State of the art

The first works related to Fault Diagnosis (FD) started at the beginning of the seventies. These works treated fault detection in lineal systems. This starting point coincides with the development reached in that decade by the computers with the birth of the first microprocessor (1972). Applications of artificial intelligence techniques, such as artificial neural networks and fuzzy logic, to FD started in the eighties. In the last decade, the interest about FD in chemical plants increased notably. The International Federation of Automatic Control (IFAC) created a Technical Committee in 1991. This Committee organises meetings every three years. This fact has permitted to standardise concepts and definitions in this area in benefit of the industrial and scientific community all over the world (Isserman and Ballé, 1997).

FD methods can be classified into three groups: historical based methods, knowledge based methods and combinations of both.

3.1. Historical based methods

Historical based methods correspond to classification methods, pattern recognition approaches and statistical techniques. Artificial Neural Networks (ANNs), Principal Component Analysis (PCA) and Qualitative Trend Analysis (QTA) are the main examples of techniques of this group.

3.1.1. Artificial Neural Networks

Among the pattern recognition methods, the Artificial Neural Network (ANN) approach is the most utilised. ANNs have many very useful properties for fault diagnosis. They can handle nonlinear and undetermined processes. They learn the diagnosis by means of the training data. They are very noise tolerant and work well with noisy measurements. Their ability to adapt during use is also an interesting property.

Figure 3.1 shows a scheme with three common ways of using ANNs for FD. The first one (Figure 3.1a) is the use of ANNs to differentiate various faults from the normal condition, and from one another, according to different fault patterns represented in the measured input-output system data, either by off-line training or on-line training by an adaptive ANN.

The second one (Figure 3.1b) is a hybrid scheme that uses an ANN to isolate faults, based on a residual generated by a quantitative model-based method.

The third approach (Figure 3.1c) uses an ANN to predict the plant output, and the prediction error is used for the residual; another ANN is then used to isolate faults.

In the petrochemical industry ANNs have been used as supervised pattern classifiers. They are trained on historical or simulated steady state process data with the aim of detecting a specified number of suspected faults.

The first reports (Hoskins and Himmelblau, 1988; Venkatasubramanian and Chan, 1989; Watanabe et al., 1989; Venkatasubramanian et al., 1990) show the application of Backpropagation networks (BPNs) using sigmoidal functions in the first layer. In more recent studies, Radial Basis Function networks (RBFNs) are preferred because they provide more reliable generalisation and fewer extrapolation errors (Gomm et al., 1998; Yu et al., 1999). The elliptical basis function neural network is similar to RBFNs with Gaussian basis function. However, it has more favourable and intuitive results in function approximation and classification (Chen and Liu, 1998).

Many successful studies have been reported on integrating wavelet transformations with neural networks (Zhao et al, 1998). Wavelets functions are more localized and pick up edge effects.

Self Organizing Maps (SOMs), which are trained unsupervised, are not always able to classify data correctly. However, their ability to classify data autonomously is very interesting and useful when real industrial processes are considered (Koivo, 1994).

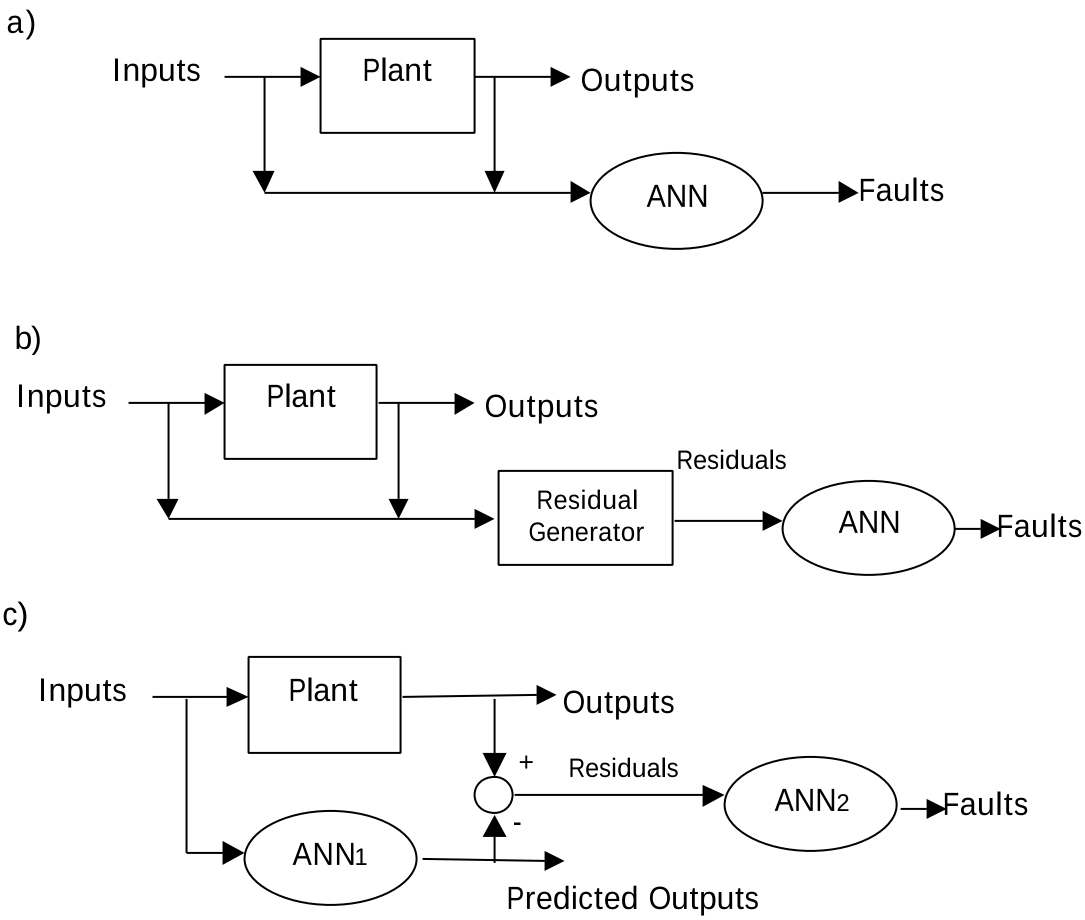

Figure 3.1. Ways of using ANNs for Fault Diagnosis. a) Recognising fault patterns in the input-output plant data; b) Isolating faults, based on residuals generated by a quantitative model-based-method; c) Predicting plant outputs to generate residuals, and isolating faults, based on such residuals.

