Results and discussion

The aim of this chapter is to demonstrate the ability of the proposed FDS to diagnose in a variety of scenarios, to discuss and compare the results obtained in each case, and also to show its potential capabilities. At the same time a step by step impolementation of the system is shown to clarify the proposed procedure.

By the different case studies already described in chapter 6, the different aspects of the proposed methodology (chapter 5) to design and implement the FDS are illustrated. The consideration of the industrial scenarios is performed in chapter 8.

In each case study, a special aspect of the methodology is highlighted and shown in detail, followed by a brief discussion of the results obtained.

7.1. Plant with recycle

First, the advantages of using a FDS consisting in a wise combination of an ANN and a FLS (subchapter 5.1.2) are shown. Then, a discussion about the election of the type of ANN is done by comparing the performance of different architectures. This comparison also contemplates the type of faults, in process or in controllers (Ruiz et al., 1999d). Finally, the special case of faults in sensors is treated by the proposed methodology (subchapter 5.4.3).

7.1.1. Implementation of the proposed combination

The step by step methodology (subchapter 5.2) has been followed. The main points of the tasks performed are summarised as follows.

Set of faults

Faults in the source of raw materials (process faults that lead to changes in the composition and in the flow rate of fresh feed) and faults in controllers have been simulated. The list of faults is presented in Table 7.1. Faults in sensors have not been considered.

Table 7.1. List of simulated faults

Fault	Nomenclature
High fresh feed flowrate (20% higher)	F1
Low fresh feed flowrate (20% lower)	F2
High fresh feed concentration of reactant A (10 % higher)	F3
Low fresh feed concentration of reactant A (10% lower)	F4
Level controller failure	F5
Composition controller failure	F6

Measurements

There are nine measured variables: reactor feed flow rate (F0) and composition (XA0), liquid volume of the reactor (VR), reactor effluent flow rate (F) and composition (XAF), recycle flowrate (D) and composition (XAD), bottom product flowrate (B) and composition (XAB).

Artificial Neural Network training

An BPN was trained with the profiles of process variables (subchapter 5.4.1). The training was performed in the following way: a change in 20% in flowrate and a change of 10% in composition are both considered to have a value of 1. The values assigned to other faults are proportional to those values. For example a decrease of 10% in the fresh feed flowrate gives a value of 0.5 to the “pre-fault” F2 *(N1(2)).* In training, it is very important a good scaling of values. Data are considered as stationary series, which means that averages and standard deviations are assumed constant. Input data are scaled by decreasing in the average and then dividing by the standard deviation.

Eight of the nine measured variables are the inputs of the perceptron multilayer (controlled variable XAB was put aside). The hidden layer has 7 neurons and the output layer has 4 neurons (the pre-faults F1, F2, F3 and F4).

The activation functions are sigmoidals in the hidden layer and linears in the output. ANN training was done using Levenberg-Marquardt backpropagation method.

As the steady state needs a long time to arrive, the ANN approach cannot diagnose some faults quickly. As an example, Figure 7.1 shows the ANN response when an increase in the fresh feed composition (Fault F3) occur at time 100.

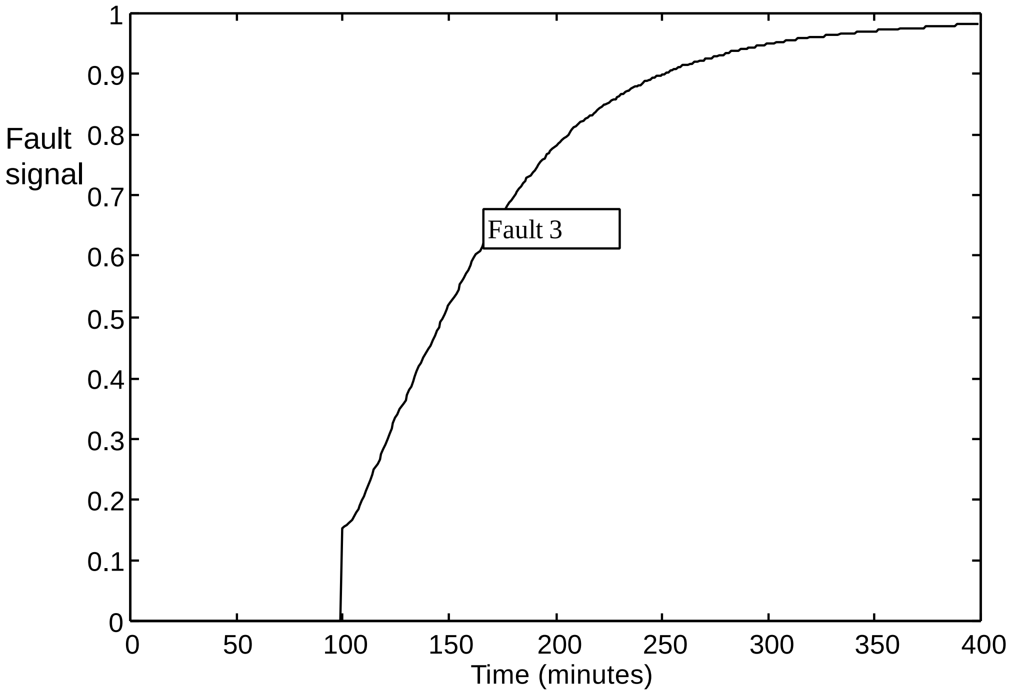


Figure 7.1. ANN approach response (Fault F3)

Fuzzy logic system

On the basis of the knowledge of the process, a set of 16 if-then rules has been defined. The inputs are some measured variables (reactor effluent flowrate *F*, holdup of the reactor *VR* and bottom product composition *XAB*, Figure 6.1) calculated variable (second derivative of *XAB*) plus the outputs of the ANN. The outputs are the six defined faults.

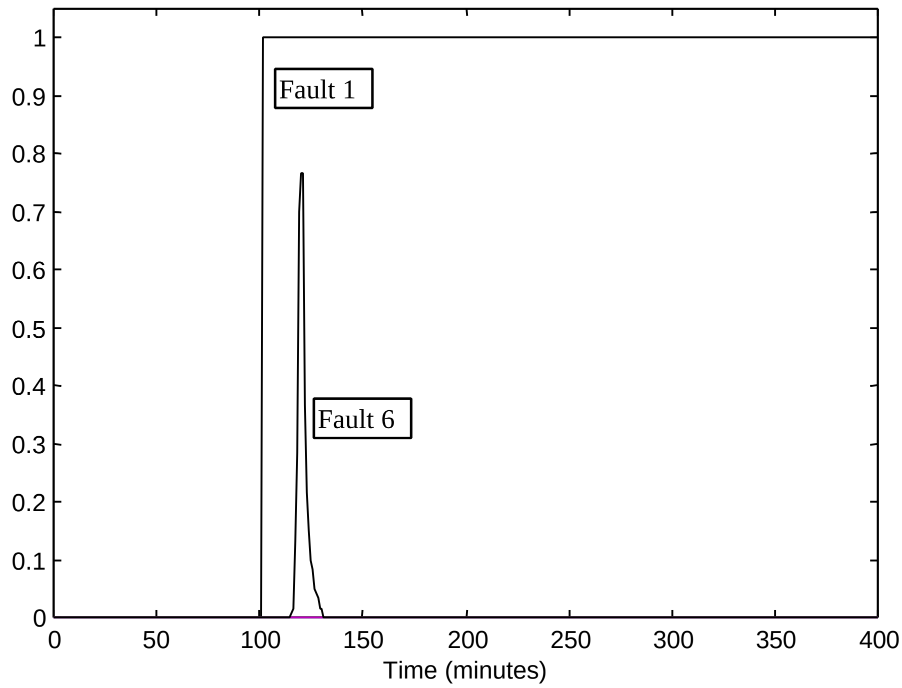


Figure 7.2. Fault Diagnosis System response (Fault F1)

Results and discussion

Figure 7.2 shows the response of the proposed neuro-fuzzy FDS when fault F1 is simulated at time 100. A fast and accurate response is observed. Between time 100 and 150, Fault F6 is suspected by the system (during this interval the composition *XAB* appears to be uncontrolled) but the failure in the controller does not exist and the system does not confirm it. A summary of the performance of the system is shown in Table 7.2. In the cases of process faults, the FDS makes the diagnosis as well as or better than the ANN approach. In addition, faults in the controllers, which are not diagnosed by the ANN, are successfully diagnosed by the FLS.

With regard to the occurrence of simultaneous faults, which the ANN approaches has problems to diagnose (Venkatasubramanian et al., 1990), the addition of rules improves the diagnosis. Only in the cases of the combination of F2-F5 and F3-F5 is there no diagnosis of the process faults (F2 and F3). In these cases the inputs are beyond the range of the ANN training, and therefore the outputs of the ANN are not taken into account by the FDS.

Calculating the average of *%P*, the ANN working alone presents 45%, the KBES: 28% and the proposed FDS: 82%. By this way, the advantages of the proposed FDS are noted more clearly.

Table 7.2. Time for diagnosis (in minutes)

Fault	I	II	III
F1	3	*	3
F2	3	*	2
F3	151	*	47
F4	15	*	1
F5	*	90	90
F6	*	33	33
F1 / F3	3 / 243	* / *	3 / 156
F2 / F4	1 / 1	* / *	1 / 1
F1 / F4	3 / 17	* / *	2 / 1
F2 / F3	3 / 3	* / *	3 / 3
F1 / F5	* / *	* / 26	7 / 26
F1 / F6	3 / *	* / 54	3 / 54
F2 / F5	* / *	* / 26	* / 26
F2 / F6	3 / *	* / 38	2 / 38
F3 / F5	* / *	* / 150	* / 150
F3 / F6	77 / *	* / 78	43 / 78
F4 / F5	* / *	* / 53	17 / 53
F4 / F6	16 / *	* / 93	2 / 93

*No diagnosis; I: ANN approach; II: KBES; III: Proposed FDS

This first attempt to test the strategy of combining an ANN and a FLS in a novel way has shown promising results. For this reason, it has been then improved and tested in batch processes as it will be shown later on.

7.1.2. *Comparison of different ANNs' performance*

In this subchapter, two supervised ANNs (BPN and RBFN) and an unsupervised one (SOM) are compared in order to evaluate the importance of the selection of the architecture of the ANN block in the FDS.

Faults in the source of raw materials (process faults that lead to changes in the composition and in the flow rate of fresh feed) and faults in controllers has been simulated.

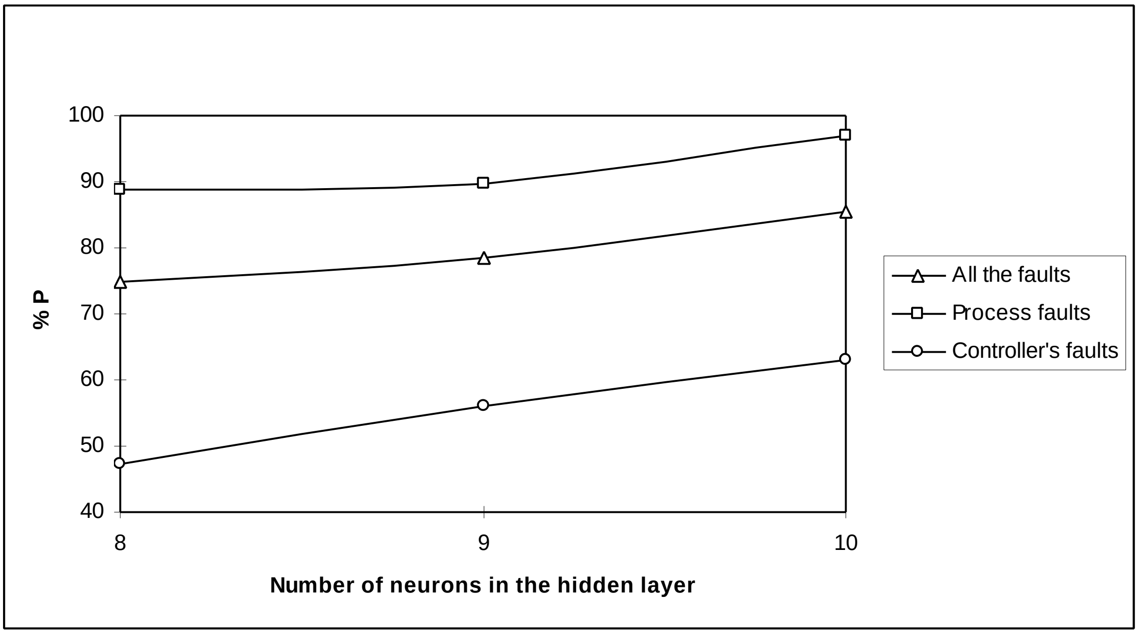
The BPNs considered have three layers. They have an input layer with as many nodes as measured variables from the plant; a hidden layer and an output layer with as many nodes as number of suspected faults. The activation function is sigmoidal in the hidden layer and linear in the output one. The number of nodes in the hidden layer has been optimized in order to find the best performance for fault diagnosis. The training algorithm was the Levenberg-Marquardt backpropagation method.

BPNs with different number of neurons in the hidden layer have been trained. Each one was tested simulating the different faults. In Figure 7.3a, the average *%P* is shown, considering process faults, controller's faults separately and all the faults.

It can be seen that the performance is increased with the number of neurons in the hidden layer. That is, faults are diagnosed quickly. One problem that BPNs have shown is the false diagnosis during the dynamic state. In Figure 7.3b it can be observed that the network shows the best results with nine neurons in the hidden layer. No cases of false diagnosis have appeared when testing the system with controller's faults. However, some cases of false diagnosis have been found in diagnosing process faults.

