, ..., 7, \end{cases}$$

where u_i is the *i*th input variable of the NARMAX model:

• model error vs. model output dispersion.

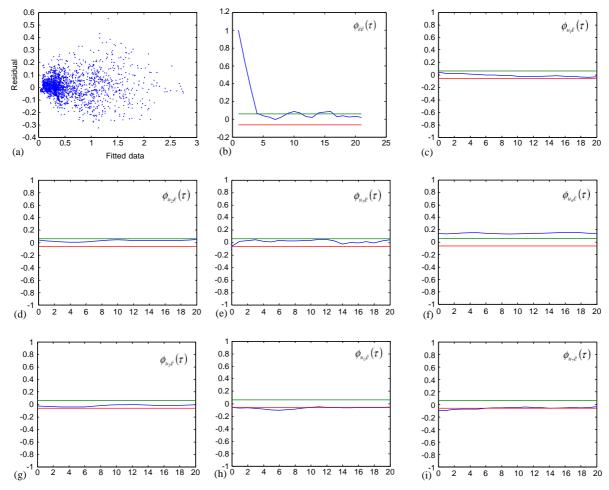


Fig. 5. Results of the correlation analysis of the neural model residual. (a) dispersion plot of the residual versus the model output; the plotted data appear quite unstructured. (b) normalized autocorrelation function of the residual. It is possible to observe that it is close to the Dirac $\delta(\tau)$ function. (c) to (i) normalized correlation functions of the residual with the model inputs u_i i = 1, ..., 7. Most of the cross correlation functions lie within the confidence interval.

The full set of plots obtained is huge. However, models proved to be very sensitive to choice of the time delay Δt . As an example, in Fig. 3 the normal plot of the residual and its normalized autocorrelation function (corresponding to the final neural model), for positive time lags ranging from 0 to 20 samples, are given for different Δt delay values along with the confidence interval. The plots obtained for delay values of $\Delta t = 20$, 30, and 40 min are shown.

Figs. 3a and d correspond to $\Delta t = 20$ min. Fig. 3a shows that the residual is far from being uncorrelated. Also, the normal plot shows a significant deviation from normality. Similar conclusions hold for the case of Figs. 3c and f, corresponding to $\Delta t = 40$ min. On the other hand, the plots reported in Figs. 3b and 3e, corresponding to $\Delta t = 30$ min, show that the residual is close to be uncorrelated and normally distributed.

The results shown in Fig. 3 allow us to argue that a suitable value for the time delay is $\Delta t = 30$ min. Such a conclusion was confirmed by most (sub optimal) structures of the neural models, with both different input lags and numbers of hidden neurons.

This consideration allowed us to fix the value of the Δt delay and to focus on the model structure.

The search procedure produced the following nonlinear fourth-order model:

$$F_{-}C5(k) = f(F_{-}C5(k-1), ..., F_{-}C5(k-4), T040(k),$$

$$P011(k), F015(k), F018(k), T004(k), ...,$$

$$T004(k-3), (T036(k) + T037(k))/2)$$
 (2)

where, as shown in Fig. 2 and Table 1:

$y = u_1 = F_C5$	C5 concentration in the top	
	flow;	
$u_2 = T040$	top temperature;	
$u_3 = P011$	top pressure;	
$u_4 = F015$	top reflux;	
$u_5 = F018$	top flow;	
$u_6 = T004$	side temperature;	
$u_7 = (T036 + T037)/2$	T036 and T037 bottom	
	temperatures.	

The number of hidden neurons is $n_h = 8$.

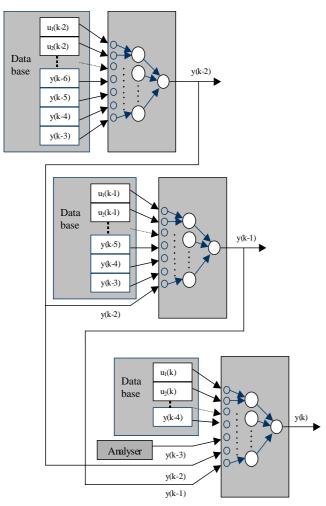


Fig. 6. Implementation of the three-step predictor for the estimation of C5 in the Top Flow.

In Section 4 a detailed description of the performance of the obtained neural model on the set of validation data, not used in the learning phase, is given (NIST/SEMATECH, 2002).

Figs. 4a and b give the C5 concentration in the top flow and its corresponding neural estimation, in separate figures for reasons of readability. Fig. 4c shows the corresponding residual. Analysis shows that no significant mean value drift nor variance value change occurs, for the data considered.

