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Change Detection in a Distillation Column Based on the Generalized Likelihood Ratio Approach

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Abstract

With increasing demands for efficiency, product quality, reliability and process safety, the field of fault detection (FD) plays an important role in chemical industries. This paper deals with a FD method based on the combination of Generalized Likelihood Ration Test (GLRT) and Artificial Neural Networks (ANNs). A reliable neural model in normal conditions, under all regimes (i.e. steady-state and dynamic conditions), is found by means of a NARX (Nonlinear Auto-Regressive with eXogenous input) model and by an experimental design. The efficiency of the combination of these two approaches used for detecting faults has been tested under real anomalous conditions on a real plant as a distillation column. From the experimental results, it is observed that the proposed FD is able to detect the process status effectively.

Keywords: Fault detection; Reliability; Safety; GLRT, ANNs; Distillation column

Introduction

Early detection of occurrence of an abnormal event, fault or failure in an operating plant is vital for ensuring plant safety and maintaining product quality in chemical industries. The necessity to improve FD methods is further underlined by the finding that about 70% of industrial accidents are caused by human errors [1]. Traditionally, the most usually implemented FD methods have been based on model-based approaches. However, in modern process industry, there is a demand for data-based methods because of the complexity and the limited availability of the nonlinear models in chemical units.

Artificial Neural Networks (ANNs) have an adaptive behavior i.e. they are able to adjust and to modify their behavior according to nonlinear dynamics of processes. ANNs can be trained to learn new associations, complex modelling, functional dependencies and new patterns [2]. Owing to their inherent nature to model and learn complexities, ANNs have been successfully applied in medicine and biomedical studies [3]. Also they have found wide applications in various areas of chemical engineering [4,5].

This paper proposes a fault detection approach, which combines a statistical test as GLRT with ANNs to quickly detect faults in a distillation column. Firstly, this study consists to obtain a reduced and reliable model of this chemical process in steady-state and dynamic conditions. The chosen model is NARX model for forecasting the process dynamics. The performance of this neural model was then evaluated using the performance criteria. Then, the abnormal behaviour of the process is inspected when it is submitted to faults. Fault detection results show that the statistical test based on the GLRT is a powerful tool to detect changes in the behaviour of the distillation column.

This paper is organized as follows: Section 2 describes the neural training and selection of neural structure, Section 3 describes the fault detection strategy, in Section 4 the experimental set-up is introduced and presents the experimental results with the proposed FD method, and Section 5 ends the paper.

Network training modelling

In many fields, there are several models representing systems that are dominated by nonlinear characteristics. Many physical processes which have nonlinear behavior can be well represented by a polynomial representation, Volterra or Wiener series, or other nonlinear techniques. It is showed that the Autoregressive with eXternal input (ARX) model can be easily identified and outperform linear models [6]. Also, Nonlinear AutoRegressive Moving Average model with exogenous inputs (NARMAX) model [7] can provide a unified and simple representation for a wide class of discrete-time nonlinear stochastic systems. The NARMAX model is an input-output recursive model where the current output depends on lagged inputs, outputs and noise terms through a suitable nonlinear function. The simpler Nonlinear AutoRegressive with eXternal input (NARX) model is often preferred, although the absence of a disturbance model may result in bias problems i.e. a NARMAX model with the noise terms excluded. Structure determination of the NARX model is to choose sufficient and necessary terms for capturing the system dynamics. This model could represent a nonlinear model with a smaller number of parameters [4,8,9]. In this study, the effectiveness of this technique for black-box nonlinear modelling is described.

