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Using A Wavelet Neural Network During The Computational Startup Procedure Of A Distillation Column

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Distillation is the most important unit operation in process industry. Due to its phase transition nature, large time delay and strong interaction between variables, the startup of distillation columns is one of the most difficult operations in the chemical industry. In many cases it is impossible to design an efficient control system due to the unavailability of online measures of crucial variables of the process. One way to make these variables to the control system is the use of a mathematical tool called soft-sensors. A powerful tool that can be used as a sensor, easy to implement and use is the neural network. In this work we chose to employ a modified wavelet neural network. Its high ability to generalize and performance is superior when compared to traditional feed-forward and radial basis nets in the identification of nonlinear process. The results showed that the neural network can be an interesting tool to operate as a sensor to avoid mathematical manipulation and possible loss of physical meaning of variables in the modeling of the distillation column.

1- Introduction

Due to the phase transition nature, large time delay and strong interaction between variables, the startup of distillation columns is one of the most difficult operations in the chemical industry. In this way, start-up operations represent very complex transient periods because of the simultaneous drastic changes in many state variables. As these dynamic transitions are always considered as non-productive periods, many researchers have been performed with the objective of minimizing the start-up time, the energy consumption or the amount of waste products and present the resulting start-up policies (Ruiz et al., 1988; Sorensen & Skogestad, 1996; Han & Park, 1997). The transient time (and its bad consequences) minimization can be achieved by making crucial variables values available to the control system. Nevertheless, in many cases, this is not possible for many reasons: concentration analyzer maintenance, or even, the inexistence of an

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online sensor. One way to cope this problem is the use of a mathematical tool called soft-sensors. Soft-Sensors are sophisticated monitoring systems that can relate state variables less accessible and the variables that can be measured during the process.

The soft sensor design involves the selection of the estimation structure and the choice of the estimation algorithm (i.e., the kind of dynamic data processor that performs the estimation task). The structural decisions (number and sensor location, set of states to estimate) play an essential role on the estimator implementation. The choice of number and sensor location still remains an open issue, with results that are not clearly connected with the estimator algorithm design and implementation (Venkateswarlu and Kumar, 2006; Oisiovici and Cruz, 2000). Soft sensors, according to Fortuna et al. (2005) have a number of attractive properties: they offer a low cost alternative to expensive hardware sensors; they can work in parallel with hardware sensors, providing useful information for fault detection tasks; they can easily be implemented on existing hardware and can easily be retuned when system parameters change; they allow real time estimation of data, overcoming the time delays introduced by slow hardware sensors, thus improving the control algorithms performance.

The present work shows the implementation of a wavelet neural network as a soft-sensor. The data for the training and validation were generated by a rigorous mathematical model of the process.

2- Neural wavelet description

Wavelets constitute a family of functions built from dilatations and translations of a basic function Ψ, known as "mother wavelet" (Claumann, 2003). Wavelets are defined as families of functions in the form:

$$\Psi_{(a,b)}(x) = |a|^{-1/2}\,\Psi\left(\frac{(x-b)}{a}\right) \tag{1}$$

with a,b $\in \Re$, $a \neq 0$. The *b* parameter performs the translation and the *a* parameter, the scale changing. By restraining the values of *a* and *b* to a discrete set it is possible to determine a family of discrete wavelets. In the direct case $a = a_0^{-m}$ and $b = nb_0 a_0^{-m}$, with $a_0 > 1$ e $b_0 > 0$. In this case, wavelet is expressed in the form:

$$\Psi_{(m,n)}(x) = |a_0|^{-m/2}\,\Psi\left(a_0^{m} x - nb_0\right) \text{com m, n} \in \mathrm{Z} \tag{2}$$

An f(x) function has its presentation in the space of functions generated by the family $\psi(m,n)$ described as an expansion in series of functions, according to:

$$f(x) = \sum_{m}\sum_{n} c_{m,n}\Psi_{m,n}(x) \text{m, n} \in \mathrm{Z} \tag{3}$$

The resolution plays the equation solution:

$$\phi(x) = \sum_{n=0}^{N} P_n \phi(2x - n) \tag{4}$$

where ϕ is known as scale function and n is the last coefficient index.