Some RBFNs were trained using different spreads. In Figure 7.4a it can be observed that the performance is rather low for controller's faults diagnosis and it decays with the spread. On the other hand, faults in the process are diagnosed faster with a high spread. Figure 7.4b shows that the networks do not present cases of false diagnosis with spreads equal or greater than 1. In the cases of the diagnosis of faults in controllers, RBFNs never shows cases of false diagnosis.

a)



b)

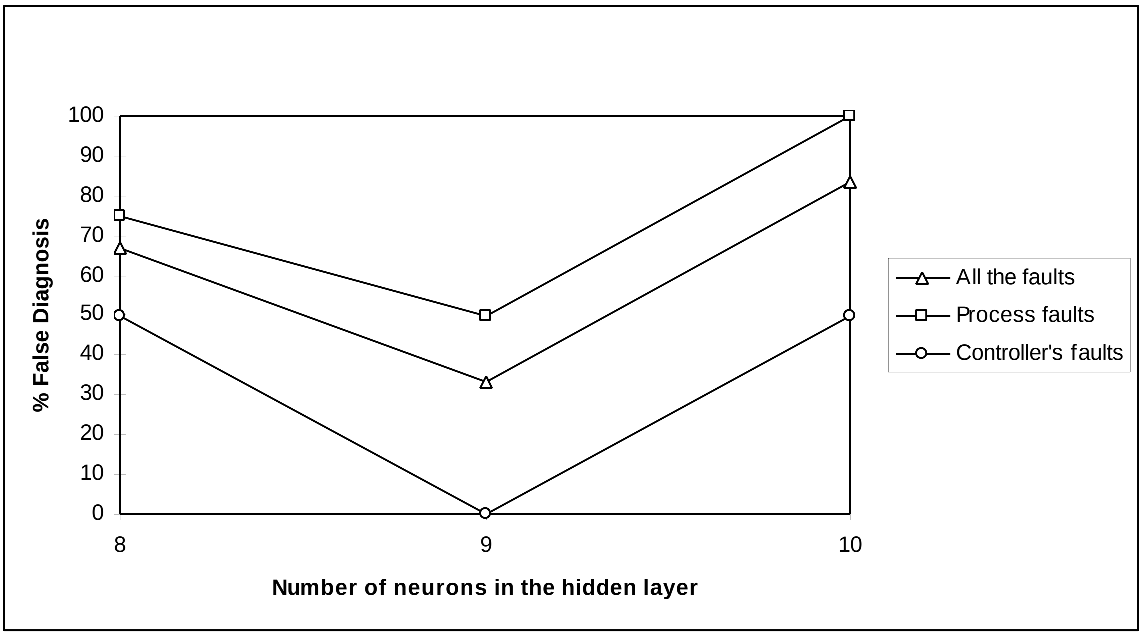
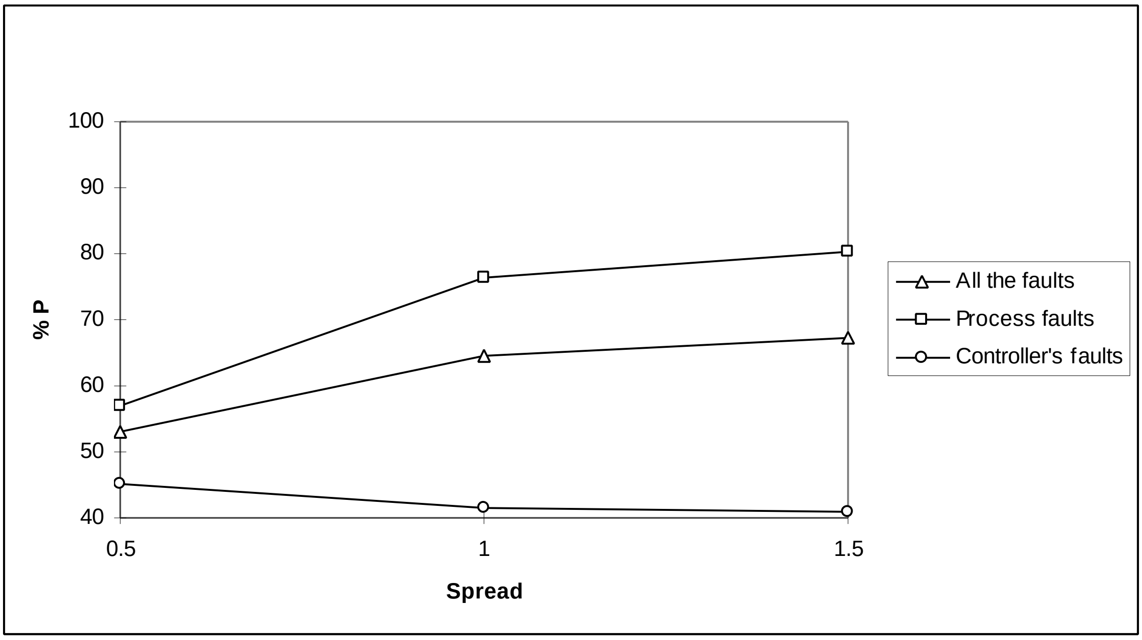


Figure 7.3. BPNs; a) Performance, b) False diagnosis

In the case of SOMs, a parameter to be optimized in this kind of networks is the number of nodes of the feature map. The training set is the same as in BPNs but without the targets.

a)



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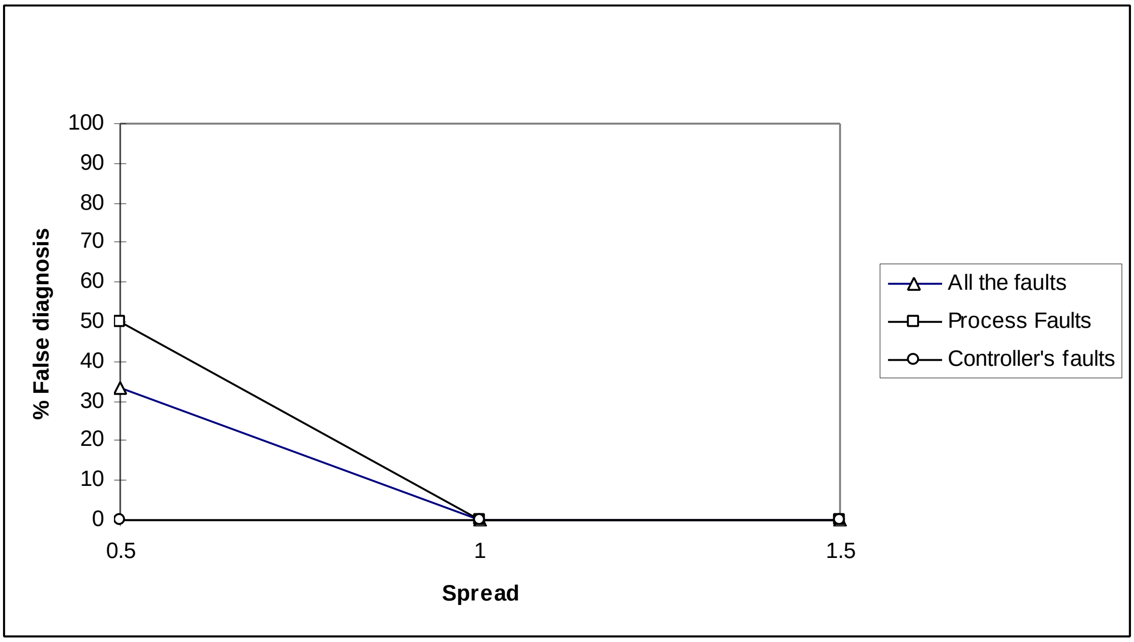
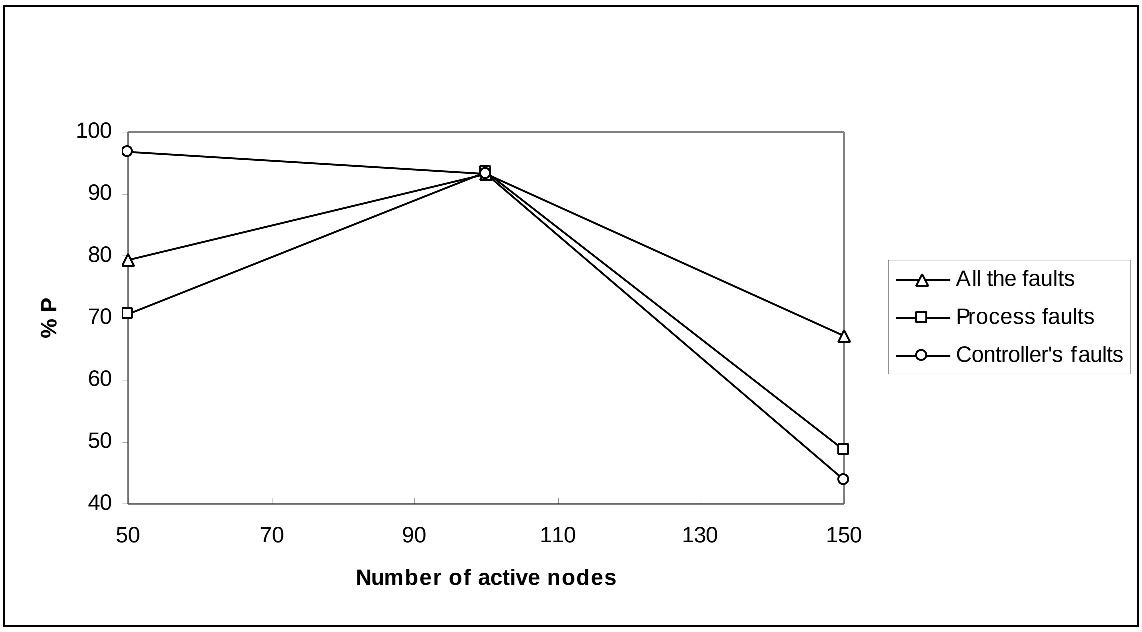


Figure 7.4. RBFNs; a) Performance, b) False diagnosis

SOMs with different number of nodes were trained. Testing results have been summarized as in the previous cases, considering an average performance. It is important to detail that SOMs do not differentiate some faults. Therefore they have low resolution. In Figure 7.5a it can be seen that a maximum performance is shown for 100 nodes for process fault diagnosis. Performance of controller fault diagnosis decays with the number of nodes. Taking into account the existence of false diagnosis, Figure 7.5b shows that there is no problem in diagnosing faults in controllers and a SOM of 100 nodes is necessary to avoid it in the diagnosis of process faults.

a)



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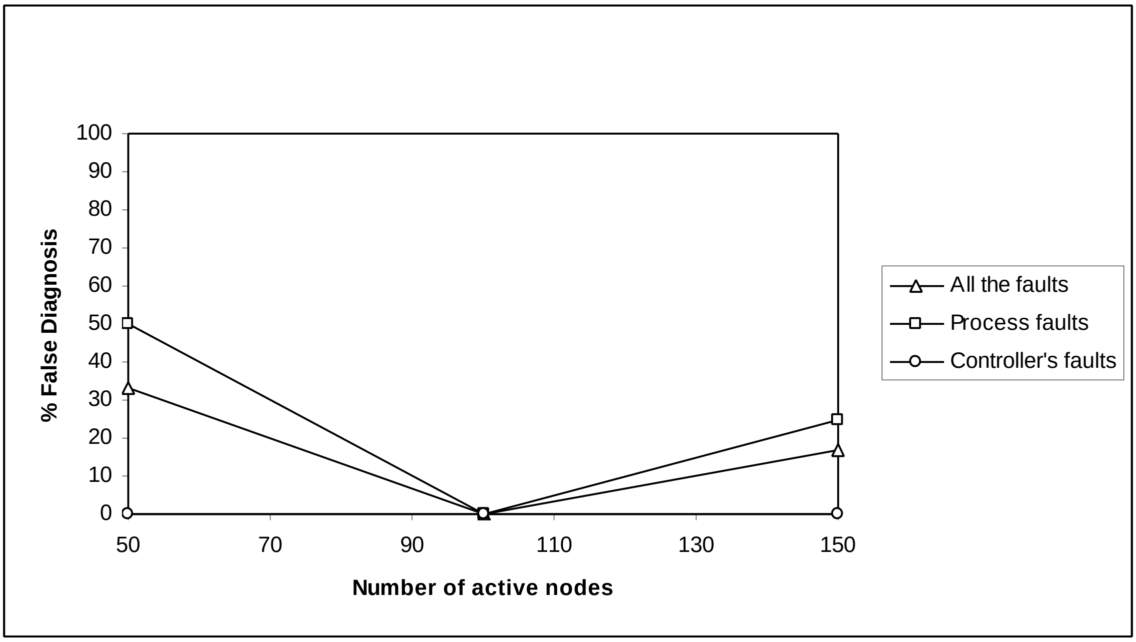


Figure 7.5. SOMs; a) Performance, b) False diagnosis

Figure 7.6 shows a comparison among the different tested ANNs using the index *%P*.* It has been considered the optimised configuration of each ANN. RBFNs have shown to be superior to the others, mainly in diagnosing process faults. In addition, BPNs have shown to be slightly better in diagnosing faults in controllers.

In summary, the use of RBFNs is recommended. However, they can present problems with high dimensional input training data (subchapter 4.1.1). SOMs have shown low resolution but they can be useful to diagnose unsuspected faults.

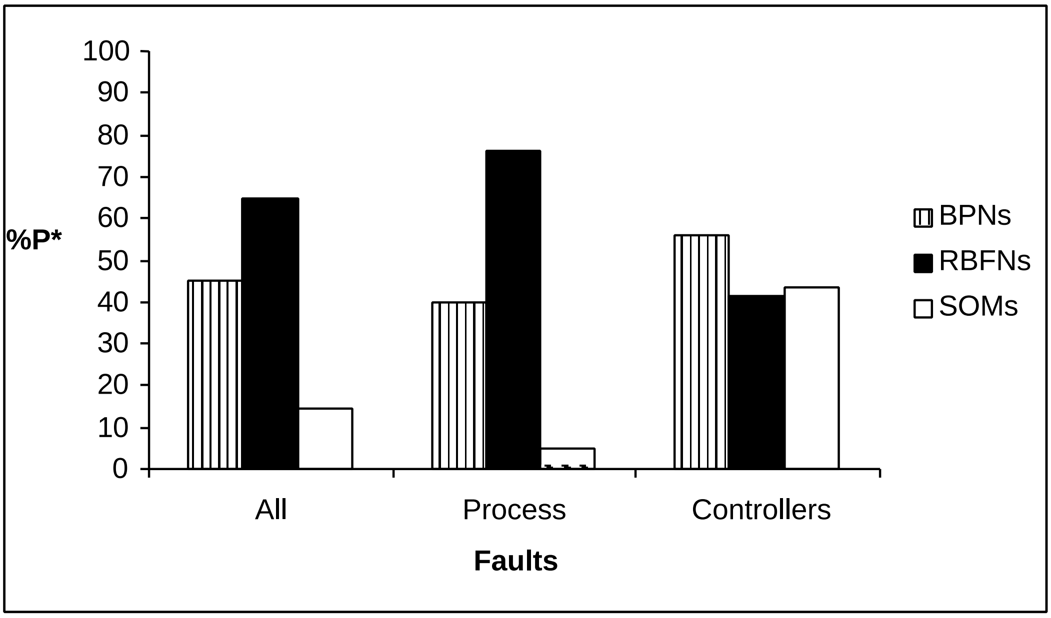


Figure 7.6. Performance of the different kinds of ANNs taking into account the false diagnosis and the resolution

7.1.3. Faults in sensors

The proposed AANN implementation for the diagnosis of faults in sensors (subchapter 5.4.3) has been tested in the plant with recycle. Bias errors in sensors have been contemplated. There are nine sensors. Their measurements in normal conditions and the bias errors considered are summarised in Table 7.3. The bias errors considered are of 50% in the cases of flowrates sensors, 25% in composition sensors and 10% in the level sensor. Big bias errors have been selected because the problem of detection of small bias errors has already been solved (Kramer, 1992; Dong and McAvoy, 1996). The reason is that the inputs are close to the input data set of AANN training in such cases.

An auto-associative neural network was trained using 40 data from normal and abnormal behavior of the process but with correct measurements. According with Equation (4.9), if *db*=3, *Ml* + *Md* << 32.6; if *db*=5, *Ml* + *Md* << 30.4 and if *db*=7, *Ml* + *Md* << 27.5 . A value of *Ml* = *Md*= 10 has been considered. The AANN has been trained using Levenverg-Marquardt backpropagation method (MSE = 0.001).