The ANN propagates the error from the output layer (y_i) to the hidden layer to update the weight matrix (w_i). Each node produces an output signal, which is a function of the sum of its inputs where *y(k)* is the Auto-Regressive (AR) variable or system output; *u(k)* is the eXogenous (X) variable or system inputs:

$$y_i = \phi_{ANN}(\sum x_i w_i) \tag{1}$$

Where $\varphi_{ANN}(\cdot)$ is the activation function. In this study, the neural model is defined as follows

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(10,11):

$$y_i = \phi_{ANN}(y(t-1),...,y(t-n_y), \\ u_i(t-n_k),...,u_i(t-n_k-n_u)) \quad 1 \le i \le m \tag{2}$$

where y(k) is the Auto-Regressive (AR) variable or system output; u(k) is the eXogenous (X) variable or system input. ny and nu are the AR and X orders, respectively. m is the number of the used inputs. nk is the time delay between u and y.

For smaller number of hidden layers and nodes, the performance of the ANN may not be satisfactory, while with too many hidden nodes, there is the risk of over-fitting the training data. In this case, the ANN generalization on the new data is poor. Different methods, both heuristic and systematic, can be chosen in order to select the number of hidden layers and the nodes. There are a large number of selection methods of the ANN. Two most popular ways of significant structures are in general used. We start with a small number of nodes in the hidden layer and add new ones when a certain criterion is met (growing algorithms). On the other hand, we can start with a large number of nodes and delete some of them under certain conditions (pruning algorithms).

In this study, the hidden layer nodes have log-sigmoid transfer hyperbolic function as the activation function and the output have linear activation function. The ANN multi-layer feed forward network is trained to capture the underlying relationship between the input *u(k)* and output *y(k)* using the training data. The input data are presented to the network via the input layer. These data are propagated through the network to the output layer to obtain the network output. The network error (generally the mean square error function) is then determined by comparing the network output with the actual output. If the error is not smaller than a desired performance, the weights are adjusted and the training data are presented to the network again to determine a new network error. The aim of this step is to find the appropriate weights which minimize the cost function. This is usually done using an iterative procedure. One of the best known learning mechanisms for neural networks is the training algorithm of Levenberg-Marquardt [12], which is used along with back-propagation (BP). In this case the ANN is trained iteratively using the training dataset to minimize the performance function of mean square error (MSE) between the network outputs and the corresponding target values. The Levenberg-Marquardt Algorithm (LMA) shows the fastest convergence during the training process based on gradient descent methods because it performs as a compromise between the stability of the first-order optimization methods (steepest-descent method) and the fast convergence properties of the second-order optimization methods (Gauss-Newton method). In many cases, LMA is able to obtain lower mean square errors than any of the other algorithms [12]. For weights initialization, the Nguyen- Widrow initialization method [13] is best suited for the use with the sigmoid/linear network which is often used for function approximation. After training, the networks thus developed are tested with the test data set to assess the generalization capability of each developed network. The best ANN model developed is trained off-line and then used on-line for detecting faults in the separation unit. All computations have been made on Matlab® 7.0.4.

Fault detection method: GLRT

GLR test is applied in order to establish an adaptive system, which achieves three important operations; fault detection, estimation and magnitude compensation of jumps generated by instantaneous changes of the process. GLRT is used for fault detection in signals and dynamic systems [14], geophysical signal segmentation [13], signals, incident fault detection on freeways [16], missiles trajectory [17], changes detection issue in a stochastic system [18]. Nikiforov [19] used GLRT when the model parameters after the change are unknown. He introduced an alternative approach to reduce the computational burden of the GR scheme. The idea of this solution is to decompose a given parameter space into several sub-sets so chosen that in each subset the fault detection problem can be solved with loss of a small part of optimalit y by a recursive change detection algorithm. This test is also proposed for estimating the time instant of muscle contraction onset via electromyographic (EMG) signal processing [20]. The proposed algorithm proves to be reasonably accurate even for low levels of EMG activity; the improved behavior of the GLRT comes with just a modest increase in the computational complexity. Keller et al. [21] developed a new GLRT based method for detecting, identifying, and estimating gross errors in steady state processes. This method improves GLRT and can be applied to all types of gross errors including leaks and biases. Boukai [22] used the GLRT to detect a local shift of parameter of a distribution function occurring at unknown point of time between consecutive independent observations. Three parametric models of distributions are considered; the one parameter exponential family, the location parameter family and the scale parameter family. The class of considered tests is based on GLRTs, appropriately adapted for such a change-point problem. Asymptotic techniques are used to obtain the limiting distribution of the test statistics, under both the null hypothesis of no change and the change-point alternative. Micera et al. [23] utilized a hybrid approach to EMG pattern analysis for classification of movements. The hybrid model included GLRT and the principal component analysis. They show that the classification method classify correctly all patterns related to the selected movements. Kay et al. [24] derived a GLRT detector for the detection of a sinusoid in complex environment where the noise variance and the signal amplitude, phase and frequency are all unknown. They derived a detector that gives an upper performance bound for the GLRT applied to this problem.