The pattern values used for a_0 and b_0 were respectively 2 and 1. According to Bakshi and Stephanopoulos (1993) those values are employed in several applications. The

functions can be specified as basis of Haar, splines and Daubechies. At the Claumann (2003) neural network development only the quadratic spline was used.
By using the multiresolution analysis, the expansion in series of functions, represented by the equation (3) is, in general, divided into two parts, and it can be expressed by:

$$f(x) = \underbrace{\sum_{n=-\infty}^{n=\infty} d_n \phi_n(x)}_{\text{scale function}} + \underbrace{\sum_{m=o}^{m=\infty} \sum_{n=-\infty}^{n=\infty} c_{m,n} \Psi_{m,n}(x)}_{\text{wavelets}} \tag{5}$$

The roughest approximation is obtained by the expansion in series of functions and, the details are generated by the walvelets. As it is composed of an f(x) limited conjunct, it is approximated in a limited domain and until a precision level. This finite number of points imposes restrictions to the number of functions used in the approximation, with only a few levels of resolutions to obtain a small approximation error.

2.1 Soft-sensor Design

The wavelet neural network used in this work has some modifications whose main objective is the improvement on the ability of generalization at the same time that it reduces the neurons number. The main modification carried out is that in a wavenet, the first level used in the approximation is constituted of scale functions and the next ones, if necessary, of wavelets, in the network used the multiresolution is carried out only with scale functions, decreasing the number of activation functions. The training data are initially approximated with activation functions (scale functions), whose support is equal to the domain of the problem (global scope function), contrary to the wavenet proposed initially, which uses only localized functions, minimizing the number of parameters to be estimated. In the case the approximation is not adequate, then, walvelets can be added with a crescent level of location according to the multiresolution. Figure 1 shows a wavelet illustration used where *y(k+1)* is the variable predicted in the time *(k+1)* and two inlets: the auxiliary variable *u(k)* and the outlet in the current instant *y(k)*. The inlet layer weights receive the value 1.

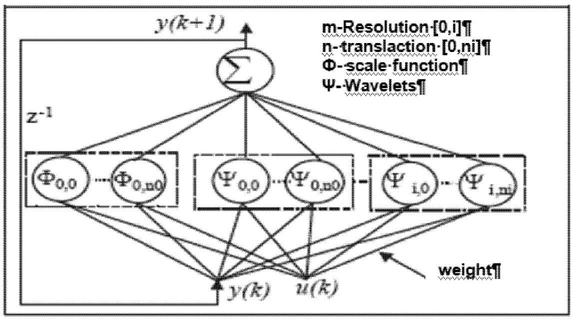

***Figure. 1** – Wavelet network used as a process simulator. Image provided by CLAUMANN (2003).*

The network has only two adjustable parameters: the regulator and the resolution levels. When a model has small errors and a deficient set of data uncertainties can be generated in the data approximation. A way to minimize them is to introduce an advance knowledge of the process, instead of just performing a data approximation. The regularization idea is to incorporate this information through a non-negative functional. For that, Tikhonov theory was used, where the problem now is to find the *s* function which minimizes the called Tikhnov functional:

$$\varepsilon(s) = \varepsilon_s(s) + \lambda \varepsilon_c(s) \tag{6}$$

with λ as the regularization parameter.

The other adjustable parameter, the resolution level, has a direct influence on the network performance, since the number of scale functions defined in the domain more parameters should be estimated, consequently increasing the possibility of numeric error. The evaluation of the results generated by the neural network was based on four parameters: quadratic average error values, maximum error, correlation coefficient and computational time, that is, CPU time.

2.2 Startup procedure

The startup procedure in the distillation column followed an event sequence: reboiler startup, feeding valve startup and modification of the infinite reflux rate for the operation value. It was considered that the column heated at a predetermined temperature of 25°C, the tray has a 10% holdup, condenser and reboiler with a level at 50%. The tray composition was considered as being the same for the feeding flow. With this procedure no overflow problem has been observed neither has the column exhaustion. The event sequence hasn't brought any numeric problems to the model resolution.