Table 7.3. Normal condition and bias errors in sensors

Sensor nº	Variable	Normal value	Bias error
1	Feed flowrate to the reactor (F0), kmol.min^{-1})	6.1	3.05
2	F0 composition, molar fraction of A (XA0)	0.64	0.16
3	Molar amount of liquid in the reactor (VAR, kmol)	750	75
4	F composition, molar fraction of A (XAF)	0.377	0.09
5	Feed flowrate to the stripper (F), kmol.min^{-1}	6.1	3.05
6	Recycle flowrate to the reactor (D), kmol.min^{-1}	4.3	2.15
7	D composition, molar fraction of A (XAD)	0.53	0.13
8	Bottom product flowrate (B), kmol.min^{-1}	1.8	0.9
9	Bottom product composition, molar fraction of A (XAB)	0.01	0.0025

By simulating the mentioned bias errors in all the sensors, interesting advantages and disadvantages of the proposed AANN implementation can be shown. The detection of a sensor fault has always been achieved. The differences appeared when the existence of cases of false diagnosis is considered. Table 7.4 shows the performance of different AANNs, each one with different number of nodes in the bottleneck layer.

Faults in flowrate sensors (sensors nº 1, 5, 6 and 8) are successfully identified by the proposed approach. The number of nodes in the bottleneck layer is not critical in these cases, except for the sensor nº6. In the case of the level sensor (sensor nº3), which is involved in a control loop, it is important to select an adequate number of nodes. Regarding with the composition sensors (sensors nº 2,4,7 and 9), some cases of no diagnosis and false diagnosis have appeared. However, it is possible to find an optimal number of nodes, except for the case of the composition sensor involved in a control loop (sensor nº 9). In the AANN training data set, the values for this sensor are very close to the set point (under normal and abnormal conditions) because it is a controlled variable. This fact is the main reason for the observed extrapolation errors. Such errors are not adequately filtered by the proposed algorithm. Therefore, the algorithm to isolate the faulty sensor should be improved for these special cases.

Table 7.4. Performance of auto-associative neural networks

Faulty sensor number	Faulty sensor number diagnosed with the following number of nodes in the AANN		
	3 nodes	5 nodes	7 nodes
1	**1**	**1**	**1**
2	4,6	**2**	4,7,8
3	4,5,6	**3**	7
4	**4**	1,**4**,5	3,6,7
5	**5**	**5**	**5**
6	2,**6**	**6**	2,3,**6**
7	1,2,5	1,5	**7**
8	**8**	**8**	**8**
9	1,2,3,5,6,8	2,4,6,7,8	1,3,5,7,8

In summary, the proposed combination of an AANN and a simple algorithm has shown to be good enough to diagnose faults in levels, flowrates and compostion sensors. Nevertheless, it may result ineffective to diagnose faults in composition sensors that are involved in control loops.

7.2. Batch Reactor

In this case study, the importance of signal pre-processing for fault pattern generation is illustrated (Chapter 5, section 5.4.2). Other important aspect also shown in this scenario is the FLS development details. The generation of if-then rules from HAZOP analysis is also discussed (Chapter 5, section 5.5.1). Then, advantages of the proposed FDS for batch process monitoring is demonstrated by its comparison against on-line MPCA (Ruiz et., 2000b). Finally, a discussion about the election of the type of FLS is done by comparing the performance of different types.

7.2.1. ANN training

The list of the suspected faults is shown in Table 7.5. These faults have been selected because they are typical abnormal situations in current industrial batch chemical reactors. The generation of patterns has been performed by pre-processing of the signals with multiscale wavelet decomposition. First, the faults at different times and with different sizes have been simulated.

Figure 7.7 shows the profiles of measured variables profiles, when Fault F2 was simulated at time 100, and when there is no fault. It can be observed the very slight difference among the profiles. The corresponding temperature and composition profiles are practically the same.

The fault patterns consist of the extrema analysis wavelet for scale 5. An eight-coefficient Daubechies wavelet has been used as a filter. Figure 7.8 shows the extrema analysis wavelets when Fault F2 was simulated at times 100 and 200 minutes with two different sizes (decrease in 50% and 25% in water flow-rate caused by a leakage in the water control valve). It can be seen how the height of the extrema are lower with lower fault sizes. Besides, the same variables presents extrema with similar patterns at different times. This feature facilitates the classification by the ANN.

The generated patterns have been used as inputs of an ANN classifier. As a target output a vector of the suspected faults has been considered. The values of 1 correspond to the fault with sizes that have been defined as unpermited deviation.

The ANN architecture used as a classifier in this study was a Probabilistic Neural Network (PNN). It is a kind of radial basis network suitable for classification problems. It has two layers (Chapter 4, section 4.1.1).

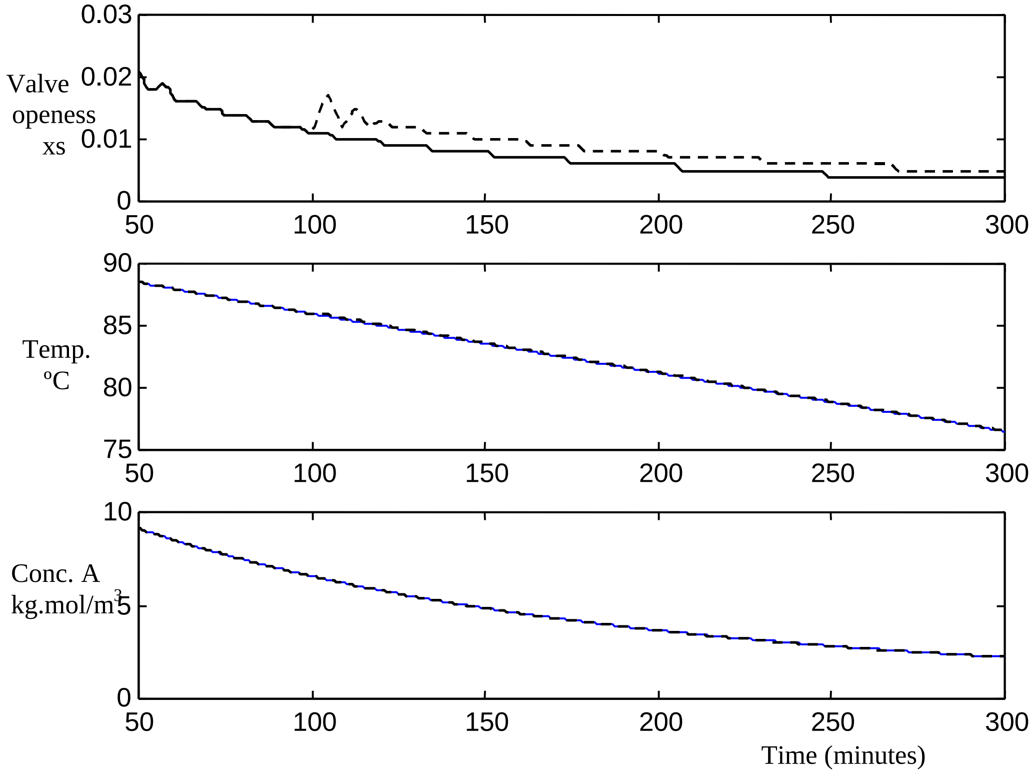
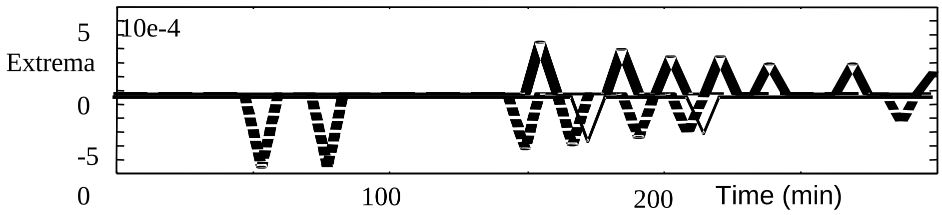


Figure 7.7. Profiles of measured variables (--- Fault F2, ——No Fault)

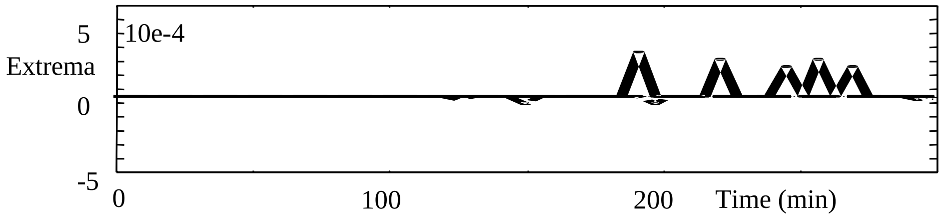
Table 7.5. List of suspected faults

Description	Nomenclature
Leaking of steam control valve	F1
Leaking of water control valve	F2
Fouling of reactor temperature probe	F3
Fouling of reactor jacket	F4
Fouling of reactor walls	F5
Incorrect master gain (higher)	F6
Incorrect slave gain (lower)	F7

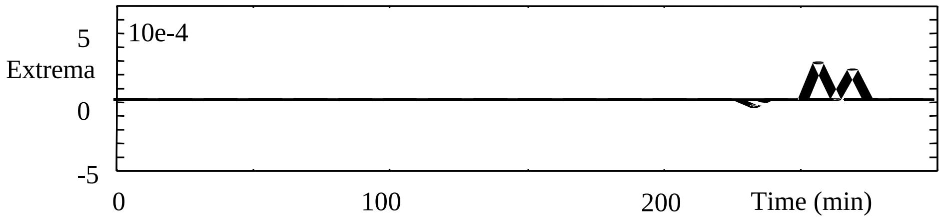
a) Fault F2, size 1, time 0 min.



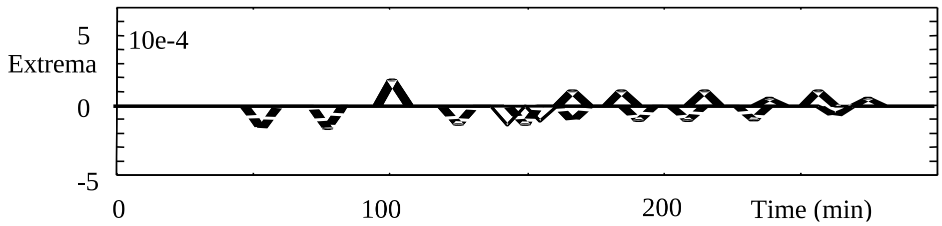
b) Fault F2, size 1, time 100 min.



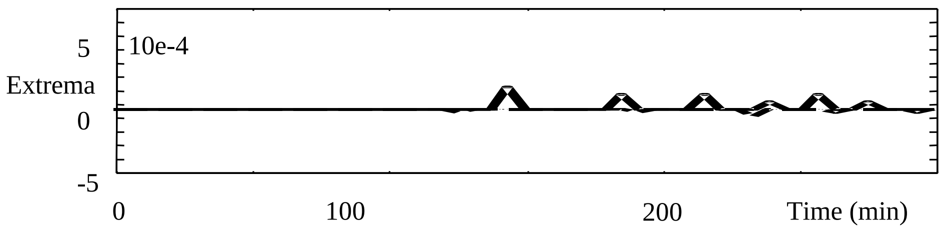
c) Fault F2, size 1, time 200 min.



d) Fault F2, size 0.5, time 0 min.



e) Fault F2, size 0.5, time 100 min.



f) Fault F2, size 0.5, time 200 min.

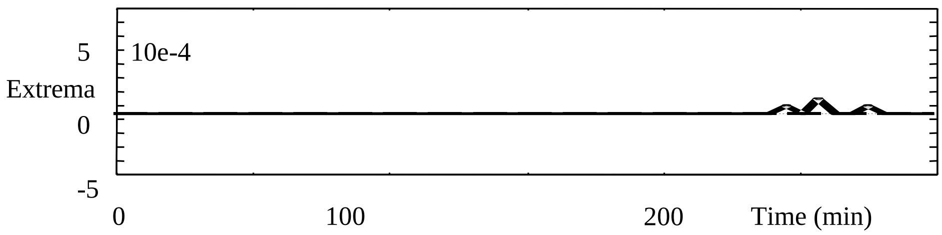


Figure 7.8. Wavelet extrema analysis of detail at scale 5; ▬▬ Water valve openesss signal (difference from reference profile); —— Water flowrate (difference from reference profile); ▬ ▬ Concentration of component A (difference from reference profile).

7.2.2. Fuzzy logic system

The set of if-then rules based on process knowledge of the operations “Reactor heating” and “Reactor cooling” are shown in Table 7.7a and 7.7b, respectively. In similar way this set of if-then rules is built for the “Reactor cooling” from the information available in the HAZOP analysis shown in Table 7.6.

Table 7.6. HAZOP analysis of two steps of the batch reactor

Stage: Reaction, Unit: Batch Reactor, Operation: Reactor heating

Node: Batch Reactor Variable: Temperature

Deviation	Causes	Consequences
High	F6	Formation of undesired product C
Low	F3, F4, F5, F7	Reaction time increased

Node: Steam line Variable: Flow

Deviation	Causes	Consequences
High	F1, F3, F4, F5	High steam consumption

Node: Steam line Variable: Steam valve openness

Deviation	Causes	Consequences
High	F1, F3, F4, F5	High steam consumption

Stage: Reaction, Unit: Batch Reactor, Operation: Reactor cooling

Node: Batch Reactor Variable: Temperature

Deviation	Causes	Consequences
High	F6	Formation of undesired product C
Low	F3, F4, F5, F7	Reaction time increased

Node: Water line Variable: Flow

Deviation	Causes	Consequences
High	F2, F3, F4, F5	High water consumption

Node: Water line Variable: Water valve openness

Deviation	Causes	Consequences
High	F2, F3, F4, F5	High water consumption

Table 7.7. Set of if-then rules based on process knowledge. a) Reactor heating operation; b) Reactor cooling operation

a) Reactor heating operation
If Reactor Temperature is High then F6 is High
If Reactor Temperature is Low then F3 is High
If Reactor Temperature is Low then F4 is High
If Reactor Temperature is Low then F5 is High
If Reactor Temperature is Low then F7 is High
If Steam Flow-rate is High then F1 is High
If Steam Flow-rate is High then F3 is High
If Steam Flow-rate is High then F4 is High
If Steam Flow-rate is High then F5 is High
If Steam valve openness is High then F1 is High
If Steam valve openness is High then F3 is High
If Steam valve openness is High then F4 is High
If Steam valve openness is High then F5 is High
a) Reactor cooling operation
If Reactor Temperature is High then F6 is High
If Reactor Temperature is Low then F3 is High
If Reactor Temperature is Low then F4 is High
If Reactor Temperature is Low then F5 is High
If Reactor Temperature is Low then F7 is High
If Water Flow-rate is High then F2 is High
If Water Flow-rate is High then F3 is High
If Water Flow-rate is High then F4 is High
If Water Flow-rate is High then F5 is High
If Water valve openness is High then F2 is High
If Water valve openness is High then F3 is High
If Water valve openness is High then F4 is High
If Water valve openness is High then F5 is High

7.2.3. Results

The proposed FDS has been tested using seven different cases corresponding to the seven suspected faults. Table 7.8 shows the list of these cases and the corresponding times required for the diagnosis by the ANN working alone and the FDS. The reference to the figures where the responses are represented is also included.