Regarding the special case of faults in sensors, auto-associative neural networks have been showing good results. Their application is based on the Nonlinear Principal Component Analysis (NLPCA) technique (Kramer, 1992). Furthermore, a robust auto-associative neural network can be used to gross error detection, identification and removal into a single step. Dong and McAvoy (1996) suggest a method that uses principal curves and three-layered neural networks. Mo et al. (1998) suggest NLPCA that is based upon functional-link auto-associative neural network (the input layer is expanded by using the concept of functional link).

Recent works enhance the use of the ANN framework for FD by big improvements in the following issues: speed of training, introduction of time explicitly into the classifier design and on-line updation using a mirror-like process model (Rengaswamy and Venkatasubramanian, 2000).

3.1.2. Statistical techniques

The use of statistical techniques for FD is based on viewing diagnosis in terms of quality control. Statistical Process Control (SPC) has been widely used in process systems for maintaining quality. PCA is a statistical technique that has a wide area of applications. Among these applications, industrial process monitoring is one of them. PCA allows to reduce the dimension of the plant models by the use of lineal dependencies among the variables. The principal components represent the selection of a new coordination system obtained by rotating the original variables and projecting them into the reduced space defined by the first few principal components, where the data are described adequately and in a simpler and more meaningful way.

Considering a matrix X (m x n), that is, m observations of n variables, PCA transforms it by combining the variables as a linear weighted sum as:

$$X = T \ P^T \tag{3.1}$$

where T is defined as principal component scores, P is defined as principal component loadings. The principal-component loadings denote the direction of the hyperplane that captures the maximum residual variance in the variables measurements, while maintaining orthonormality with the other loading vectors. The principal component scores are the coordinates for the objects in the reduced space. They are uncorrelated and therefore are measuring different underlying "latent structures" in the data. By plotting the scores of one principal component vs. another, one can easily see which objects have similarities in their measurements and form clusters, and which are isolated from the others and therefore are unusual objects or outliers.

The X data may be decomposed by singular-value decomposition as follows:

$$X = UA^{1/2}V \tag{3.2}$$

where A is a diagonal matrix of eigenvalues of X; P^T=V and T=$UA^{1/2}$.

In practice, the measured variables are usually contaminated by errors, and none of the eigenvalues are exactly zero, but loadings and scores corresponding to small eigenvalues are composed of the errors only. Thus, the contribution of the errors in the data matrix may be decreased by eliminating the loadings and scores corresponding to the small eigenvalues, and reconstructing the filtered or rectified matrix as:

$$\widehat{X} = \widehat{T}\widehat{P}^T \text{ ,} \tag{3.3}$$

where $\widehat{T}$ and $\widehat{P}^T$ represent the selected scores and loadings, respectively. Principal components are the projections of original variables along the directions determined by the *h* eigenvectors {p_1, p_2, ..., p_h } (*h*<n) corresponding to first *h* largest eigenvalues of the covariance matrix of *X*. An important decision is to select the appropriate number of principal components that capture the underlying relationship, while eliminating the errors. Some techniques are available for this task (Jackson, 1991).

Basically, the application of PCA to FD consists in the calculus of the Squared Prediction Error (SPE) of residual space as:

$$Q_i = \sum_{i=1}^{\widehat{P}} (x_{ij} - \widehat{x}_{ij})^2 \tag{3.4}$$

where Q_i is the SPE value for the *i*th sample of process variables.

The process is considered normal if Q_i is between the control limits. These limits are calculated by:

$$\text{95\% control limits} = Qmean \pm 2s \text{ ,} \tag{3.5}$$

for 95% confidence limits, being s the standard deviation, and

$$\text{99\% control limits} = Qmean \pm 3s \text{ ,} \tag{3.6}$$

for 99% confidence limits for SPE.

Another index often used for fault detection is the Hotelling T^2 test. It is an overall measure of variability. For new data, the score space is monitored by computing the T^2 value as the sum of the squares of the selected scores scaled by the respective eigenvalue computed from data representing normal operation as:

$$T_i^{\,2} = \sum_{j=1}^{\widehat{p}} \frac{t_{ij}^2}{l_j} \text{ ,} \tag{3.7}$$

where T_i^2 is the T^2 value for the *i*th row of measurements, $\widehat{p}$ is the number of scores selected, t_{ij} is the *j*th score for the *i*th row of measurements and l_j is the eigenvalue of the *j*th score. Assuming Gaussian distributed measurements, the detection limits are calculated in the same way described for *Q* -Equations (3.5) and (3.6) -. It is important to note that the principal component loadings and detection limits for the scores and residuals are computed from data representing normal operation.

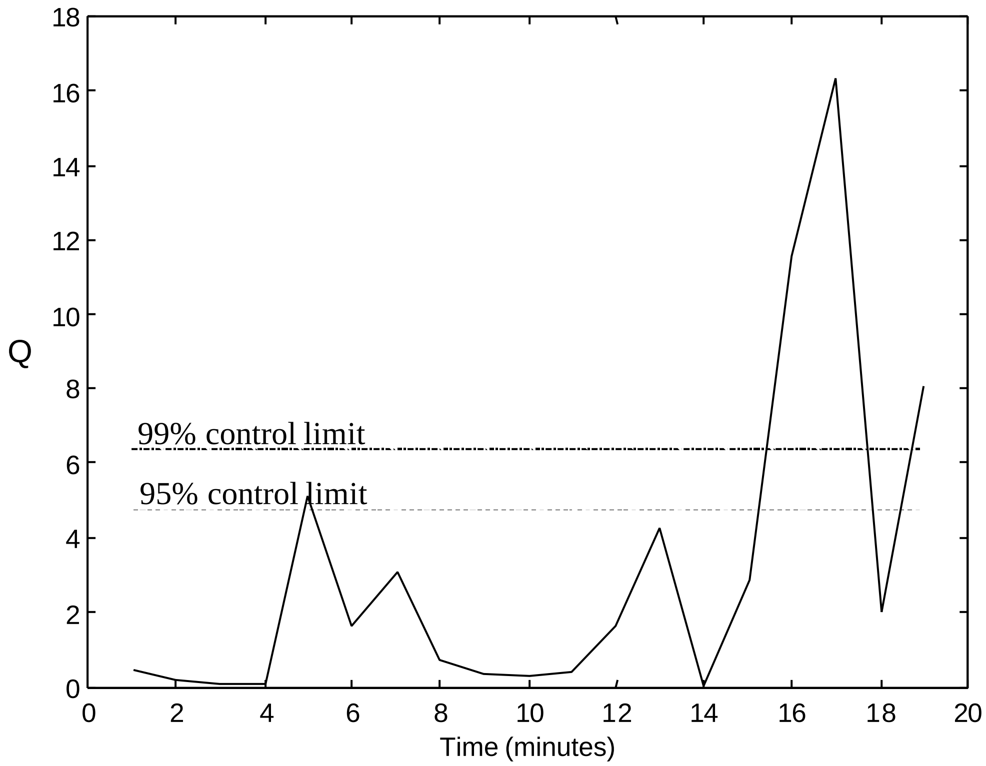

Figure 3.2. Example of a Q plot. Fault detected at time 15 (minutes)