Fig. 5 gives the results of the correlation analysis of the residual. Fig. 5a shows the dispersion plot of the residual versus the model output; the plotted data appear to be quite unstructured. Fig. 5b shows the residual autocorrelation function, for positive time lags ranging from 0 to 20 samples, along with the corresponding confidence level. It is possible to observe that, for the proposed model, the residual autocorrelation function is close to the Dirac $\delta(\tau)$ function. Figs. 5c to i show the normalized correlation functions of the residual with the model inputs u_i i = 1, ..., 7. It is possible to observe that for the proposed model, most

of the cross-correlation functions lie within the confidence interval. Similar results hold for the $\phi_{\hat{\epsilon}(\hat{\epsilon}u_i)(\tau)}$ correlation functions, the corresponding graphs are not shown for reasons of space.

The model in Eq. (2) allows estimation of the output sample at the sampling time k, on the basis of a number of previous samples of both the input and output signals. Samples of the input signals at each time instant are recorded in the plant data base. They are then available for neural processing. On the contrary, a threestep predictor is used to obtain the required output data. In fact, to perform output estimation at the sampling time k, Eq. (2) requires the samples $F_{-}C5(k-1)$, $F_{-}C5(k-2)$, $F_{-}C5(k-3)$, $F_{-}C5(k-4)$, the sampling time being $T_s = 10 \text{ min.}$ Taking into account the value $\Delta t = 30$ min, at time k the samples available in the plant data base are $F_{-}C5(k-3)$, $F_{-}C5_{-}(k-4)$. The output values $F_{-}C5(k-1)$, $F_{-}C5(k-2)$ are estimated recursively by a three-step predictor implemented using the neural model in Eq. (2), as represented in Fig. 6.

The proposed soft sensor is currently implemented on the debutanizer column at the ERG Raffineria Mediterranea s.r.l (ERGMED), in Syracuse (Italy) and is used for monitoring purposes. The online performance of the sensor is discussed in the next section.

3.2. Estimation of C4 concentration in the bottom glow

The C4 concentration in the bottom flow was estimated using a procedure similar to the one described in Section 3.1. The model obtained is

$$F_{-}C4(k) = f(F_{-}C4(k-1), \dots, F_{-}C4(k-4), T040(k),$$

$$P011(k), F015(k), F018(k), T004(k), \dots,$$

$$T004(k-3), (T036(k) + T037(k))/2), \quad (3)$$

where the variables have the same meaning as in Eq. (2). In this case the sampling time was $T_s = 15$ min, due to different performance of the gas chromatograph used. The procedure for determination of the time delay gave $\Delta t = 45$ min while the obtained number of hidden neurons is $n_h = 13$.

Figs. 7a and b give the C4 concentration in the bottom flow and its corresponding neural estimation on a set of validation data, in separate figures for reasons of readability. Fig. 7c gives the corresponding residual. The results of residual analysis are very similar to those obtained for the estimation of C5 in the top flow.

The recursive structure shown in Fig. 6 is again used in this case to implement the soft sensor on the debutanizer column.

The on-line performance of the C4 sensor is described in Section 4.

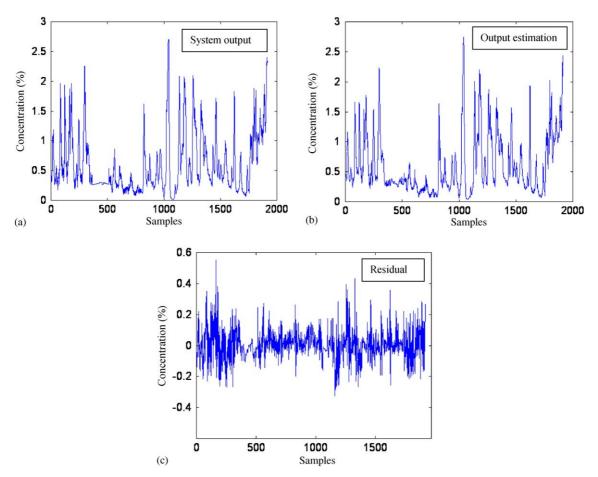


Fig. 7. Comparison between the neural network estimation of the concentration of C4 in the bottom flow and the corresponding actual data on a set of validation data. (a) actual data; (b) neural network estimation; (c) residual.

4. Soft sensor on-line performance

Both sensors are currently implemented for the online estimation of C5 and C4 in the debutanizer output. The on-line performance for a period lasting one week, collected 6 months after installation of the sensor, is shown in Fig. 8. Plant experts judged the sensor performance to be satisfactory.