The first case corresponds to a batch with an initial problem of a leaking in the steam control valve (Figure 7.9) The ANN needs a long time to recognise the pattern. The FLS plays an important role in this case diagnosing the fault during the period of heating. In fact, as it has been explained before, there is a FLS for heating operation and other one for cooling operation. During cooling operation, the FDS response shows the existence of the fault, but with some delay. This isolation is possible due to the ANN support which recognise the pattern, according to the signal features.

The second case corresponds to a batch with a leaking in the water control valve 100 minutes after the beginning of the stage Reaction (Figure 7.10). The ANN needs some minutes to classify the fault and the FLS improves the performance of the whole FDS by diagnosing the fault very quickly. Note that the correct response of the ANN, in this case, must be a value of 0.5 according to the suspected size of the fault.

The third case corresponds to a batch with the problem of the fouling of the temperature probe (Figure 7.11). The ANN needs a long time to correctly diagnose the fault. However, the FDS diagnosed the fault quickly thanks to the FLS support.

The fourth case corresponds to the fouling of the reactor jacket (Figure 7.12). The ANN supports the FLS to maintain the fault signal at time 78. Previously, the firing of if-then rules based on process knowledge is enough to give a successful response, except for a brief period from time 70. The behaviour of process variables, according to available measurements, is not very different from normal operating conditions from that time. The signal features for this fault are recognised by the ANN at the mentioned time 78.

The fifth case corresponds to a fouling of reactor walls (Figure 7.13). The ANN delays more than fifty minutes in diagnose the fault but the FDS responds quickly. It has been observed the influence of the ANN response on the FLS again (time 50).

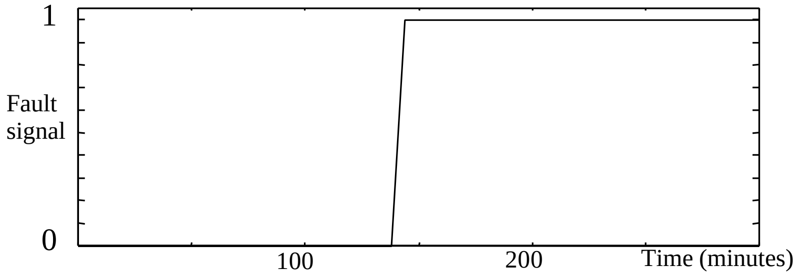
The sixth case corresponds to a fault in the control system, a higher master gain, at time 200 (Figure 7.14). The ANN classifies correctly and rapidly this fault and the FDS makes the diagnosis almost instantaneous. Note that the signal jumps before time 200 because of the discrete sample time, and the dyadic length of the window (Chapter 4, section 4.4.1) when performing on-line wavelet multiscale filtering.

The last case that has been considered corresponds to a deviation in the control system, too. In this case, a lower slave gain at time 200 (Figure 7.15). The ANN needs more time than in the previous case to diagnose the fault but the FDS shows to be very efficient again. The discrete sample time originates the jump of the signal before time 100.

Table 7.8. Cases used for testing the FDS and times for diagnosis

Case	Fig. Nº	ANN (min.)	FDS (min.)
Leaking of steam control valve (50% decrease in steam flow at 0 min; F1=1)	7.9	144	6
Leaking of water control valve (25% decrease of water flow at 100; F2=0.5)	7.10	26	2
Fouling of reactor temperature probe (F3=1 at time 0 min)	7.11	144	6
Fouling of reactor jacket (F4=1 at time 0 min)	7.12	78	6
Fouling of reactor walls (F5=1 at time 0 min)	7.13	66	6
Incorrect master gain (10 % higher at time 200)	7.14	16	4
Incorrect slave gains (50 % lower at time 100 min)	7.15	56	2

a)



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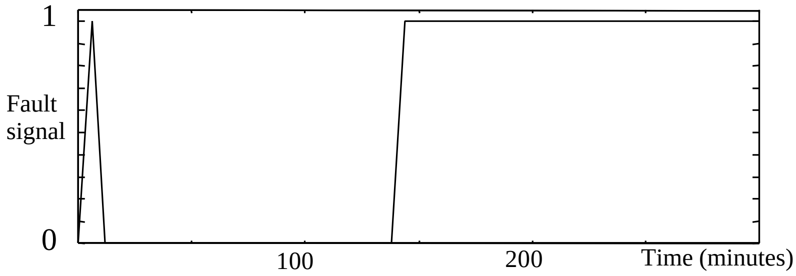
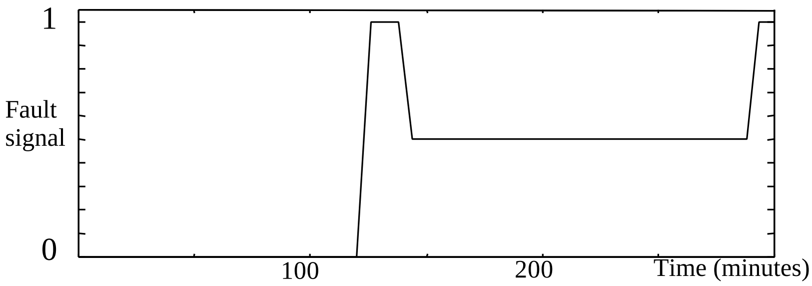


Figure 7.9. Initial steam control valve leakage, responses of a) ANN, b) FDS

a)



b)

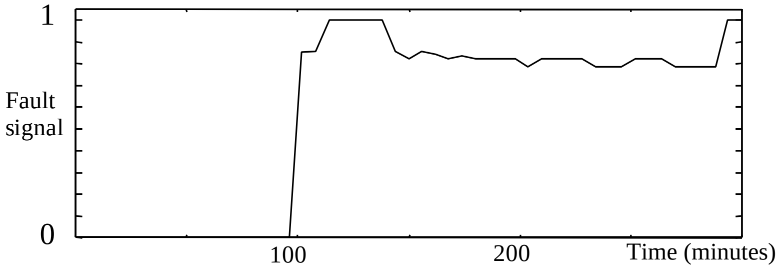
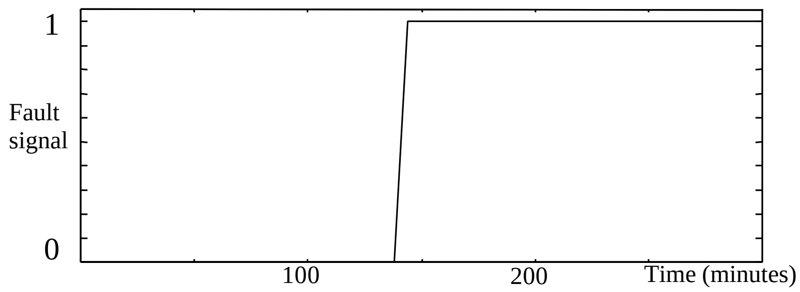


Figure 7.10. Water control valve leakage at time 100, responses of a) ANN , b) FDS

a)



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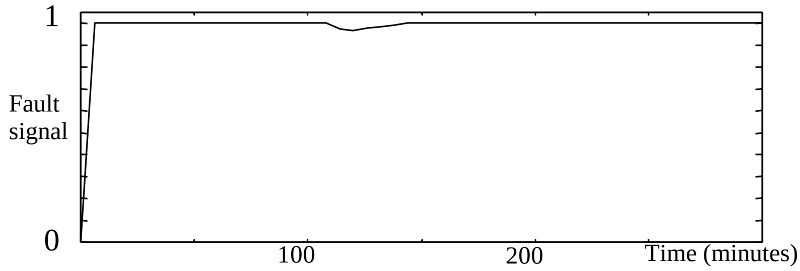
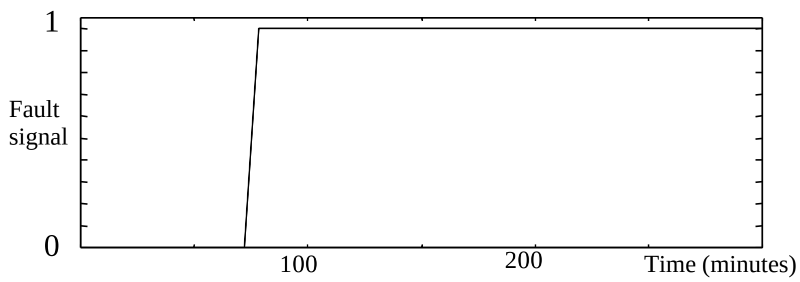


Figure 7.11. Fouling of the reactor temp. probe, responses of a) ANN, b) FDS

a)



b)

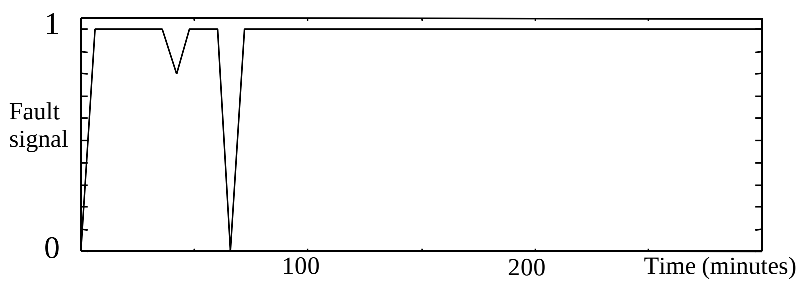
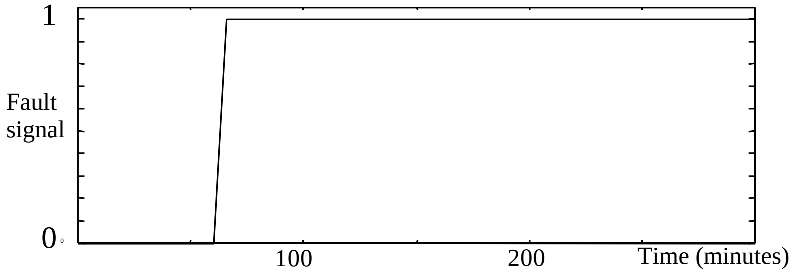


Figure 7.12. Fouling of the reactor jacket, a) ANN response, b) FDS response

a)



b)

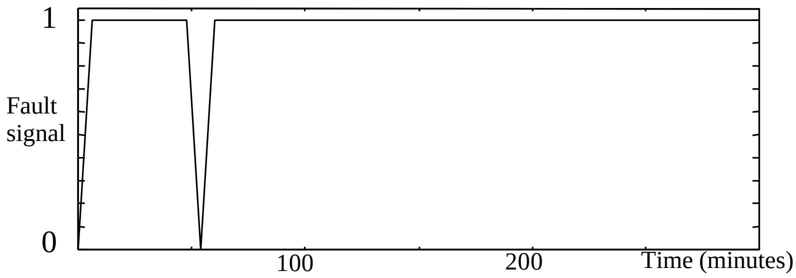
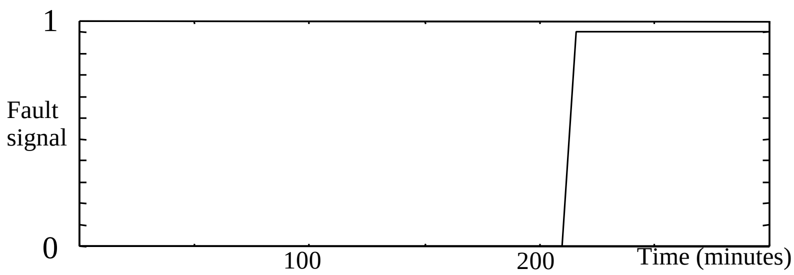


Figure 7.13. Fouling of reactor walls, a)ANN response, b) FDS response

a)



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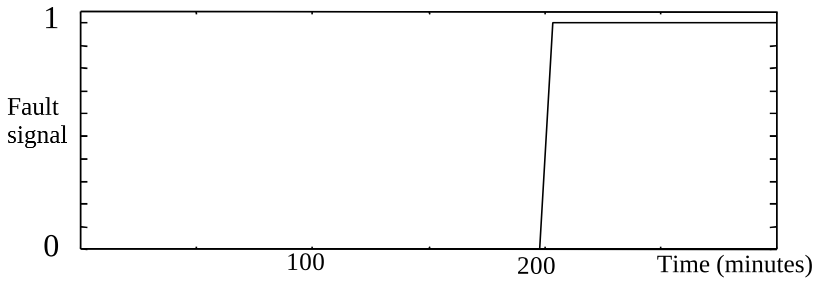
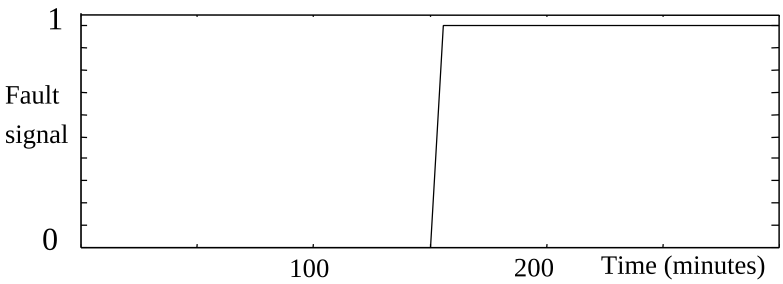


Figure 7.14. Incorrect master gain (higher) at time 200, a) ANN , b) FDS responses

a)



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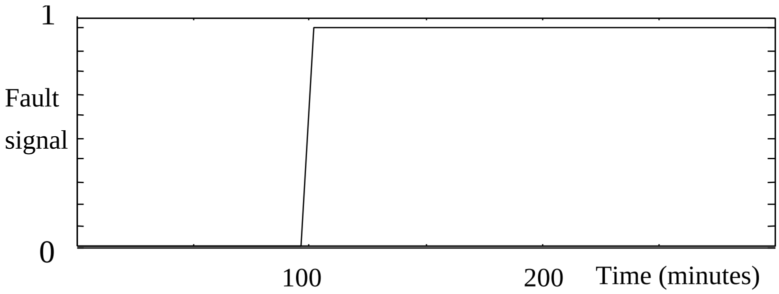


Figure 7.15. Incorrect slave gain (lower) at time 100, a) ANN response, b) FDS response

Comparison against on-line MPCA

MPCA allows to extract information in the multivariate trajectory data by projecting them onto low-dimensional spaces defined by the principal components. This leads to simple monitoring charts, consistent with the philosophy of Statistical Process Control, which are capable of tracking the progress of new batch runs and detecting the occurrence of observable upsets (Chapter 3, section 3.4).

Using a database of 81 different batch runs, with different initial conditions (variations in the reaction volume, initial concentration, jacket temperature and initial reactor temperature) the MPCA has been implemented determining the different control limits. Figure 7.16 shows the Square Prediction Error (SPE) of a normal batch run and the corresponding control limits. On-line MPCA was implemented (Nomikos and MacGregor, 1994) in order to have a reference with respect to the FDS system performance. The on-line MPCA technique allows detecting abnormal situations but is not able to properly isolate the fault.