In this study, the recursive algorithm of the GLRT is established according to normal conditions of the operating plant (null hypothesis) vs. an alternate hypothesis. This letter is normally distributed (where variance (σ^2) is unknown). The problem is described in terms of a hypothesis test H_0, with the null hypothesis denoted by with plant behaviour belonging to the normal region Ω_0, and the alternate hypothesis H_1 denoted by with this behaviour belonging to Ω_1. One way to distinguish between these two hypotheses is to build the likelihood ratio test where $P(l \le \lambda / H_0 \text{ is true}) = \alpha$. The main aim is to detect a change in the behaviour of a conditional probability distribution (P_0), from the known value of the parameter (θ_0) to the unknown value (θ_1) which occurs at an unknown time of fault (t_f). The detection rule of GLRT is defined as following:

$$lk - \max_{1 \le j \le k} \sup_{\theta_1} \sum_{i=j}^{k} \log\left(\frac{P_{\theta_1}(\gamma_i)}{P_{\theta o}(\gamma_i)}\right) \tag{3}$$

With $t_f = \min(k: k \ge \alpha)$

In the case of the Equ 2, the GLRT test rule is given as follows:

$$lk - \max_{1 \le j \le k} \sup_{\theta_1} \left[\frac{1}{2}\log(\sigma_0^2 / \sigma_1^2) + \frac{(\gamma_i^o)^2}{2\sigma_0^2} - \frac{(\gamma_i^1)^2}{2\sigma_1^2}\right] \tag{4}$$

where $\gamma(k) = y(k) - y^{\wedge}(k)$ is the sequence of the residuals between the actual and predicted output of the system. During a normal operation, innovations fluctuation $\gamma(k) = y(k) - y^{\wedge}(k)$ is low and corresponding to random variations in measurements. Moreover, when a fault occurs, the innovation evolves differently according to the type of fault and its influence on the general state of the plant. In order to limit the computing time, it is decided to detect changes in a window of fixed size (*M*). The window size is chosen according to the process dynamics,GLRT sensitivity, and to the delay in detection.

Experimental Results

Experimental set-up

The proposed FD scheme is applied to a distillation unit. The feed tank contains a mixture to be separated (toluene-methylcyclohexane) with amass composition at 23% in methylcyclohexane. The operation in continuous mode involves charging the still with the mixture to be separated, bringing the column to equilibrium under total reflux. The product is introduced through the optimal feed tray so that the light components are volatilized, while the heavy part goes down again with the reflux in the column reboiler. The quality of the collected top product of the column depends on the reflux flow rate. The reflux ratio is varied through the magnetic valve by changing the relative quantities of material returning to the column and flowing to product storage. Feed preheating system is constituted by three elements of 250 W each one. In addition it has a low liquid level switch in order to avoid the running if the level is excessively low. The reciprocating feed pump is constituted by a membrane allowing firstly the suction of the mixture and the discharge towards the tank with a flow capacity F = 4.32 L.h-1. The column has also a reboiler of 2 liters hold-up capacity, an immersion heater of a power Qb = 3.3 kW and of a level liquid switch sensor which allows the automatic stop of heating if the level is insufficient. The column can be used in atmospheric (Patm) or in vacuum conditions (Pr). The stirring of the mixture in the reboiler is ensured by the boiling mixture. The internal packing is made of Multiknit stainless 316L which enhances the mass transfer between the vapor and liquid phases. In order to approach the adiabatic conditions, a heat-insulating made of glass wool is laid around the column. A condenser is placed at the column overhead in order to condense the entire vapor coming out from the column. The cooling (Q_c) used in exchangers is water. The heat transfer area of the total overhead condenser is 0.08 m^2. Moreover the reflux timer (R_t) allows to control the reflux ratio (R_r). It is monitored by the overhead product temperature (T_d). When the required distillate temperature (T_d) is attained, the reflux timer opens. In the opposite case, it remains closed. Distillation supervision control system allows to modify the parameters and to follow their evolution such as the pressure drop (ΔP), the flow or the temperatures at different points of the distillation column. This control system, therefore, must hold product compositions as near the set points as possible. The thermocouples are coupled to a calibrated amplification circuit (4-20 mA, 0-150°C) whose signals are inputted to the computer on-line, which permits the bottom and top temperatures to be obtained. The unit has twelve sensors which measure continuously the temperature throughout the column.