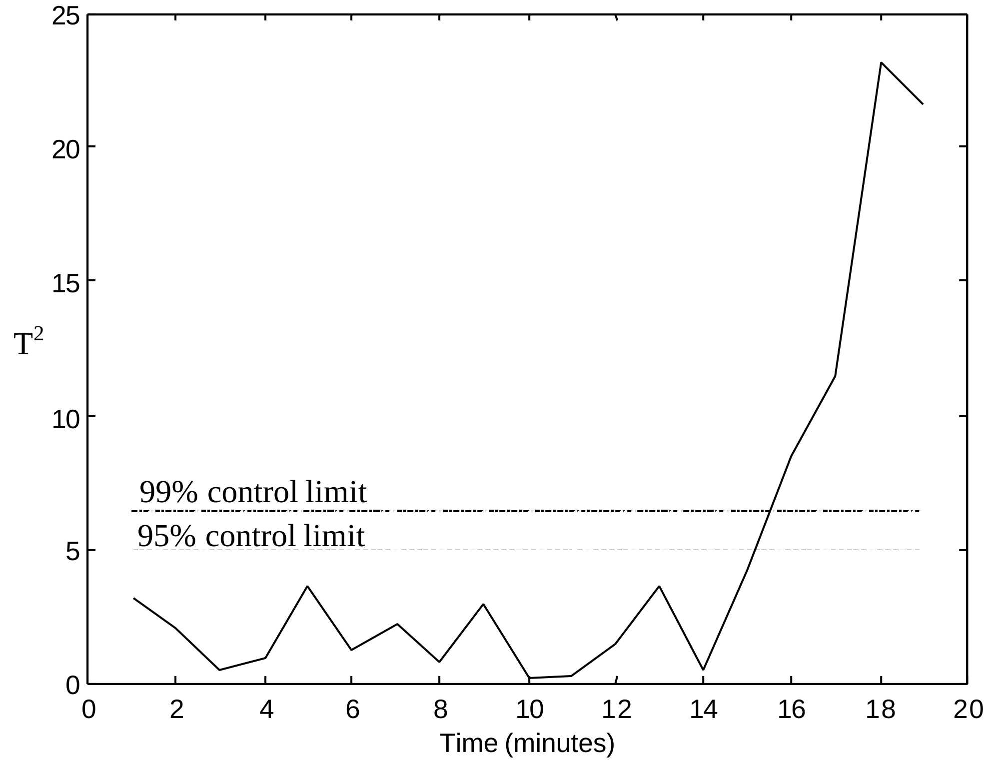

Figure 3.3. Example of a T^2 plot and the control limits. Fault detected at time 15 (min.)

Therefore, the on-line determination of T^2 and Q allows to detect a fault. Figures 3.2 and 3.3 show an example where the explained process monitoring charts permit to detect a fault. Other monitoring charts can be displayed (e.g. plots of one principal component against other). From the analysis of different monitoring charts a fault can be diagnosed.

Multiway Principal Component Analysis (MPCA) has been proposed for batch process monitoring (Nomikos and McGregor, 1994). It will be discussed later on (section 3.4. Fault diagnosis in batch plants).

PCA has problems to handle a nonlinear process because it is a linear technique. Some modifications of conventional PCA are being investigated in order to be applied to the monitoring of chemical plants. A combination of Multiscale PCA with wavelet analysis shows to be superior to conventional PCA (Bakshi, 1998).

Other difficulty of basic PCA method is the isolation of deviations from normal operating conditions when the shifts are relatively small. The *summed-scores construct* have been proposed to improve conventional PCA in this respect (Wachs and Lewin, 1999). Since it can be expected that disturbances propagate in a dynamical system with a given directionality, the summed-scores construct leads to a reinforcement of this directionality, and thus improves the disturbance detectability. Basically, the summed scores approach is an extension of the moving-average technique, to the multidimensional space of scores, obtained from applying the PCA model.

The main drawback of PCA in FD is the fault isolation. Hence, research is focused in this aspect. By using the equivalence between PCA and the parity relation method in order to generate structured residuals, faults can be isolated better (Gertler et al., 1999).

A recent study combine the best of linear PCA and Nonlinear PCA. A multiscale wavelet decomposition is first performed on process data. Then, linear PCA and NLPCA are performed separately. Finally, an ANN is trained using the linear PCA transformed data set as the input layer and the non-linear principal scores as the output layer (Fourie and de Vaal, 2000).

3.1.3. Trend Analysis

QTA transforms the process variable's data in descriptions of its trends in an explicit and meaningful form, in real time (Cheung and Stephanopoulus, 1990). Its application to FD has been performed through a methodology based on the multiscale extraction of process trends (Bakshi and Stephanopoulus, 1994). Its application to real cases is more recent (Vedam and Venkatasubramanian, 1997) and continues being matter of research.

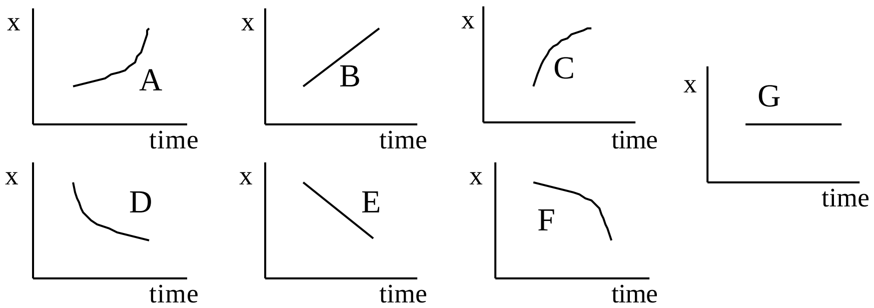

Figure 3.4. Fundamental elements, primitives, the language for sensor trends

The QTA-based monitoring and diagnostic methodology has three main components: the language used to represent the sensor trends, the method used for identifying the fundamental elements of the language from the sensor data and their use for performing fault diagnosis.