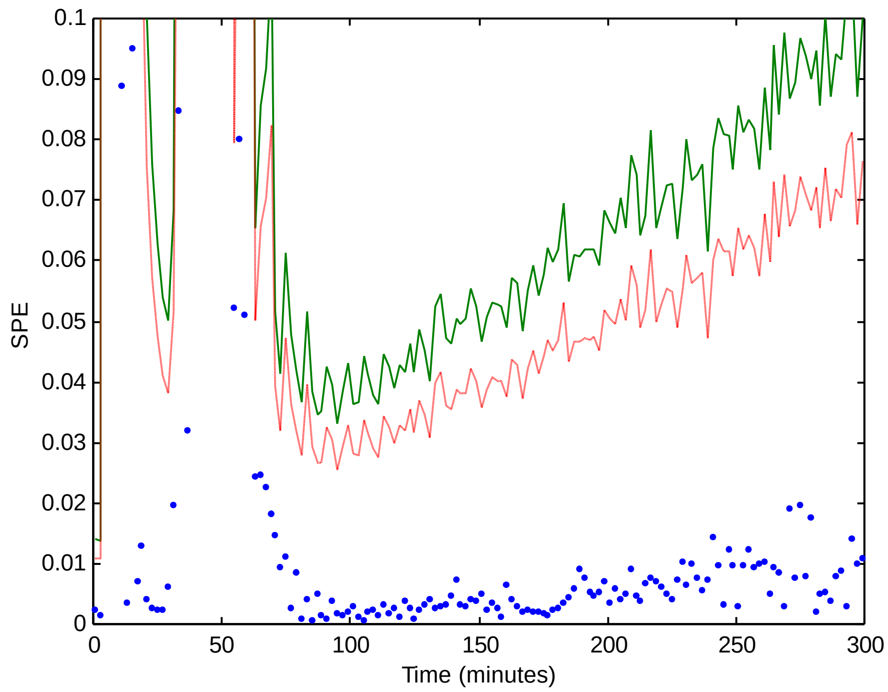


Figure 7.16. SPE plot for a normal batch, on-line MPCA; SPE (by points) under the 95% an 99% control limits (____ 99% control limit; _ _ _ _ 95% control limit)

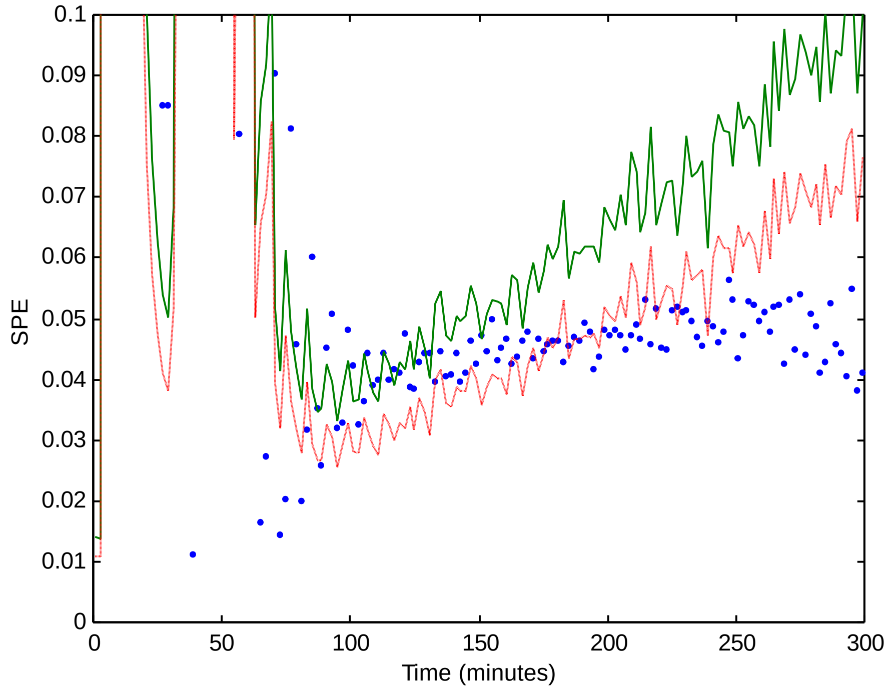


Figure 7.17. SPE plot for a batch with the initial problem of leaking in the steam control valve, Fault 1 (____ 99% control limit; _ _ _ _ 95% control limit)

It has been found that the SPE control limits have been overcome in the different simulated cases except for the first case. Figure 7.17 shows the monitoring chart that corresponds to this case. Actually, this case presented problems to the ANN in order to diagnose the fault quickly. However, the implemented FDS, with the FLS support manage to diagnose the fault quickly during the heating phase.

Discussion

The FDS implementation for batch processes has been illustrated. The main aspects detailed in this work correspond to the signal pre-processing using wavelets and the generation of if-then rules in the FLS from HAZOP analysis.

The application using as case study a batch reactor demonstrates the ease of implementation and its good performance by the correct identification of the faults. These two aspects makes the difference with respect to the on-line MPCA which is being used in the last years as good choice in batch process monitoring.

During the tests and tuning of the FLS, a problem (not shown in the presented plots) has been the existence of cases of false diagnosis. For this reason, one additional aspect, the selection and tuning of the FLS is considered in the following section.

7.2.4. Types of Fuzzy Logic Systems

The selection of the type of FLS has been evaluated by trying different types of FLSs. Table 7.9 shows a list of six cases corresponding to the operation Reactor cooling in the Batch reactor scenario. Different types of FLSs have been tested using those cases.

Table 7.9. Cases where the FLSs have been tested for comparison purposes

Case nº	**Description**
1	Leaking of water control valve (25% decrease of water flow at 100; F2=0.5)
2	Fouling of reactor temperature probe (F3=1 at time 0 min)
3	Fouling of reactor jacket (F4=1 at time 0 min)
4	Fouling of reactor walls (F5=1 at time 0 min)
5	Incorrect master gain (10 % higher at time 200)
6	Incorrect slave gains (50 % lower at time 100 min)

The two main types of FLSs have been considered: Mamdami and Sugeno (Chapter 4, section 4.2.3). Table 7.10 summarises the parameters that have been considered in each FLS. Results of the tests are shown in Table 7.11 in terms of the performance index.

By using the "Min-max" fuzzy reasoning method, the obtained performance has been very good but in the case of the Mamdami fuzzy model, many cases of false diagnosis have appeared. On the other hand, by using the Sugeno fuzzy model, the fuzzy reasoning method is not critical (the same acceptable performance has been obtained either by the min-max or the prod-sum fuzzy reasoning method). No cases of false diagnosis have appeared using the FLS of the Sugeno type.

The use of input-output data for the FLS tuning has also been investigated. According to available techniques, the Adaptive-Network-based-Fuzzy-Inference-System (ANFIS) method could be used (Jang and Sun, 1995). This is the major training routine for Sugeno-type FLS. ANFIS uses a hybrid learning algorithm to identify parameters of Sugeno fuzzy models. It applies a combination of the least-squares method and the backpropagation gradient descent method for training MFs parameters to emulate a given training data set. In order to use that method a FLS with only one output is required. This is the first limitation. It implies the use of one FLS for each fault. There are two alternatives:

1) To give the input MFs and the output MFs, and the algorithm ANFIS optimise the output MFs;

2) To give an input-output data set and the algorithm ANFIS generates the MFs of inputs and outputs.

The first alternative has the limitation that the number of MFs has to be equal to the number of if-then rules. The second alternative implies that the very intuitive recommended way (Chapter 5, section 5.5.2) cannot be used. The mentioned limitations make the use of ANFIS difficult to adequate to the presented FDS methodology of design. Furthermore, preliminary results do not show an improvement.

Table 7.10. FLSs considered

Fuzzy system Nomenclature →	FLSm1 (Mamdami)	FLSm2 (Mamdami)	FLSs1 (Sugeno)	FLSs2 (Sugeno)
AND method	Min	Prod	Min	Prod
OR method	Max	Sum	Max	Sum
Defuzzification	Centroid	Centroid	Weighted average	Weighted average

Table 7.11. Performance of the FLSs (%P)

Case nº	*FLSm1*	*FLSm2*	*FLSs1*	*FLSs2*
1	98,0*	87,0	84,0	84,0
2	96,5*	54,5	67,1	67,1
3	100,0*	77,1	77,1	77,1
4	98,3*	81,5	81,5	81,5
5	84,0*	84,0	84,0	84,0
6	72,0	72,0	72,0	72,0

(*) False diagnosis

7.3. Fluidised bed coal gasifier

In this case study, the use of historical data of past faults is contemplated. ANN training is based on the profiles of variables directly (Chapter 5, section 5.4.1). After analysing the FDS performance, a comparison against a statistical technique (PCA) is shown (Ruiz et al., 1999d; Ruiz et al., 2001a). Finally, the special case of faults in sensors is treated (Chapter 5, section 5.4.3).

7.3.1. Process faults

Two faults occurred in the past have been considered. Figure 7.18 shows the evolution of reactor temperatures and gas output compositions when a fault occurs at time 102 min. This fault corresponds to a melting of ashes at the reactor bottom and the subsequent obstruction in the air distributor. It can be seen the increase in temperature T2 and the shutdown of the combustion (%CO2 low) at that time.

Figure 7.19 shows the profiles of reactor temperatures and gas output compositions when a high flow-rate of water is fed to the reactor at time 62 min. A slow decrease of temperature T1 can be observed.

7.3.2. ANN training

Following the described methodology (section 5.4.1), a RBFN was selected. It was optimised with a spread of 0.9, in the same way shown in subchapter 7.1.2. Inputs were five: the three reactor temperatures (T1, T2, T3) and the gas output compositions (%CO2 and %O2).

Responses are shown in Figure 7.20 and Figure 7.21 for each fault.

As can be seen in Figure 7.20a, the diagnosis of Fault 1 by the ANN is very fast. In this case, the FLS, confirms the fault at the same time (Figure 7.20b). However, in the case of Fault 2 (Figure 7.21), the ANN needs more than 6 minutes to diagnose the fault (Figure 7.21a). In this case, The FLS plays an important role accelerating the diagnosis and improving the performance of the FDS (Figure 7.21b).

Therefore, in both faulty cases, operators have a support system for quick decision making. The corresponding corrective actions can be automated following the indications of the HAZOP analysis.

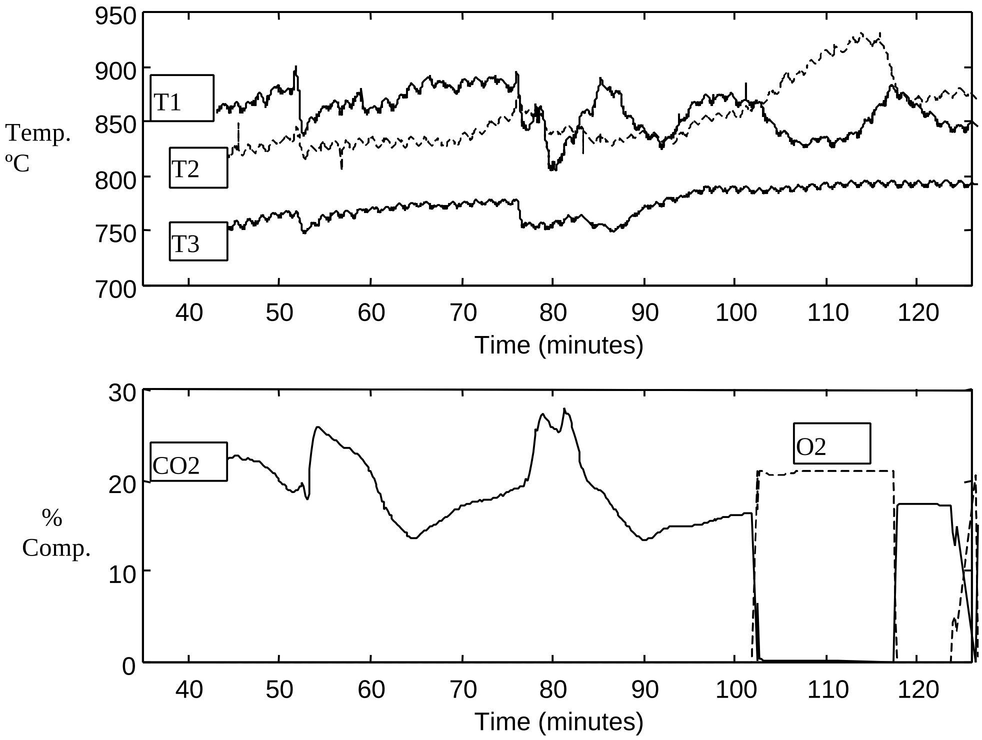


Figure 7.18. Fault 1: Melting of ashes at the reactor bottom and the subsequent obstruction in the air distributor, at time 102 min.

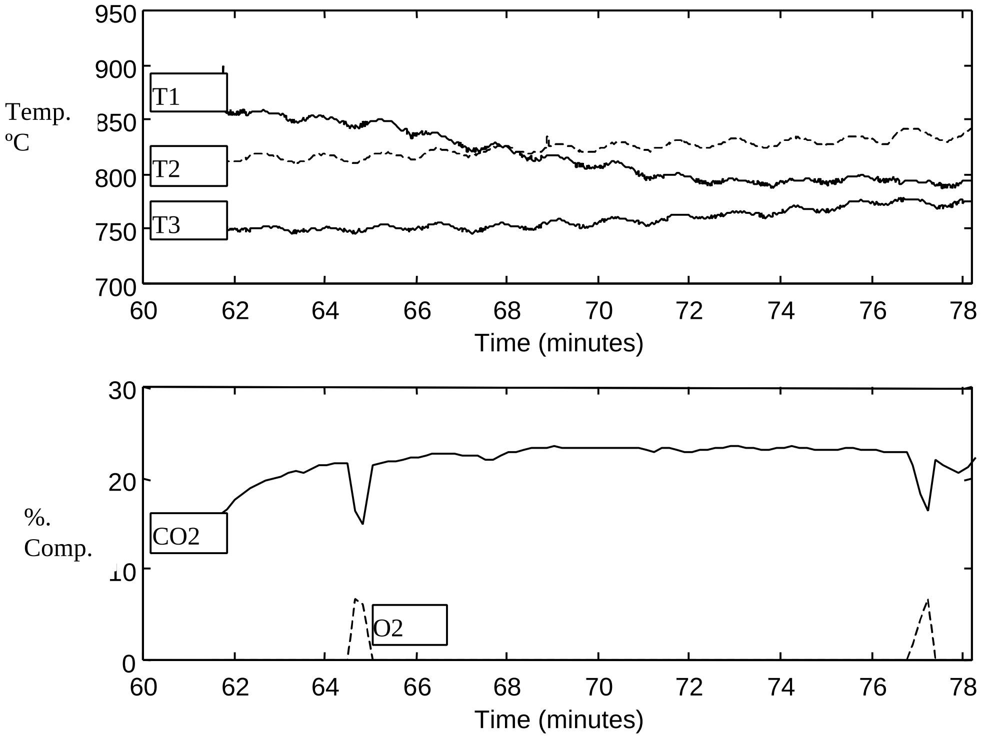
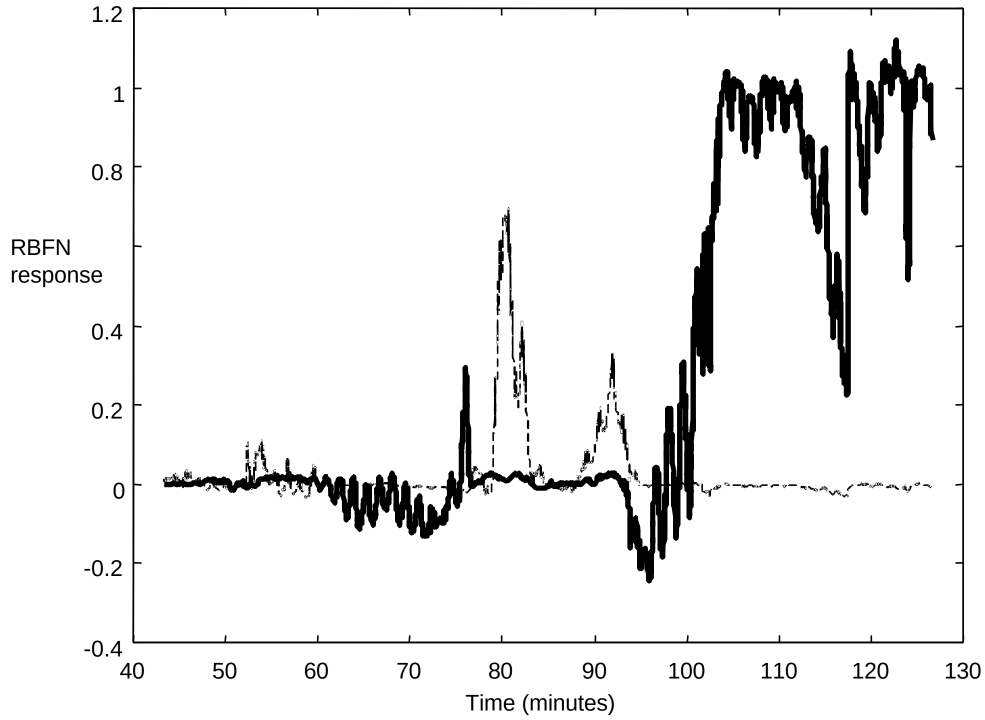