Selection of the reliable and reduced structure of the ANN model

For ANNs learning, it is very important to appropriately choose the input and output variables, determination of the relative importance of inputs and time delay [25]. For the experimental application as this used distillation column, it is often faced with the challenge of pre-processing a huge set of possible inputs. However, many variables possess redundant information and not all variables are relevant or even necessary. The strategy adopted here is the most relevant input variables are those preferentially define the most influential rules appearing in the model. For this reason, each input variable is modified and the variation relevance on the output variables is examined. It has to be bear in mind that this analysis of the relative importance is based on an experimental work but it takes the real physical nature into account as well. This analysis is based mainly on the physical knowledge of the industrial processes. The fact of changing an input and only one allows to visually observing the delay between this input and the outputs of the process. If the delay exists, therefore there is dependence between this input and the observed output. Otherwise, there is no correlation between these quantities. For this particular reason, the distillation unit operates at T_d = 95°C from the isobar diagram of the toluene-methylcyclohexane by using the Wilson thermo-dynamic model for vapor-liquid equilibrium (VLE). In order to define this nominal mode, all the regulation systems of the column are put in a closed-loop configuration. When the steady-state regime is achieved, the column was operated for approximately four hours in steady-state mode (T_d = 95°C) in order to collect a sufficient number of data. The data are taken every 11 s. The set of the most important measurable variables of the process are (R_t, Q_b, P_r, ΔP, Q_f, T_f, F, Q_c). Amongst the remaining variables, an experimental analysis of the process is carried out in order to observe the influence of each input variable on the output variables. This analysis aims at reducing more the system. Table 1 gives the values of the measurable variables calculated on average from the nominal steady-state regime.

Influence of all input variables

This part summarizes the experimental variation of all inputs as seen previously in 4.2. Table 2 collects the mean time delay measured between each input variable and the output variable [25]. The lower time delay is, the higher the relative importance is, because if a variation of the input variable occurs the output variable would be disturbed afterwards a time delay. On another side, it is important to highlight that the time delay between the reflux timer and the distillate temperature is 44 s. The feed flow rate has an influence on (T_d); however the response of this temperature is especially low to a feed variation (210.6 s). Therefore, the feed flow rate has less influence on (T_d) than the other input variables. When a time delay is called infinite (represented by "∞"), it means that there is no influence of the input variable upon the output variables.

Pattern generation

This study aims at modelling the overhead product temperature (T_d) according to the input variables of the process such as ΔP, R_t, Q_b, Q_f, Q_c, T_f, P_r and F. To have this database which is rich in amplitudes and in frequencies, the column behaviour is modified in both in a steady- state and dynamics conditions in the chosen temperature range (T_d = 93.4 → T_d = 95.9°C).

The test data are a set of independent data used to verify the consistency of the efficiency of the model. For more legibility of figures, the parameters of the distillation column are represented in Figures 1 and 2. The operation duration of the distillation column is 12 hours continuously.