The qualitative representation of the trends has fundamental elements called primitives. Examples of them are shown in Figure 3.4. Groups of primitives form episodes and episodes combined form a trend.

The method utilised for primitive identification can be based on first and second derivatives of the process trend calculated using the finite difference method. Other method is the use of an ANN, taking advantage of its ability to learn from examples and its tolerance to noise.

The primitives thus identified are used in a knowledge base (KB) to perform fault diagnosis. A key consideration is the window over which the trend is being identified. The window should be large enough to capture the process dynamics. Vedam and Venkatasubramanian (1998) used a B-Spline based compression method to identify piecewise linears from the trend wherein the window is adaptive to the sensor trend.

The general scheme of a QTA framework is shown in Figure 3.5 (Dash and Venkatasubramanian, 2000). The approach consists of extracting out the features (trends and frequencies) from the sensor data. The identified trends (Primitive identification) are used for the purpose of matching against a knowledge base for the diagnosis of known events. Hence, the known events are reported. The unknown events are characterised by abnormal frequencies (Window size distribution). These novel events are reported as high certainty events if they are significant in terms of magnitude. Otherwise, they are logged as medium certainty events. Once the operator annotates the novel high certainty events, using annotations and the historical data, the current knowledge base is updated. Thus, the system is capable of on-line learning/adaptability. Honeywell has licensed this technology developed at Purdue University for incorporation into an intelligent control system called Abnormal Events Guidance and Information System (AEGIS). The development of the AEGIS is being carried out with the support of the ASM Joint Research and Development Consortium led by Honeywell. It was formed in 1992 to develop the technologies needed to allow plant operations personnel to control and prevent abnormal situations (http://www.honeywell.com). The problems with this technique for real-time implementation on large-scale processes are: the large amount of data to be processed, the need to distinguish between operational and abnormal events, unclear definition of normal operation, and incomplete annotations, among others.

Process trending is being exploited as key tool for process monitoring. A statistical approach to wavelet-based trending has been recently proposed (Bakhtazad et al., 2000). That system uses hidden Markov models.

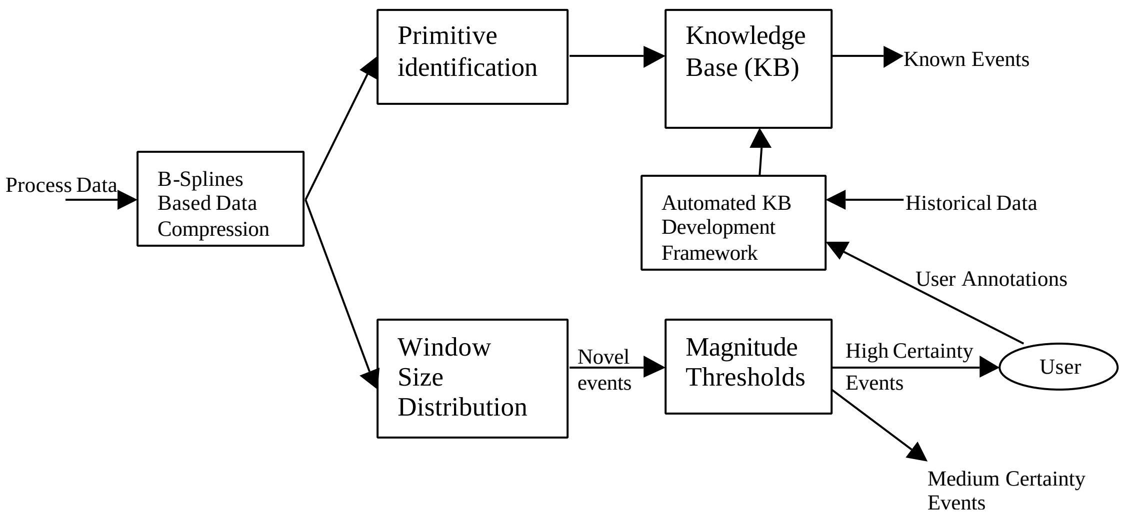

Figure 3.5. Qualitative Trend Analysis framework

3.2. Knowledge-based methods

The second group of methods correspond to the techniques that require a more detailed knowledge about the process. Model based methods and inference systems are included in this group. Observer Based Methods -OBMs- (Patton, et al., 1989), Assumptions Based Methods -ABMs- (Petti et al., 1990), Signed Directed Graph (SDG) method (Wilcox and Himmelblau, 1994), and fuzzy logic expert systems (Tarifa and Scenna, 1997) are the most representative of this group. They are difficult to implement, require a lot of work for maintenance but their structure is transparent.

3.2.1. Observer based methods

It is one of the most known residual based technique. It consists of two steps: residual generation and decision process to identify the cause. Figure 3.6 shows a simple scheme of an OBM. Faults are detected by setting a (fixed or variable) threshold on each residual signal. A number of residuals can be designed, each having a special sensitivity to individual faults occurring in different locations in the system. The subsequent analysis of each residual, once a threshold is exceeded, then leads to fault isolation. Therefore, the essential issue is the residual generation.

The residual generation can be performed in different forms: hardware redundancy using parity equations, state and parameter estimation. The OBMs use state estimation for residual generation. A model of the process in state-space form is needed:

$$\frac{dx}{dt} = Ax + Bu + Ed + Ff \tag{3.8}$$

$$y = Cx + Du \tag{3.9}$$

x: states; *u*: inputs; *y*: outputs; *d*: disturbance; *f*: faults; and *A, B, C, D, E, F* are the corresponding matrices to be determined.

The basic idea behind the OBM is to estimate the outputs of the system from the measurements (or a subset of measurements) by using either Luenberger observer(s) in a deterministic setting or Kalman filter(s) in a stochastic setting. Then, the (weighted) output estimation error (or innovations, in the stochastic case), is used as a residual.

With respect to the estimation using Kalman filters, some techniques are being investigated in order to perform simplifications and to consider non-linear systems using Extended Kalman Filters -EKFs- (Chang and Hwang, 1998). These EKFs linearise about the current mean and covariance.