Figure 7.19. Fault 2: High flow-rate of water is fed to the reactor at time 62 min.

a)



b)

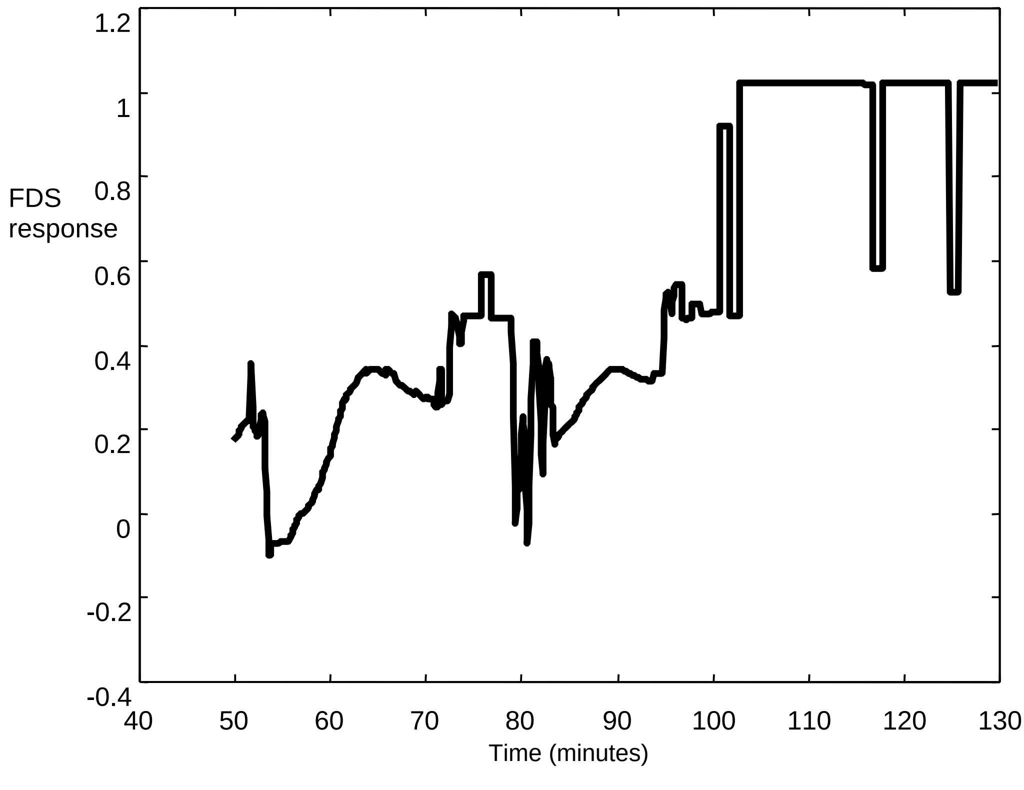
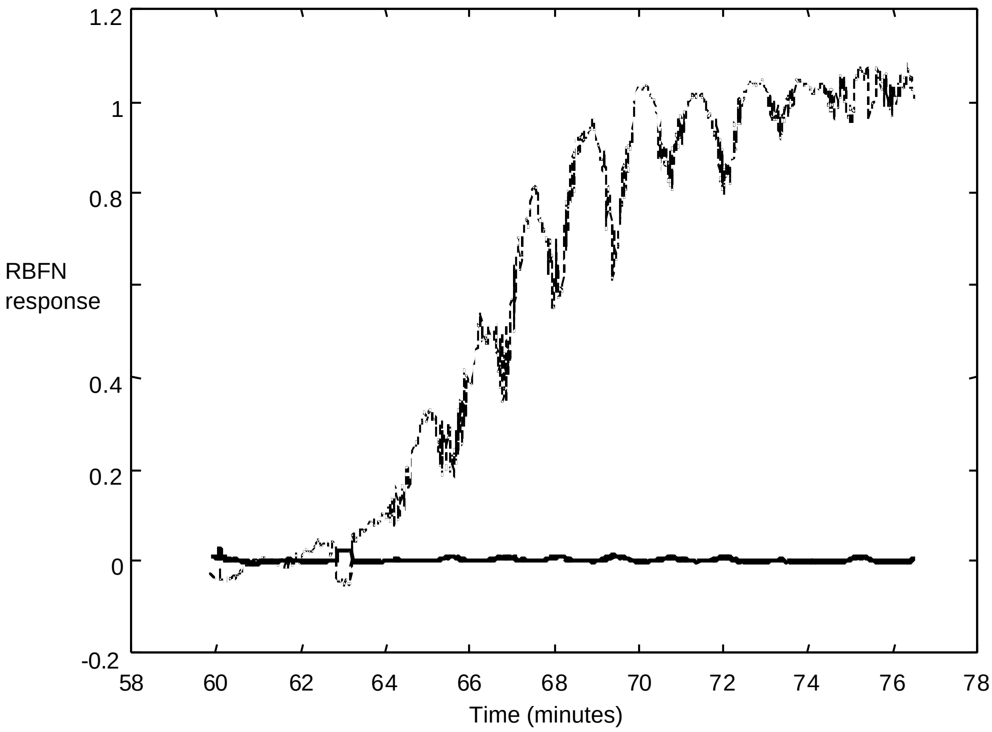


Figure 7.20. Fault 1 at 102 min.; a)ANN and b) FDS responses (Fault 1: ▬▬ ; Fault 2: _ _ _)

a)



b)

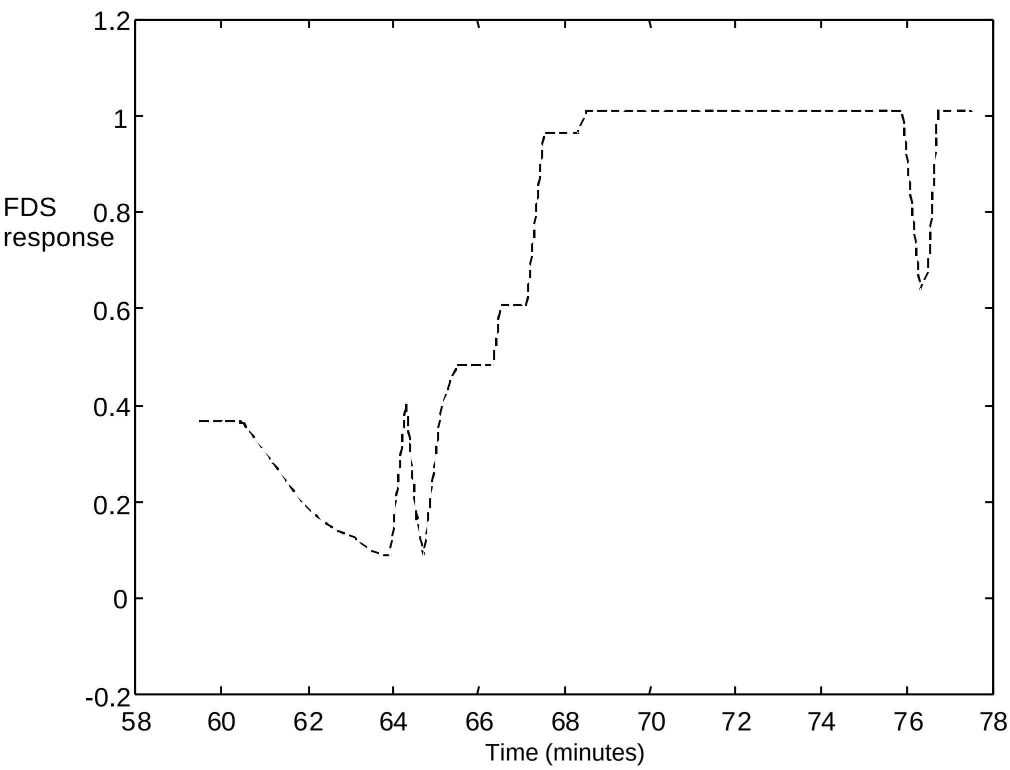


Figure 7.21. Fault 2 at 62 min.; a) ANN and b) FDS responses; Fault 1: ▬▬ *; Fault 2:* _ _ _

7.3.3. Comparison against Principal Component Analysis (PCA)

Among the historical-based techniques, PCA is one of the main competitors of ANNs. This data-analytic technique has been used to compare the performance of the ANNs. In order to detect the abnormal behavior of the process, two parameters already introduced in section 3.1.2 have been considered: the overall measure of variability (T^2) and the residual analysis (Q). Figure 7.22 and Figure 7.23 show the profiles of these parameters with their respective control limits.

In the case of Fault 1, there is slight difference in time detection with respect to the ANNs. On the other hand, in the case of Fault 2, where the RBFN approaches needs 6 minutes to adequately detect and diagnose the fault, PCA requires more than 8 minutes for the detection.

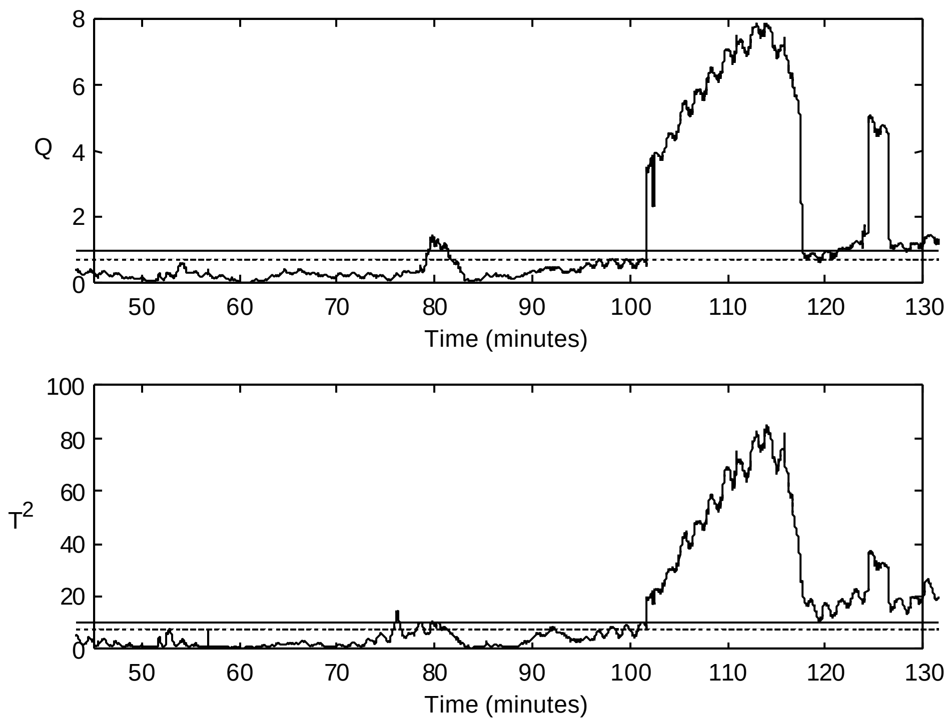


Figure 7.22. Fault detection by conventional PCA; Fault 1 at time 102 min.

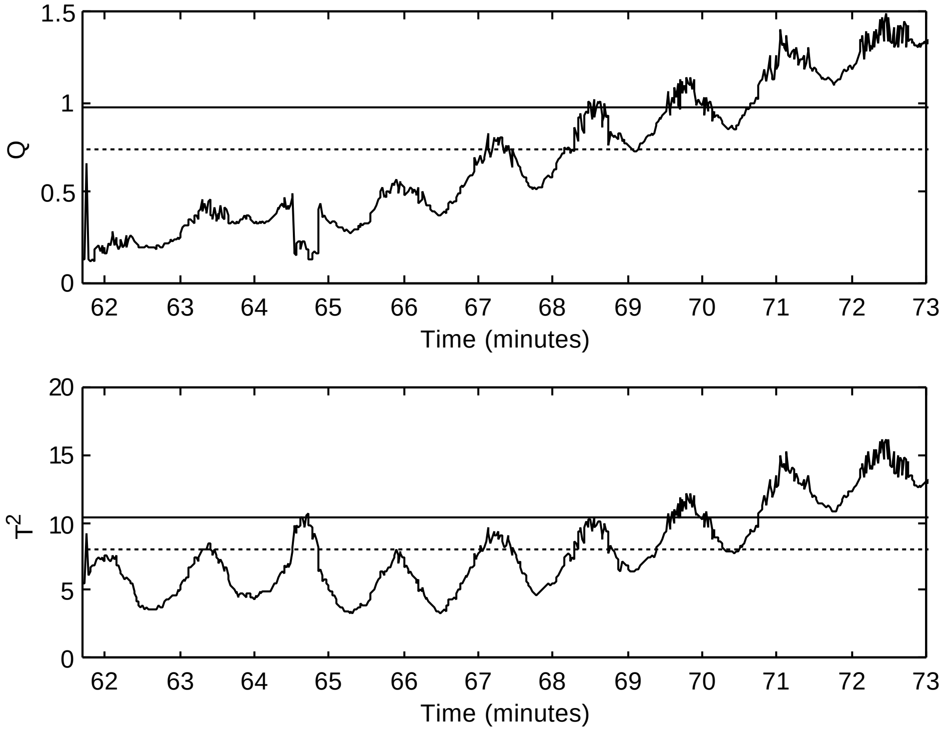


Figure 7.23. Fault detection by conventional PCA; Fault 2 at time 62 min.

7.3.4. Discussion

Table 7.12 summarises the performance of the proposed FDS in comparison with the ANN and a KBES working alone, taking into account the time for diagnosis.

The combination of the ANN and the FLS notably improves the diagnosis. The calculated average *%P* is 78%, higher than the ANN working alone (68%), the KBES (47%) and the conventional PCA (53%).