Data normalization

To maintain the influence of smaller data values in comparison to higher input values, the generated experimental data are no-directly introduced in the network as training patterns. For this reason, the

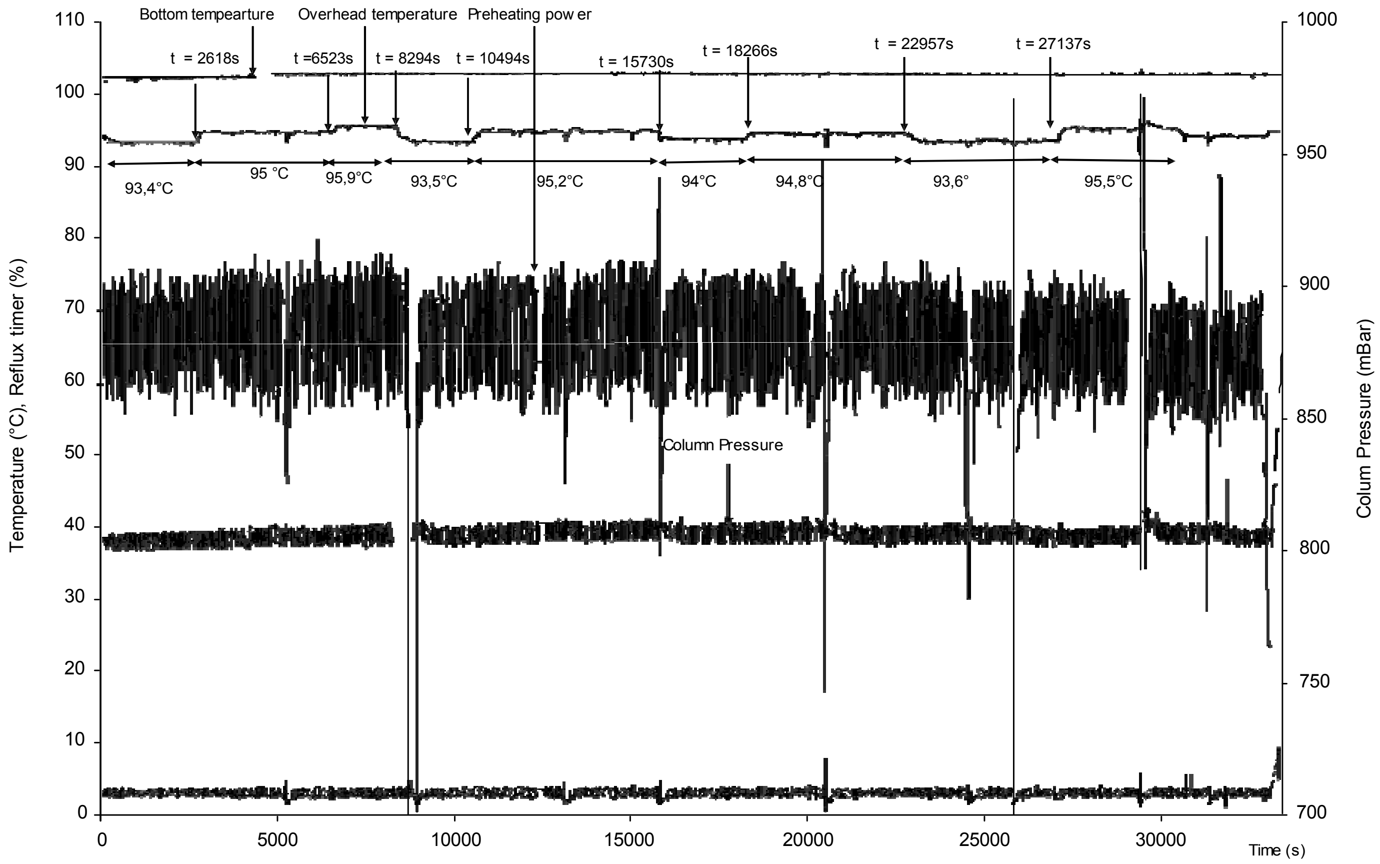

Figure 1: The operating conditions of the nominal steady-state regime.

experimental data are normalized before being presented to the ANN which gives equal priority to all the inputs variables. In our study, data normalization compresses the range of training data between 0.1 and 0.9.