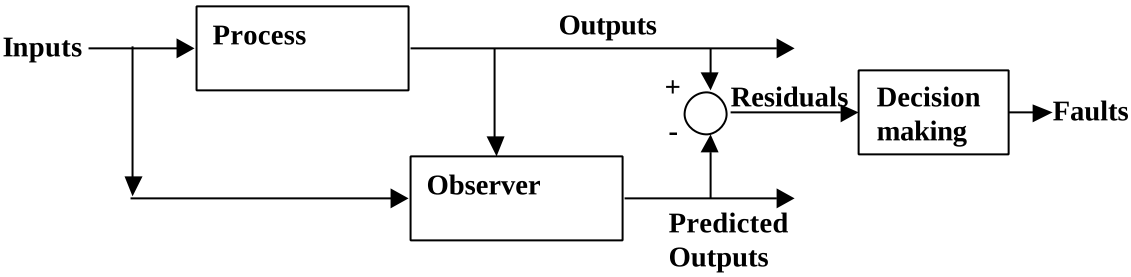

Figure 3.6. General Observer based method scheme

There are robustness problems with respect to modelling errors and disturbances. They are being considered in recent works (Patton and Chen, 1997; Chen and Patton, 1998).

The extension of the existing results of this linear technique to the non-linear case is not an easy task. With the application of non-linear observer theory some results have been obtained, principally in the detection and, with some restrictions, also in the isolation of faults. Some problems taking into consideration more general models as well as the design of the corresponding non-linear observers are still open, because of the difficulties of estimating the state or the measurement vector of a non-linear system, even if the nonlinearities are known and no disturbances are present.

Alcorta García and Frank (1997) present a survey of the principal observer-based approaches to FD for deterministic non-linear dynamic systems. A complete solution to the fault detection problem for a general non-linear model is still unsolved. Some approaches can solve non-linear problems but expressed in special forms. Because the detection of faults is a necessary condition for their isolation, the general fault-isolation problem for non-linear systems is still also unsolved.

The use of adaptive observers could provide a solution to the fault isolation problem. With respect to the threshold selector, an optimal one which finds a compromise between robustness and fault sensitivity could improve the solutions to the FD problem.

In summary, the main drawbacks of the OBMs are the following. First, it is difficult to obtain adequate models. And second, most work is restricted to linear systems and although theory is well developed for such systems, methods for non-linear chemical processes are restricted.

3.2.2. Assumption based methods

These methods attribute the residual to the violation of certain assumptions regarding the normal behaviour of the system.

An algorithm called the diagnostic model processor has been introduced by Petti et al. (1990). It uses the satisfaction of model equations from process plants to arrive at the most likely fault condition. The KB consists of a vector of model equations. These statements are merely listed as a series of governing equations that describe the process. Associated with each model equation are tolerance limits, which give an indication of when the equation is no longer representative of the process. Also needed is an expression for determining the sensitivity of each model equation to various parameters. A set of assumptions is associated with each model equation. A simple example of the formulation of a model equation and the associated assumptions (possible faults) is illustrated in Figure 3.7. A model equation can be written for the mass balance about the tee:

$$e_1 = (r_1 F_1) + (r_2 F_2) + (r_3 F_3) \qquad (3.10)$$

where e_1 is the residual, r the density and F the flow rate of the streams.

The assumptions associated with this equation would be:

- The sensors are functioning and correct
- The fluids have the expected densities
- There are no piping leaks

The method uses the fact that violation of a model equation indicates that at least one of its associated assumptions is invalid. By examining the direction and extent to which each equation is violated, and by considering the assumptions on which they depend, the most likely failed assumption can be deduced. An assumption that is common to many violated equations is strongly suspect, whereas satisfaction of equations provides evidence that associated assumptions are valid. The system architecture is shown in Figure 3.8. An important drawback of the system implementation is that balances that require unavailable measurements can not be used.

Dhurjati (1998) summarised the lessons learned with the implementation of an assumption based system in industrial plants. Not only the non-availability of sensor measurements is a difficult but also the accessibility to experts, non-availability of knowledge in the form of heuristics or models, complicated process dynamics, knowledge validation, exclusive dependence on a simple methodology and human factors are important challenges.

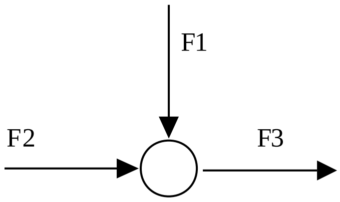

Figure 3.7. Mixing tee example for model equation formulation

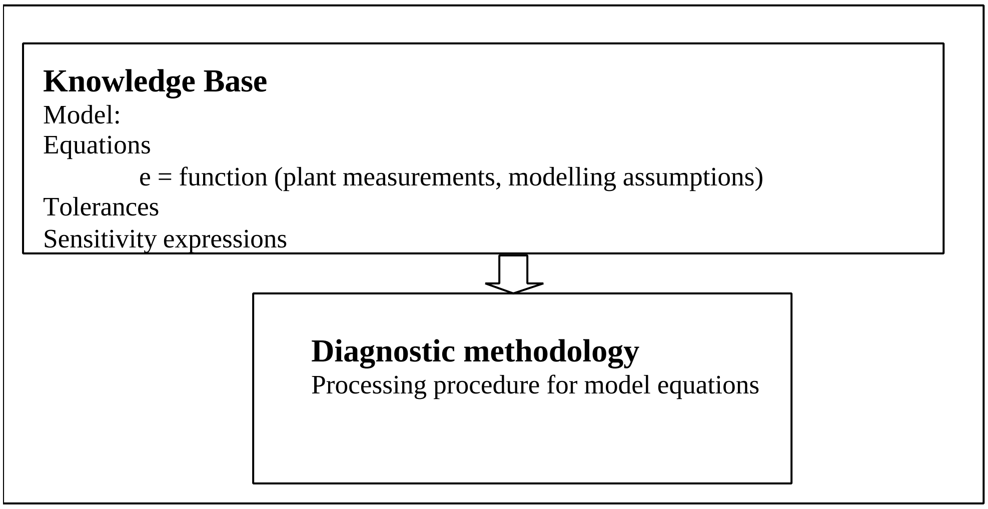

Figure 3.8. Diagnostic model processor, an Assumption Based Method

3.2.3. Signed Directed Graphs

SDG is a representation of the causal information, similar to fault trees, which is other strategy. The process variables are represented as graph nodes and causal relations by directed arcs. Figure 3.9 shows the signed digraph for the simple example of two tanks in series, also shown in the same Figure 3.9. *F0*, *F1* and *F2* represents flows and *L1* and *L2* represents levels.