Table 7.12. Time for diagnosis (in minutes) and %P

Fault	ANN	KBES	PCA	FDS
Fault 1	0.5 min. / 97%	1 min. / 93%	2 min. / 87%	0.5 min. / 97%
Fault 2	6 min. / 40%	* / 0%	8 min. / 20%	4 min. / 60%
%P* (average)	**68%**	**47%**	**53%**	**78%**

*No diagnosis

7.3.5. Faults in sensors

Two sensor faults were considered: fault S1: a bias sensor fault in T1 of about 5% (+50ºC) and fault S2: a bias sensor fault in %CO2 (+10%). They have been simulated separately at time 68 min. Figure 7.24 shows the square prediction error (SPE) calculated from the response of the AANN, when fault S1 was simulated. It overcomes the control limits largely and quickly. Table 7.13 shows the isolated faulty sensors by the proposed additional algorithm. Such algorithm generates a multiple fault diagnosis: faults S1 (correct) and S2 (false diagnosis). Figure 7.26 shows the SPE when fault S2 was simulated. ANN detect and diagnose successfully the sensor fault. As can be seen in Figure 7.25 and Figure 7.27, conventional PCA was unable to detect properly the sensor faults S1 and S2 (only during few minutes the control limits have been overcome).

Table 7.13. Isolation of faulty sensors

Fault	Fault diagnosed
S1 (Sensor T1)	S1, S2 (sensors T1 and %CO2)
S2 (Sensor %CO2)	S2 (sensor %CO2)

Discussion

The use of the proposed methodology to diagnose faults in sensors by using an AANN has been compared against conventional PCA. As conventional PCA is a linear technique, its performance is very poor when detecting sensor faults even if the bias errors are large. Otherwise, in spite of the fact that AANNs can receive the measurements outside the range of training data set, they can detect these bias errors. However, the proposed algorithm to isolate the faulty sensors has some problems (false diagnosis) for this experimental case that require further consideration.

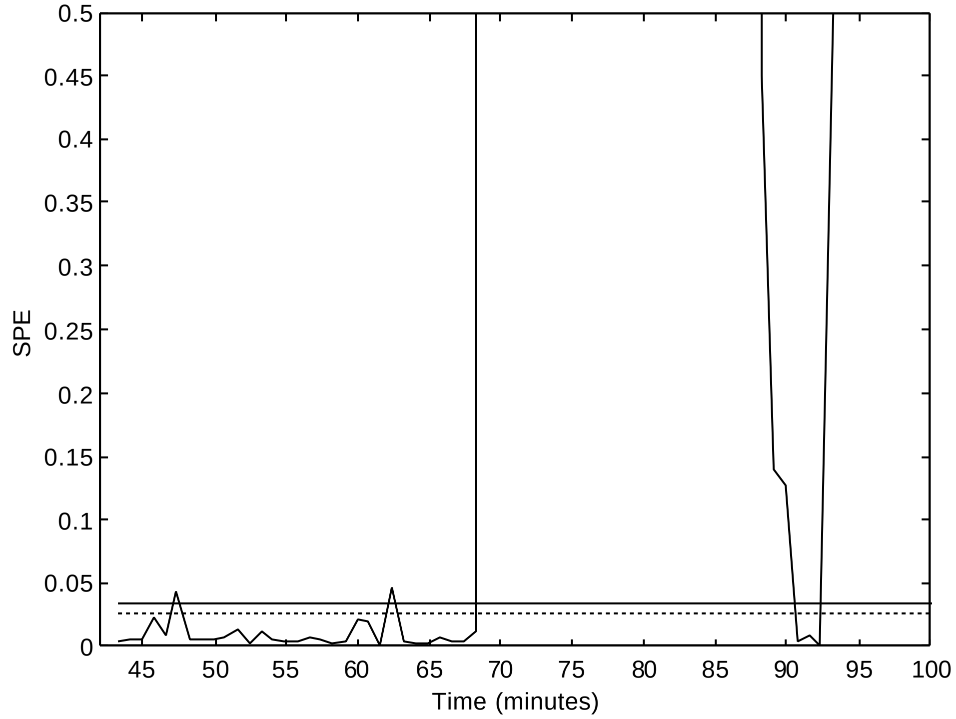


Figure 7.24. Fault in sensor T1 at time 68 min. Detection using NLPCA by an AANN

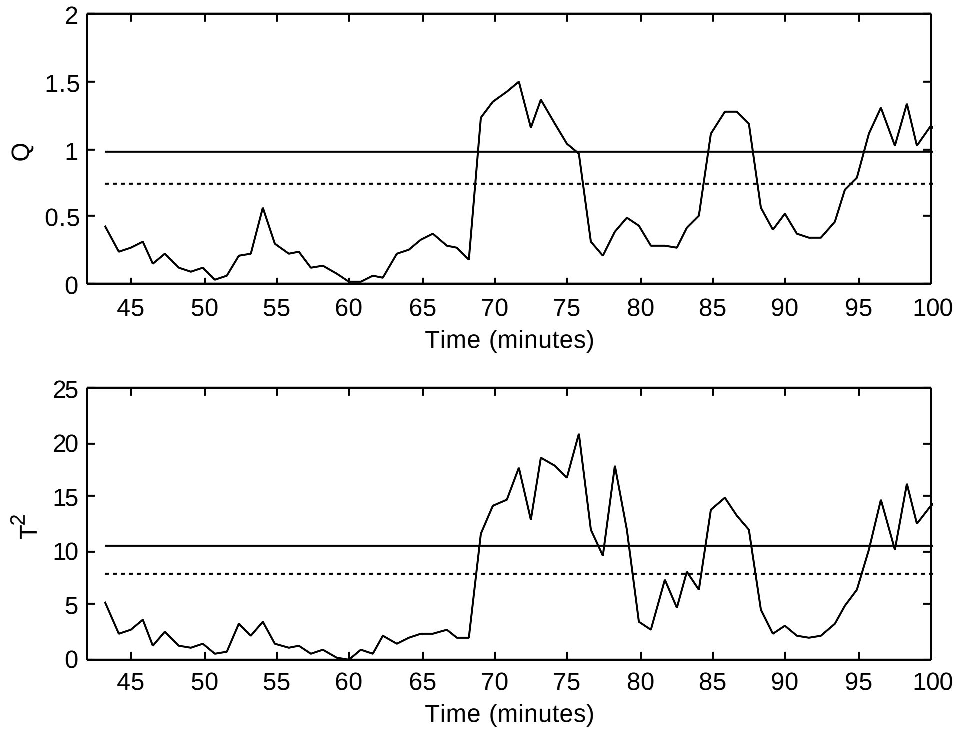


Figure 7.25. Fault in sensor T1 at time 68 min. Detection using conventional PCA

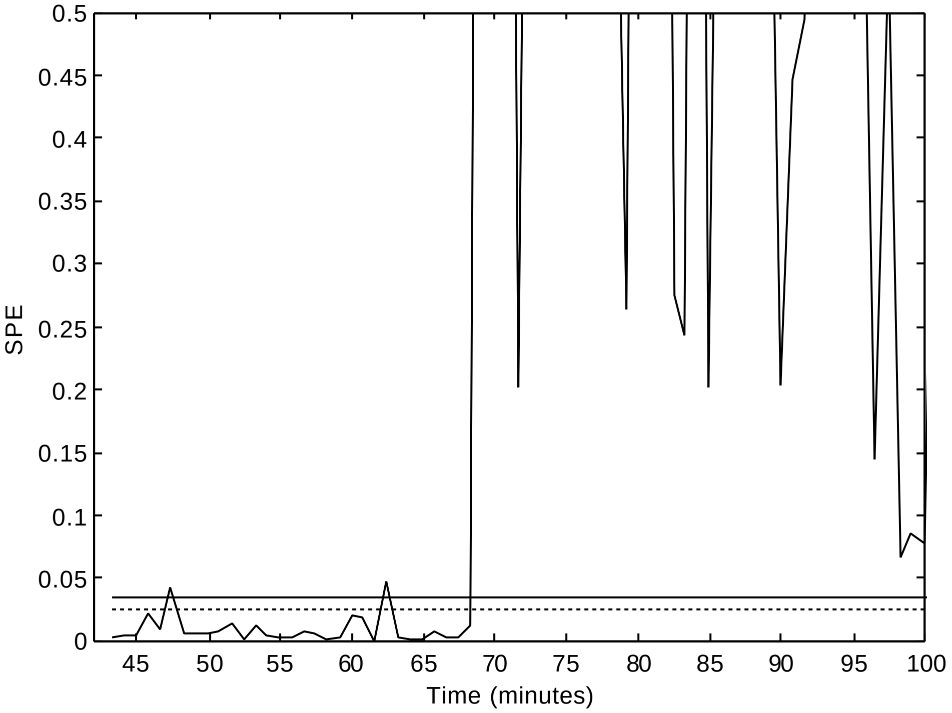


Figure 7.26. Fault in sensor %CO2 at time 68 min. Detection using NLPCA by AANN

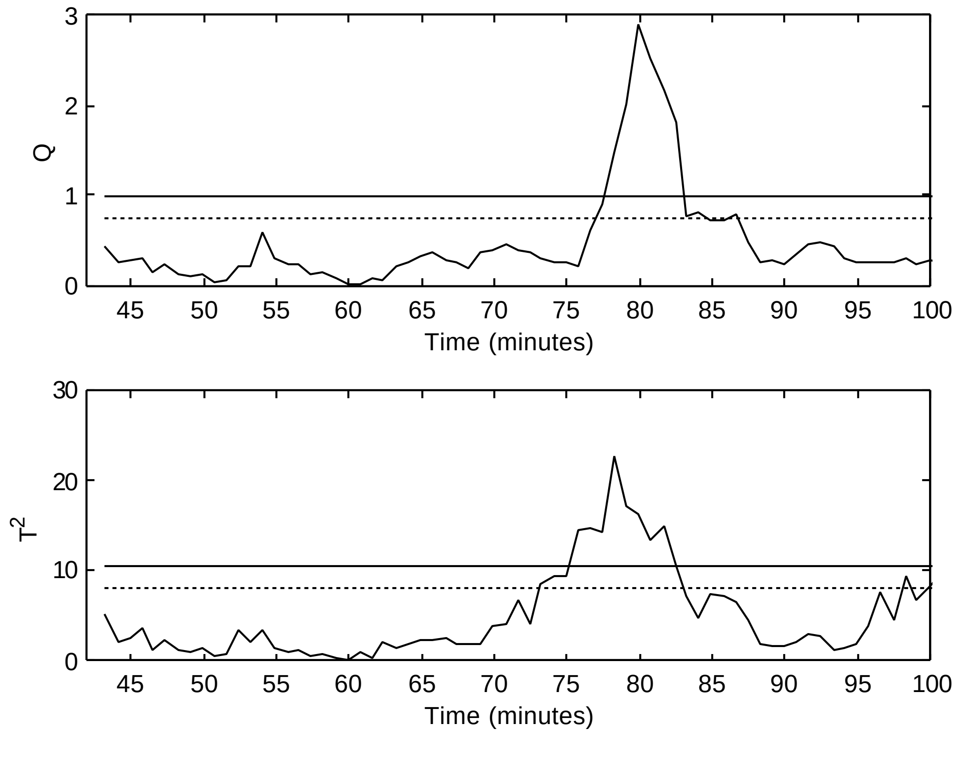


Figure 7.27. Fault in sensor %CO2 at time 68 min. Detection using conventional PCA

7.4. Batch plant at pilot plant scale

The proposed FDS has been tried in two different scenarios of a batch chemical plant. In the first case, the fed-batch reactor, ANN training based on the profiles of variables (subchapter 5.4.1) is shown. The advantages of this alternative against on-line MPCA is demonstrated (Ruiz et al., 1999c; Ruiz et al., 1999e).

In the second case study, the integration of the FDS into the information system is shown (Ruiz et al., 2000a; Ruiz et al., 2000c; Ruiz et al., 2001b).

7.4.1. Fed-batch Reactor

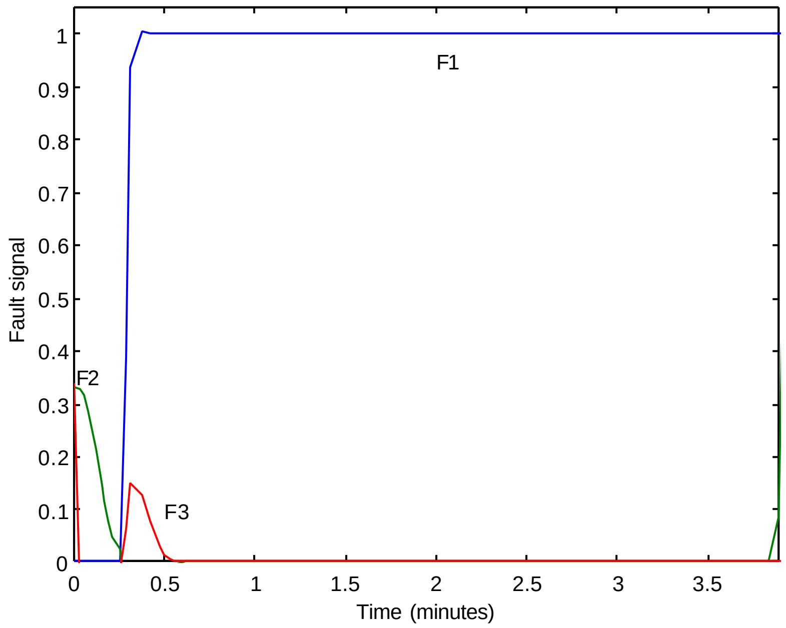
ANN training was performed with data from simulated abnormal situations in the plant. The inputs to the ANN block are the following: Mixer level, Reactor level, reactants concentration (observable by inference), reactor temperature and the time from the start of the operation. The outputs are the suspected faults:

- Low feed reactant concentration (F1)
- Fouling of reactor temperature sensor (F2)
- Cooling system failure (F3)

Figure 7.28a shows the response of the ANN block when a low reactant concentration in the feed is simulated. The ANN needs 14 seconds to recognise the fault F1 pattern. In the first seconds a low signal of Fault F2 appears but decays immediately. Furthermore, a very low signal of Fault F3 appears with Fault F1 signal. In this case, both low signals could be considered as false diagnosis cases. However, the FDS response is free of those signals (Figure 7.28b). This fact confirms the importance of the use of the supplement (FLS) in order to eliminate any possibility of cases of false diagnosis.