Reliability of modelling of the overhead product temperature (T_d)

The number of nodes in the input and the output layers depend on the number of input and output variables, respectively. In this study, the adopted strategy is chosen as follows; the initial model has a low number of parameters and hidden nodes were gradually added during learning until the optimal result is achieved in the test subset. In the present work, the number of hidden nodes was modified from 1 to 12. Also, one hidden layer was used. The complete training process of networks took approximately 80,000 epochs using the Levenberg-Marquardt algorithm. In this case, the model composed by the set of inputs (ΔP, R_t, Q_b, Q_f, Q_f, T_f, P_r and F) and the output (T_d) is reduced according the equation 2 and tables 1 and 2.

$$T_d(t) = \varphi\,(T_d(t-1), T_f(t-3), R_t(t-4), \Delta P(t-8), Q_t(t-8)) \qquad (13)$$

The difficult trade-off between model accuracy and complexity can be clarified be clarified by using model parsimony indices from linear estimation theory (Ljung, 1999) such as Akaike's Information Criterion (AIC), Final Prediction Error (FPE) and Bayesian Information Criterion(BIC). A strict application of the indices would select a number Nh=5 because it exhibits the lowest of three indices for all the model structures compared. In conclusion, the developed network architecture used consisted of 5 nodes in the input layer and 5 nodes for the hidden layer. This reduced neural model is considered as a reliable one for describing the dynamic behaviour of the studied distillation column. In conclusion, the identified model is reduced from a (9-9-1) neural structure to (5-5-1)

Application of the developed fault detection

Once the identified ANN is trained and tested, it is ready for detecting faults. This neural model developed in part 4.5. is used both for the prediction and the FD procedure using the analysis of residuals. The proposed method is based on the GLRT as described in Section 3. This test should be processed to detect any real fault condition, rejecting any false alarms caused by noise. In this section, the proposed FD is applied to an experimental fault to verify its workability and effectiveness under real measurement conditions.

Statistics concerning the incidents which occurred in the distillation column showed that the most frequent faults are due to an inadequate heating power, feed pump, feed preheating, reflux or pressure used in the column. Consequently, the choice was carried out on this type of faults. To illustrate the adopted approach for the fault detection, it was decided to attempt among these faults to detect a sudden closing of the reflux timer (R_t=0%). This fault is frequent in the distillation operation and introduces a large deviation in comparison with the normal behaviour. It is important to notice that this fault occurs at 8173 s causes a large decrease of the overheat temperature (T_d). This evolution is showed in Figure 4.