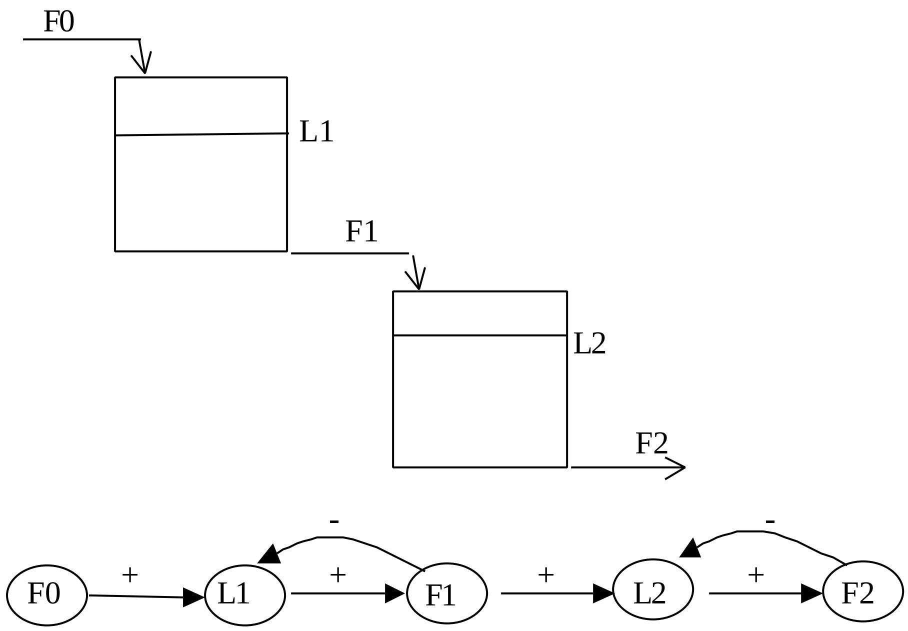

Figure 3.9. Two tanks in series and the corresponding signed digraph

The state of the system is described qualitatively by a pattern. Table 3.1 describes a possible pattern for the two tanks in series. The cause-effect graph is a subgraph of the signed digraph consisting of valid nodes (any node which is abnormal) and consistent branches (a consistent path for the propagation of the influence of its initial node to its terminal node). Given the pattern in Table 3.1 and signed digraph in Figure 3.9, the corresponding cause-effect graph is shown in Figure 3.10.

Table 3. 1. A possible pattern for two tank in series

Variable	F0	L1	F1	L2	F2
Pattern	High	High	High	Normal	Normal

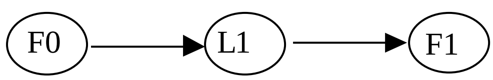

Figure 3.10. The cause-effect graph for the pattern of Table 3. 1.

The Possible Cause-Effect Graph (PCEG) was introduced by Wilcox and Himmelblau (1994) as a generalization of the SDG. There are two concepts involved in representing the process state relative to the PCEG: the representation of the complete state using a pattern, and the representation of incomplete knowledge of the process state using a constraint. An example of a constraint is shown in Table 3.2. With the definition of the patterns and the constraints, the diagnostic problem can be defined as a composite of these two structures. Diagnosis or generation of an explanation sketch occurs through the determination of the cause-effect graph.

Table 3.2. An example of a constraint representing incomplete knowledge of the process state for the example of the two tanks in series

Variable	Constraint
F0	High, Normal, Low
L1	High, Normal, Low
F1	High
L2	High, Normal, Low
F2	Normal

Implementation of the PCEG model requires three basic capabilities:

- The ability to construct the PCEG
- The ability to construct the constraint representing the current state of the process
- The ability to implement an effective inference strategy

A number of approaches exist that can be used to construct the PCEG and the constraints: direct specification in a general-purpose programming language, use of a structure editor, or implementation of a special purpose language. However, the most important part of the implementation of the PCEG model is the inference strategy.

A big drawback of techniques based on cause-effect reasoning is the generation of a large number of hypothesis. The high computational requirements are high, too. Therefore, low resolution but high completeness is the feature of these kind of approaches which facilitate explanation generation.

Recent works considered the use of wavelets as signal preprocessors in order to perform SDG in processes with load-fluctuations (Tsuge et al., 2000).

3.2.4. Fuzzy logic expert systems

There is a great improvement respect to the Rule-Based (RB) methods. RB methods are made up of an antecedent part (series of events) and a consequence part, which maps these events to a known fault. The main advance corresponds to the use of fuzzy logic in the RB methods. In the case of Fuzzy Logic Systems (FLSs) the rules are put in a fuzzy way. Some authors include this technique in the group of historical-based methods because this information is useful to construct the rules. Historical data can be used to tune the FLS.

Tarifa and Scenna (1997) reported the development of a method consisting in fuzzy logic expert system. It has been shown good performance with large and batch processes (Tarifa, 1995). The method has two stages, the first one is done in off-line mode while the second one is carried out in on-line mode. In the off-line stage a SDG is used to model the process to be supervised. Besides, all the potential faults are determined using tools of the Reliability Engineering (e.g. Hazard and Operability analysis). Afterwards, all the possible patterns of each potential fault are found out by a Qualitative Simulator. Finally, these patterns are compiled into IF-THEN rules, one rule for each potential fault. This set of rules is the KB to be used by an Expert System. The off-line stage must be done only once for each new process to be supervised, and the time is not a critical variable. Conversely, the on-line stage must operate with the supervised process, and the time is a critical variable. In this stage, an Expert System evaluates the set of rules using data about the actual process state. Fuzzy logic is used in the evaluation to overcome the problems caused by the data noise, compensatory response, inverse response, and the model limitations. Moreover, additional information from the Qualitative Simulation is used to explain the diagnosis. If it is necessary, this information is also used to improve the diagnosis. Previous methods have not these important feature.

3.3. Combinations

Finally, in order to combine the strengths of both pattern recognition and inference methods, adaptive Neuro-Fuzzy (NF) systems are being developed. The idea is to obtain an adaptive learning diagnosis system with transparent knowledge representation. Some combinations are subject of current research (Leonhardt and Ayoubi, 1997): ANNs influenced by fuzzy logic (e.g., fuzzy models within ANNs), fuzzy systems influenced by ANNs (e.g., serial configuration), and hybrid NF systems. In the last years, the application of combined methods for fault diagnosis has steadily been growing (Issermann and Ballé, 1997).