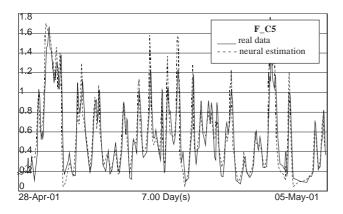
The soft sensors were designed taking into account data referring to the whole set of working conditions, collected over a period of three years, significantly expressing the plant history. However, the range of input values is continuously monitored in order to detect whether one of the input/output variables goes beyond the ranges observed in the data base used for neural network training. If new data exceed the respective ranges, retuning of the soft sensors is programmed (during a period of 18 months, such an event occurred only once, after a plant stop for maintenance purposes).

In Fig. 9 the records of T-036 and T-037, both before and after the plant stop are given. It is possible to

observe that T-037 has an abrupt change after the restart of the plant. The corresponding new trend is outside the range considered for the design of the sensors.

The performance of the C4 sensor after the stop, without any tuning intervention, is shown in Fig. 10. It is possible to observe from the time records that, although the variance of the estimate of the system output is comparable to that of actual data, the mean value of the predicted data is affected by a large bias.

During the programmed retuning procedure, two-day data were collected and randomly inserted into the learning file to retrain the neural networks. In this way, wider working ranges for the sensors can be assured. In this phase the previously established number of hidden neurons and model order were maintained. The retrained neural models recovered prediction capabilities comparable with the ones obtained before the plant stop. However, during the retuning period the system is also monitored by experts in order to detect anomalies in the system.



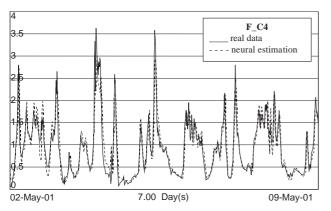


Fig. 8. On-line performance of the C5 and C4 soft sensors.

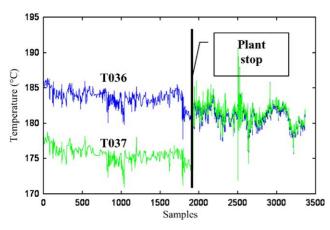


Fig. 9. Records of the temperatures $T_{-}036$ and $T_{-}037$ both before and after the plant stop. It is possible to observe that the mean value of $T_{-}037$ undergoes a change after the plant stop. The new values lie outside the range considered during the neural network learning phase.

5. Conclusions

Government laws enforce hard limits on the product specifications and effluent discharges of refineries as a result of the ever-growing interest in air quality and pollution phenomena. Increasingly efficient control

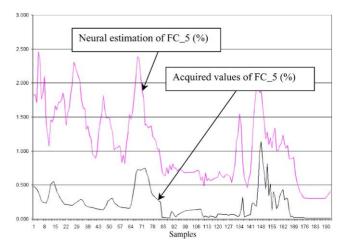


Fig. 10. Performance of the soft sensor for the estimation of C5 after the plant stop, before soft sensor retuning.

policies require a large set of data acquired from the plants to be processed. An increasing number of expensive measuring devices would therefore need to be installed. An effective solution to this drawback is represented by the availability of powerful low-cost data processing systems. This makes it possible to implement soft sensors, i.e., to use mathematical models to estimate unmeasured variables, using data on a set of measured variables.

A general procedure for the real-time estimation of variables acquired with large and unknown measuring delays has been proposed in the paper. The proposed procedure, based on neural soft sensors, was applied to estimate the concentrations of top and bottom products in a debutanizer distillation column. The soft sensors provide a fast, cheap real-time estimate of the variables of interest and hence make it possible to design fault-tolerant and effective control policies.

A set of historical time series of relevant variables, collected at the ERG Raffineria Mediterranea s.r.l (ERGMED), was used to design the neural network based soft sensors.

Dynamic nonlinear models were introduced to describe the relationship between a number of input variables and the estimated quantities.

An in-depth description of the strategy used, to find both the relationship between the measured variables and the delay introduced by the location of the actual measuring devices, is given in the paper.

The sensors are currently implemented in the plant and are used to monitor the production process, avoiding the long delay introduced by the gas chromatographs. The availability of the gas chromatographs gave us the opportunity to check the quality of soft sensor estimation that is considered satisfactory by experts. As a first point, the implementation of the soft sensor allows experts to monitor the plant performance

in real time. Also, the quality of the soft sensor performance suggests the possibility of using their real time estimates in a control loop to improve the column performance. Technologists are currently designing the control algorithms that will exploit the soft sensor capabilities. This was not possible with traditional sensors (gas chromatographs) because of the long delay introduced by the measuring cycle.

Great care was taken in both selecting the appropriate set of training examples, which covered all the operating conditions of the plant, and the on-line maintenance of the sensors. In particular, changes in the operating conditions are continuously monitored in order to decide whether retuning of the sensors is required. Experimental evidence of this occurrence is shown in the paper.

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