Table 7.14 summarises the FDS performance taking into account the three suspected faults for this case. The main feature is the rapid and correct diagnosis.

a)



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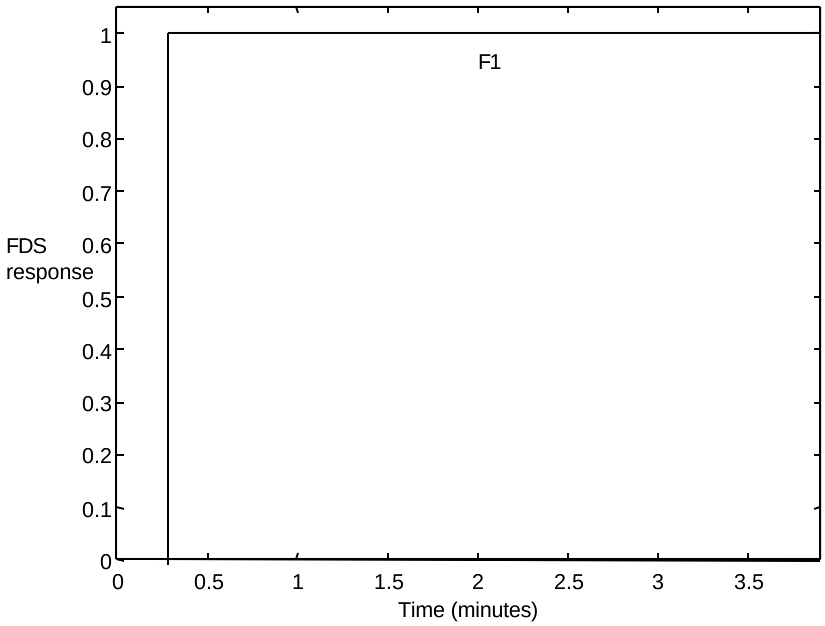

Figure 7.28. Responses for a batch run with the initial problem of low reactant concentration in the feed; a) ANN; b) FDS

On-line MPCA (Nomikos and Mc Gregor, 1994) was performed in order to have a reference for the ANN performance. Figure 7.29 shows one of the monitoring charts that allow detecting a fault in a batch process using the on-line MPCA. The points correspond to the score (t) of the first principal component while the continuous and dashed (upper and lower) lines correspond to the 95 and 99% control limits, respectively. The lower limit of 95% is overcome three minutes after the fault occurs while the overcoming of the 99% control limit requires almost 4 minutes. The Square Prediction Error (SPE) chart allows detecting the simulated fault quickly, but the isolation of the fault is difficult because the on-line MPCA technique requires an additional complex expert system to do that. On the other hand, the ANN isolates the fault in less than a quarter minute (Figure 7.28a). After passing through the FLS, the final signal has a value of 1 only for the output corresponding to this suspected fault F1 (Figure 7.28b).

Table 7.14. FDS performance

Fault	**Time needed by the FDS to isolate the fault (seconds)**
Low feed reactant concentration	**14**
Fouling of reactor temperature sensor	**8**
Cooling system failure	**19**

Discussion

This short introduction of the results obtained with the FDS implementation in the fed-batch reactor illustrates the following aspects.

The ANN has been trained with the profiles of variables including the time from the start of the batch (subchapter 5.4.1). It allows the obtention of better results in comparison with conventional PCA.

The use of a FLS which can "filter" the ANN response, in order to eliminate possible false diagnosis signals, has also been observed.

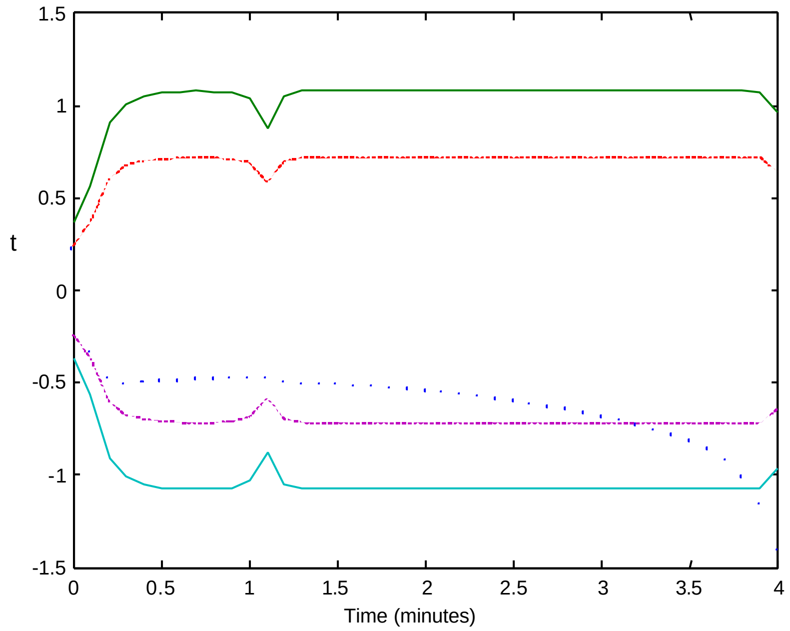

Figure 7.29. Monitoring chart with its 95% and 99% control limits for a batch run with the initial problem of low reactant concentration in the feed

7.4.2. Multipurpose batch chemical plant

This case study allows to show the use of the information provided by the proposed FDS. In Chapter 5 (section 5.6), the strategy has been explained and illustrated by a simple example. In this subchapter, the implementation strategy is tested in the multipurpose batch chemical plant.

Implementation results

Two different faults have been considered to test the implementation strategy. The first one corresponds to a delayed operation caused by a pump malfunction. Figure 7.30 shows the tank level profiles, comparing a regular batch, an abnormal batch in the absence of FDS and an abnormal batch with the FDS implemented. It can be observed that the rapid diagnosis and communication to the supervisory control level allows reducing the delay. The discharge of tank T1 (and loading of Reactor R1) needs almost 0.15 hours instead of the suspected 0.06 hours. With the support of the FDS a switch to other pumps and the checking of the corresponding pump by the operator can be done and the consequences of the abnormal situations are reduced (approximately 0.08 hours). Furthermore, the scheduling system can perform reactive scheduling (schedule optimiser) taking into account the delay.

The second abnormal situation considered is the unavailability of a piece of equipment, in this case the Reactor R2. The whole schedule considered in this study consists of 5 batches of product A (recipe 1) and 8 batches of product B (recipe 2). It has been simulated that the unavailability of Reactor 2 lasts for fifty minutes since the beginning of the schedule. Figure 7.31 shows three Gantt charts. The first one corresponds to the initial schedule. The makespan of this initial schedule is 4.37 hours. The second one corresponds to the abnormal situation without the FDS support. Finally, the third Gantt chart considers the implementation of the FDS and the reactive scheduling. Event Operation Network model was utilised for the scheduling system (Graells et al., 1998; Cantón et al., 1999a; Cantón et al., 1999b). In the initial schedule, reactor R2 always runs with recipe 2. In the presence of the abnormal situation diagnosed, the schedule optimiser selects the reactor R2 to perform the rest of batches with recipe 1 when this piece of equipment is available again.

Table 7.15 shows a comparison of the results taking into account the plant functioning without a FDS and with the FDS support for the first considered abnormal situation. In this case of a simulated delayed operation, the energy consumption grows a 1% with respect to normal operation. This growth is reduced by the adequate integration of the FDS and the supervisory control system to only 0.3%, representing energy savings of 0.7%.

Table 7.16 summarises a comparison of the results taking into account the plant functioning without a FDS and with the FDS and reactive scheduling for the two considered abnormal situation. In the case of the simulated delayed operation (the first simulated abnormal situation), the makespan is increased only a 0.5% with the FDS support (0.9% less than the case without the FDS support). On the other hand, the FDS support to reactive scheduling reduces the impact of the second abnormal situation simulated. The makespan is increased a 7.6% that is 2.9% less than the scenario without the FDS support. Savings of this order (2.9% and 0.9%) can represent a big improvement in terms of productivity in modern batch chemical plants like pharmaceutical and fine chemicals manufacturing. Furthermore, taking into account that different abnormal situations can appear in the different batches, the potential savings may be much more bigger.

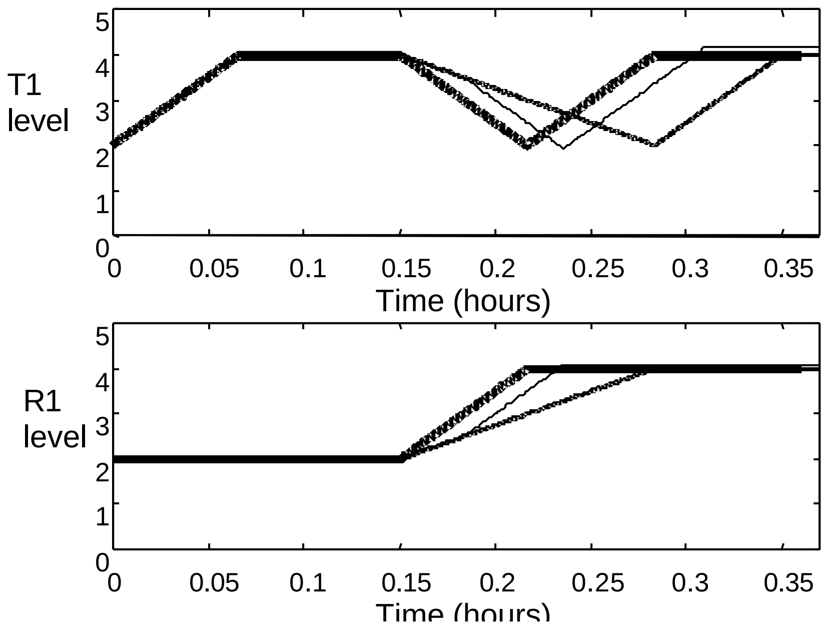

Figure 7.30. Tank levels profiles, Normal batch; Abnormal batch without FDS; Abnormal batch with FDS support

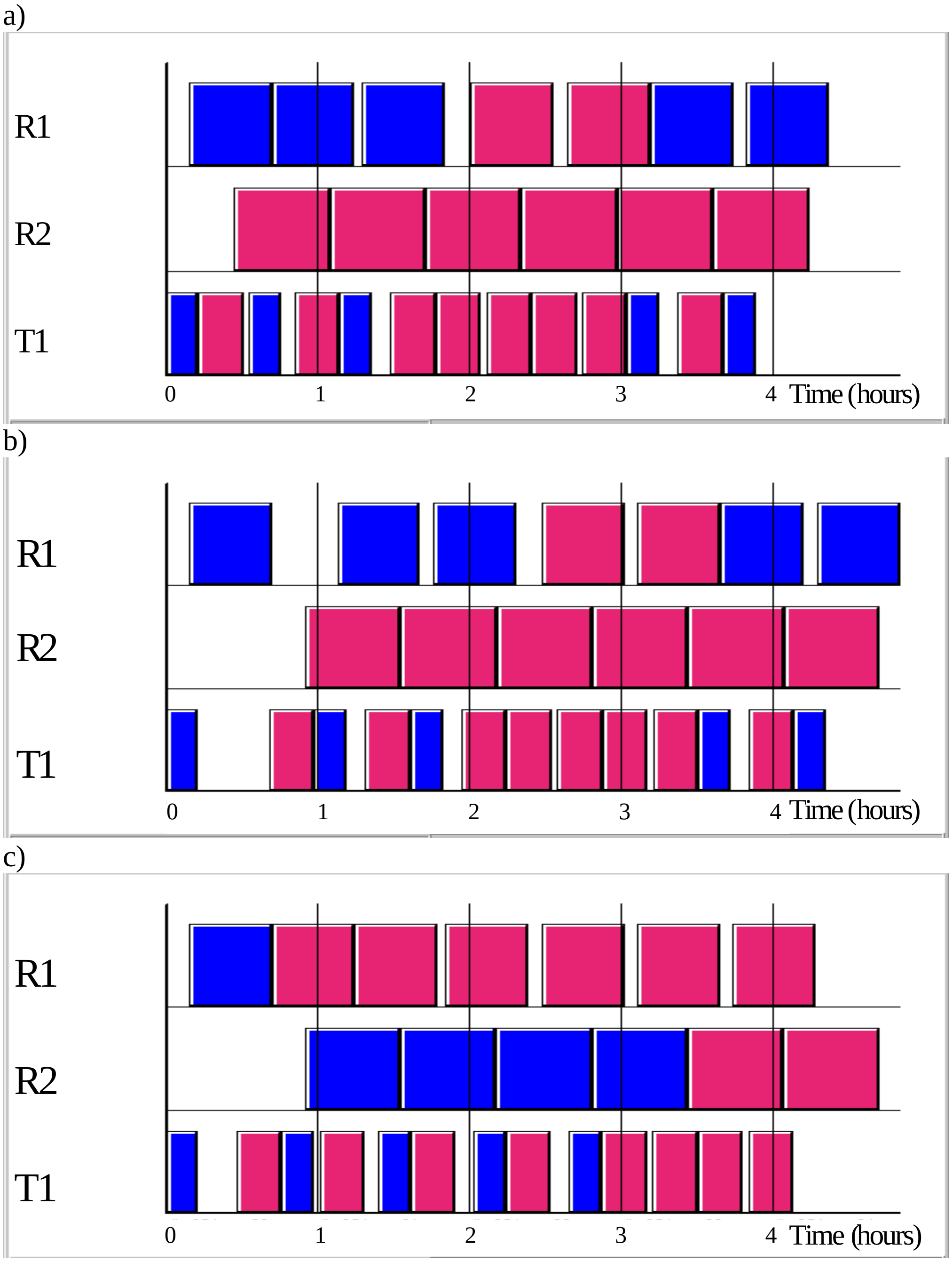

Figure 7.31. Comparison of Abnormal situation management: a) Initial schedule, b) Schedule performed without the FDS support and c) Schedule with FDS and reactive scheduling. Recipe 1: Recipe 2:

Table 7.15. Energy consumption comparison (Abnormal situation: Delayed operation)

Normal operation	Without the FDS support	With FDS support
21982 Kw.sec	22198 Kw.sec (+1%)	22054 Kw.sec (+0.3%)

Table 7.16. Performance comparison -makespan-

Abnormal situation	Without the FDS support	With FDS & reactive scheduling
Delayed operation	4.43 h (+1.4%)	4.39 h (+0.5%)
Unavailability (R2)	4.83 h (+10.5%)	4.70 h (+7.6%)

Discussion

The proposed simple implementation strategy for the development and implementation of the FDS integrated to the scheduling system has been tried in the pilot plant scale scenario of a multipurpose batch chemical plant.

The results correspond to the simulation of two abnormal situations. The proposed integration of the FDS in the information system shows promising results by significant improvement in the production efficiency. Preliminary results show the possibility of important energy savings.

Industrial applications of the proposed system are straightforward because of the simplicity of implementation.

Acronyms

AANN	Autoassociative Artificial Neural Network
ANN	Artificial Neural Network
BPN	Backpropagation Artificial Neural Network
DCS	Distributed Control System
FDS	Fault Diagnosis System
FLS	Fuzzy Logic System
HAZOP	Hazard and Operability study
KBES	Knowledge Based Expert System
MF	Membership function
NLPCA	Nonlinear Principal Component Analysis
PCA	Principal Component Analysis
PNN	Probabilistic Artificial Neural Network
RBFN	Radial Basis Function Neural Network
SOM	Self Organising Map
SPE	Squared Prediction Error

Notation

db	Number of nodes in the bottleneck layer of an AANN
Md	Number of nodes in the demapping layer of an AANN
Ml	Number of nodes in the mapping layer of an AANN
N1	Output vector of the ANN in the proposed FDS
%P	Performance parameter for FDS
*%P**	Modified %P which takes into account cases of false diagnosis
Q	Sum of squares of the residuals
$SPE_{js}\%$	Percentage relation between SPE_j of a new measurement and SPE_{js}
t	Principal component scores vector
T^2	Overall measure of variability