Table 3.3. Classification of FD methods and their attributes

Methods' classification ▸ Attributes ▾	**Historical based**			**Knowledge-based**					**Cs**
				Inference		*Model-based*			
	ANN	PCA	QTA	FLS	RB	SDG	ABM	OBM	NF
Fastness	✓	✓	✓	✗	✗	✗	✗	✓	✓
Isolability	✓	✗	✗	✓	✗	✗	✗	✓	✓
Robustness	✓	✗	✗	✓	✗	✗	✗	✓	✓
Novel identifiability	?	✓	✓	?	?	✓	✓	✓	?
Multiple fault ident.	?	✓	✓	✓	?	✓	✓	✓	✓
Explanation facility	✗	✗	✗	✓	✓	✓	✓	✗	✓
Adaptability	✓	✓	✓	✓	✓	✓	✗	✗	✓
Computational Req.	✓	✓	✓	?	✗	✗	✗	✗	?

Cs: Combinations; ✓: Favourable; ✗: Not favourable; ?: Situation dependent

A comparison of the methods can be seen in Table 3. 3. A single method is inadequate to handle all the attributes of an ideal FDS.

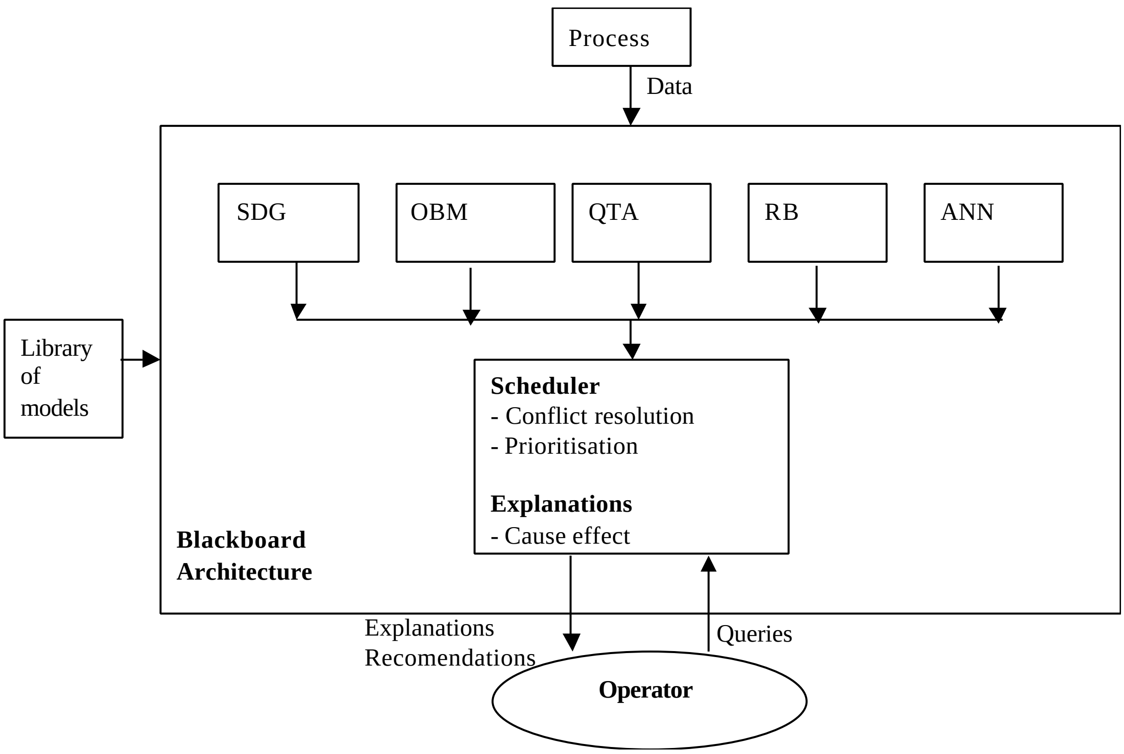

Figure 3.11. Blackboard architecture for a hybrid framework

A hybrid framework, in which different diagnosis methods are integrated to perform collective problem solving has been shown to display a lot of promise (Myralaswamy and Venkatasubramanian, 1997). The philosophy behind it is similar to using a panel of expert physicians to diagnose a complex illness. Following this idea, a blackboard architecture has been proposed. Figure 3.11. shows it schematically. The components are a collection of one or more diagnostic methods discussed earlier, the blackboard (a placeholder for various process states), a scheduler which mainly resolve the possible conflicts in the results from the experts, the plant input-output interface and the operator interface. However, its implementation does not seem very easy. Otherwise, industrial implementations of such system have not been reported, only some simulation results have been shown.

Recently, Vedam et al., 1999, presented a combination of PCA-SDG and a system based on QTA. An algorithm based on rules solve the possible conflicts that can exist between the individual results from each of the previous systems.

An agent-based framework for the diagnosis of chemical processes, based on spatially distributed diagnosis architecture, has been recently proposed (Soo Young Eo et al., 2000). It uses only the information about process topology and control structure.

The problems of maintenance and implementation of individual methodologies makes industrial implementation of hybrid frameworks difficult. A complex task is the conflict resolution. On the other hand, the use of combinations, where methods are adapted to each other in order to enhance the advantages and to reduce the drawbacks seems to be the right choice.

3.4. Fault Diagnosis in batch processes

Most of the FD approaches presented so far show to be applicable to steady-state processes. These approaches, as explained before, can be divided in three groups: historical based methods, knowledge based techniques and combinations of both. However, the application of these diagnosis approaches to batch chemical processes is usually difficult.

In the past decades, research was focused on the use of either fundamental models or detailed knowledge based models. The first monitoring procedure is based on estimation methods. The second relies on the knowledge of the operators and engineers about the process.

More recently, the use of pattern recognition methods based on ANNs and the use of statistical techniques are matter of research. There are few applications reported in relation to the use of ANNs for FD in batch processes. Some interesting results have been obtained at pilot plant scale and in simulated cases (Tsai and Chang, 1995). The problem of the traditional ANNs related to totally capture the space and time characteristics of process signals is overcome with the use of wavelet functions. Studies on wavelet functions, of extensive use in signal processing, have advanced rapidly in the last years. Its application to fault diagnosis is being performed in two ways:

- For feature extraction; the wavelet function outputs are then processed either by an ANN (Chen et al., 1999), by Qualitative Trend Analysis (Vedam and Venkatasubramanian, 1997), or by a Principal Component Analysis approach (Bakshi, 1998);
- As an activation function of the ANN (Zhao et al., 1998).

With respect to the use of statistical techniques, there are several procedures developed and under investigation to apply PCA on the batch process monitoring.

MPCA has shown good results for on-line batch process monitoring (Nomikos and Mc Gregor, 1994; Lee et al., 1999). The only information needed is a historical database of past batches. However, it has some drawbacks like the difficult isolation and localisation of the fault.