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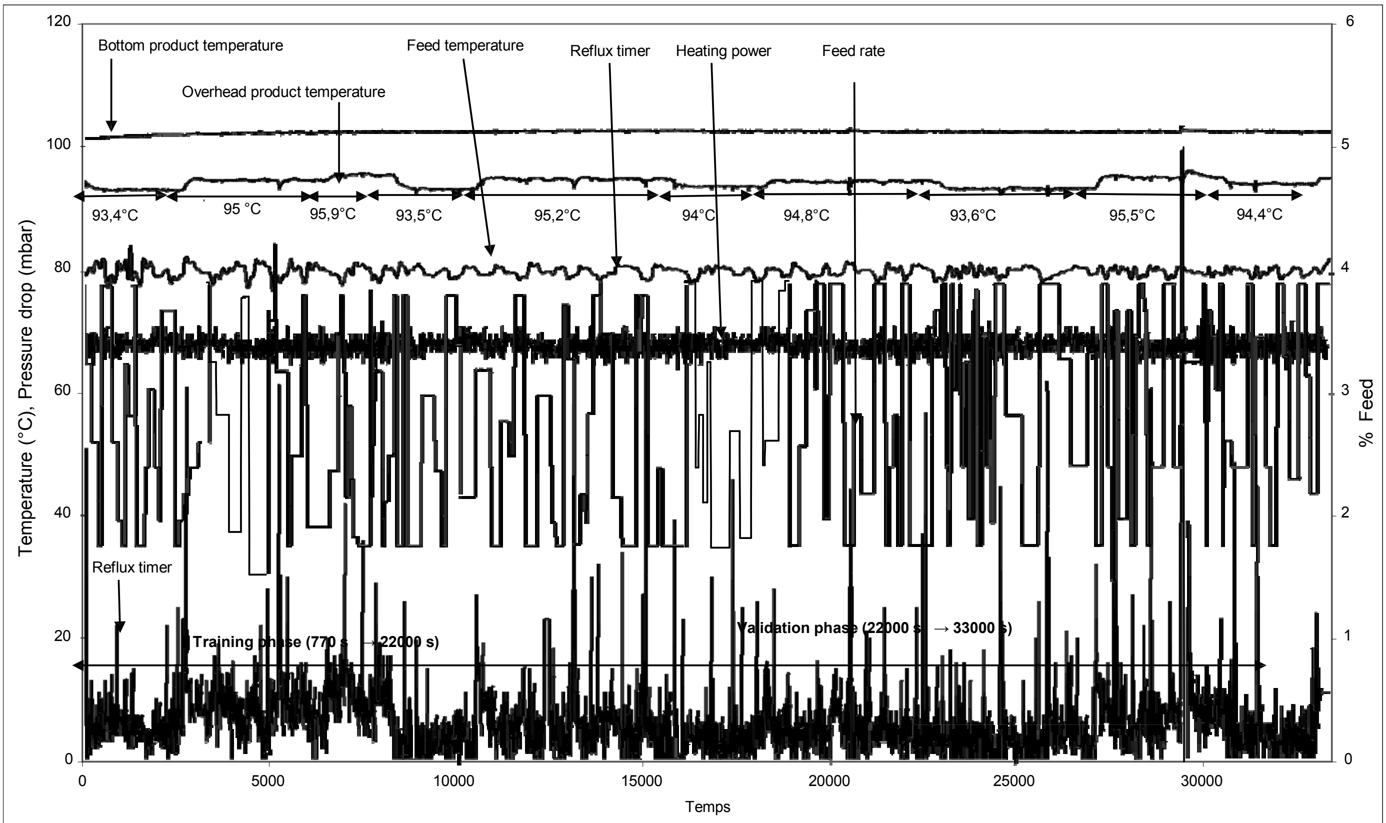

Figure 2: Mean time delay (seconds) between input and output variables.

Rt	*Qb*	*Tf*	*Td*	*F*	*Qc*	ΔP	*Pr*	*xb*	*xF*	*Qf*
7 %	68 %	80.1 °C	95.15 °C	80 %	250 $L.h^{-1}$	3.02 mbar	800 mbar	0.25 [-]	0.25 [-]	16 %

Table 1: The operating conditions of the nominal steady-state regime.

Input / Output	*Rt*	*Qb*	Δ*P*	*Qf*	*Tf*	*F*	*Qc*
Td	44	104.5	93.5	95.3	29.3	201.6	∞

Table 2: Mean time delay (seconds) between input and output variables.

This decrease should be detected by the GLRT because it exceeds a statistical threshold (3.841). The statistical threshold of decision is chosen according to the physical description of the process. It considers the different noises resulting from the process and the imperfections. Of its modeling. Indeed, it must be chosen too high in order to avoid generating false alarms due to the variations of the measurement equipment. By analyzing the various rates of false alarms probability, a rate of 5% represents a good threshold of decision. This statistical acceptance threshold is shown clearly in Figure 5 which represents the evolution of the GLRT. The size of the window is chosen according to the system dynamics. The analysis of the GLRT algorithm shows that the size value M =10 is a judicious compromise between the process dynamics, the delay time in detection and the GLRT sensitivity.