3. Results

A distillation column sensitiveness analysis has been carried out in order to observe the variables of greatest impact on the desired composition profiles. The size of the data set selected for training and testing followed the recommendation of Pinheiro (1996) whose proportion is respectively 70% and 30% of the set. The results obtained by the simulation of a 5 tray, binary column (n-butane and n-pentane) were presented, whose feeding tray is the number 4. The flow gets in as saturated liquid and the column operates at atmospheric pressure.

3.1 Estimation of concentration in the top stream

Several tests have been carried out in order to select the variables that generate the best predictions of top composition. It is probable that the influence of the disturbance on the reflux rate is adequately quantified through the temperature measurement on the tray 2, rate by which the results were better. As it gets away from the top of the column, the influence of the reflux rate variation becomes less intense, not aggregating any improvements in the results of prediction and inclusion of new measurements as the network inlet variables. Figure 2 shows the results of the tests carried out in the neural network after it is worked out and validated.

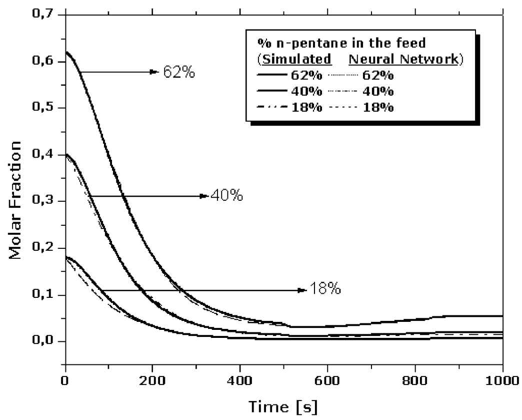

Figure 2 *– Results obtained by simulation and the network to predict the n-pentane composition in the top stream*

From the observation of the figure 2, it is observed a qualitative and quantitative agreement of the resulted obtained by the neural network. By calculating the absolute error errors in the order of 0,006% are obtained.

3.2 Estimation of concentration in the bottom stream

The tests have shown that only temperature measurements weren't enough for an adequate prediction of the bottom stream. The need for the inclusion of an auxiliary variable was observed. The same way that the temperature measurements were used by the readiness of online measuring, the choice for the auxiliary variable, essential for the case of the bottom composition prediction, has also considered the availability and the readiness of the measuring.

The many tests carried out have shown that temperature measurement on the tray 6 and the inclusion of the reboiler load measurement as an auxiliary variable generated the best results. Figure 3 shows the results found during the validation of the neural network.

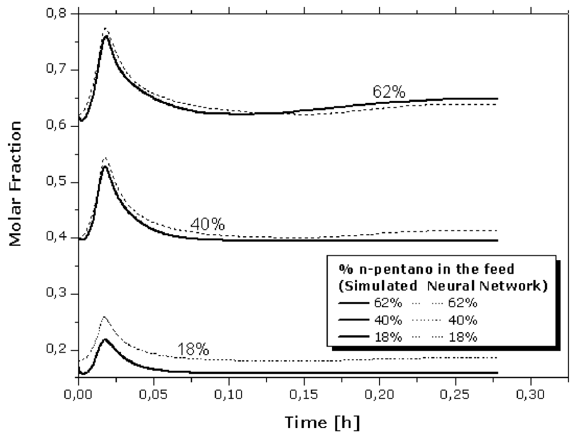

Figure 3*– Results obtained by simulation and the network to predict the n-pentane composition in the bottom stream*

A greater difficulty in carrying out the composition prediction of the column bottom stream. According to Lang and Gilles (1990) it is about the region of greatest mass transfer in the column, fact that can make only the measurement of the temperature an insufficient data to predict the composition. It is also a region strongly influenced by variations in the reboiler load and the feeding conditions, one more time being a region that needs more information of the process to predict the composition.

4 Conclusions

The proposed soft-sensor, represented by a wavelet neural network was able to predict, within the desired precision, the variables of interest during the startup procedure. With the sensor tested and validated it is possible to make available the variable values for a control system and in this sense, to minimize the transient time of the startup procedure. Thus, this work presents a robust tool, of simple usage and able to increase the set of mathematic solutions whose main goal is to minimize the problems caused by the column startup.

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