Figure 5 shows two operating zones: a fault region and a confidence one. It is important to notice that the fault which occurs at 8173 s, is detected at 8195 s i.e. with a delay of 33 s which corresponds to a difference ($\Delta T \approx 0.5°C$) between the temperature of the desired overhead temperature (T_d =95°C) and the fault one (T_d =94.5°C). This delay in detection defined as the difference between the time of the fault occurrence and the time of its detection, depends essentially on the evolution of the process dynamics.

Conclusion

Faults that change the system dynamics by causing surges of drifts of components, abnormal measurements, sudden shifts in the measurement channel, and other difficulties such as the decrease of instrument accuracy, an increase of background noise, reduction in actuator effectiveness etc., effect the characteristics of the likelihood ratio. This study shows that the combination of the ANN and the GLRT solves efficiently the FD problem. The experimental results show that the one-layer perceptron network provides promising assignments

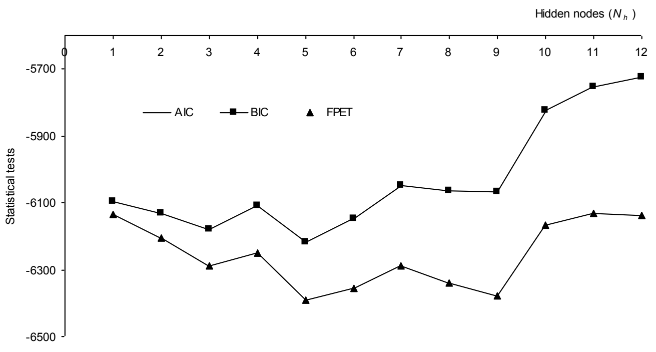

Figure 3: Evolution of the statistical criteria.

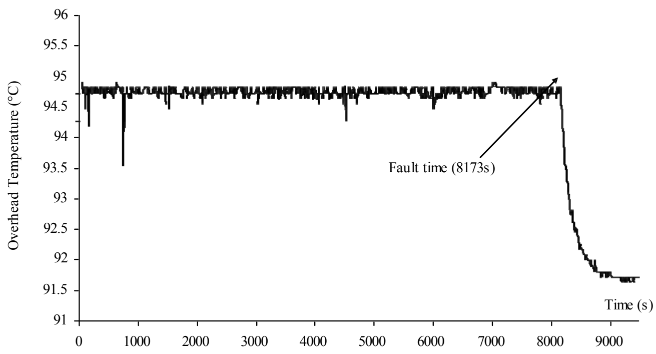

Figure 4: Evolution of the overheat temperature (*Td*) caused by the chosen fault.

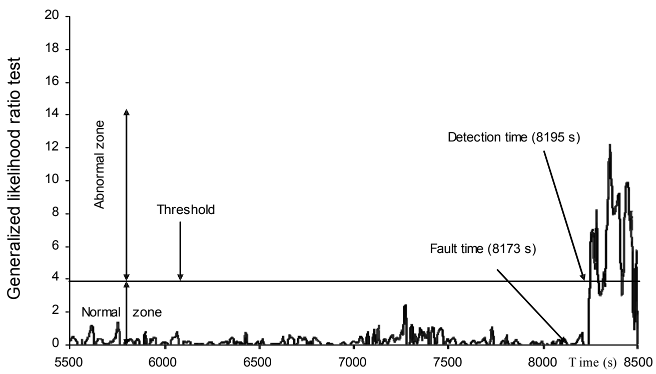

Figure 5: Fault detection test based on GLRT.

to normal and faulty states of the investigated reference process. The dedicated example indicates the strength of the proposed approach for reliability of models, prediction of the future data and fault detection. It makes this combination very attractive for solving the modelling issues and fault detection in real time operation of complex plants as a distillation column. GLRT is used to advise the operator of an abnormal behavior of the process by setting-on the suitable alarm. Such alarm could be used in order to initiate the back-up procedure, to stop the operating plant or even to begin the diagnosis algorithm of the fault physical origin.

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