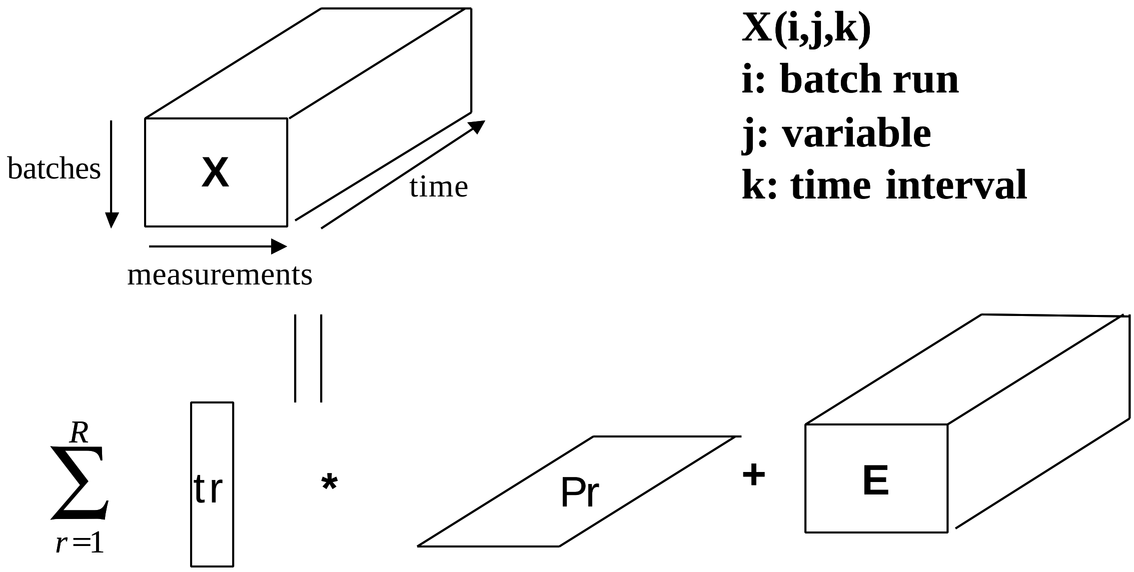

Figure 3.12. Arrangement and decomposition of a three-way array by MPCA

MPCA consists in treating multidimensional matrices in a better way than the conventional PCA. The relation between MPCA and PCA is that MPCA is equivalent to performing ordinary PCA on a large two-dimensional matrix formed by unfolding the three-way array $\underline{X}$. The matrix $\underline{X}$ is built in the following way. Consider a typical batch run in which $j=1,2,...,J$ variables are measured at $k=1,2,\ ...,\ K$ time intervals throughout the batch. Similar data will exist on a number of such batch runs $i=1,2,\ ...,\ I$. All the data can be summarised in the $\underline{X}$ *(IxJxK)* array illustrated in Figure 3.12. The objective is to decompose the three-way array $\underline{X}$ into a series of principal components consisting of score vectors (t_r) and loading matrices (P_r), plus a residual matrix $\underline{E}$. The *ith* elements of the *t*-score vectors corresponds to the *i*th batch and summarise the overall variation in this batch with respect to the other batches in the database over its entire duration. The *P* loading matrices summarises the time variation of the measurement variables about their average trajectories. Once historical data of normal batches are treated in the explained way, the implementation of the on-line MPCA is as follows:

1) Take the new vector of measurements at time interval *k*.

2) Substract the means and divide by standard deviation, which corresponds to the *k*-th time interval from the normal database to get the vector with the current deviation.

3) Set the rows of X_{new} from *k* onward equal to the current deviation vector.

4) $$t_{r,k} = X_{new} \circ P_r \qquad (3.11)$$

$$E = X_{new} - \sum_{r=1}^{R} t_{r,k} \otimes P_r \qquad (3.12)$$

$$SPE_k = \sum_{j=1}^{J} E(k,\ j)^2 \qquad (3.12)$$

The matrix operations are:

$$t = \underline{X} \circ P \text{ ----->} \ t(i) = \sum\sum X(i,\ j,k)P(k,\ j) \qquad (3.13)$$

$$\underline{X} = t \otimes P \text{ ---->} \ \underline{X}(i,\ j,k) = t(i)P(j,k) \qquad (3.14)$$

5) Return to step 1.

If the batch that is being monitored is normal, the residuals *E(k,j)* should be small, and its score values ($t_{r,k}$) should continue to fall within the region of variation defined by the reference distribution.

The use of this technique is illustrated in the present thesis (see the Chapter 7. Results and discussion, section 7.2.3) because it has been used for comparison purposes.

Batch analysis and monitoring method based on MPCA and Multiway Partial Least Squares (Multiway PLS) have been extended by using multi-block-multiway Partial Least Squares (Kourti et al., 1995). This extension allows one to utilize the historical data on the measured process variable trajectories, the measured feed-stock properties and other variable initial conditions and the final product quality measurements at the end of each batch.

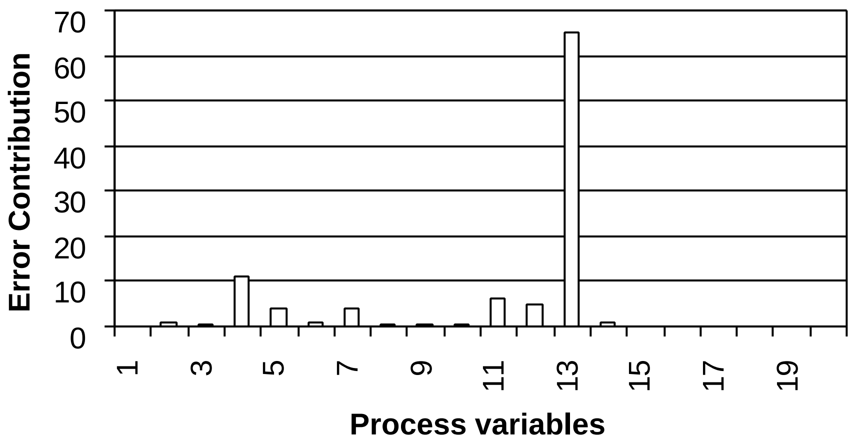

Figure 3.13. % Contribution to the SPE value for all processes variables at a time k for an abnormal batch (taken from Tates et al., 1999)

Recent works in the area of on-line batch process monitoring based on MPCA are related to fault isolation. It is performed by analysing the monitoring charts. Tates et. al, 1999, consider the use of batch contribution plots. They consist in the plot of the contribution of process variables to the SPE value at each time instant. By this way, the deviated process variable can be analysed to determine the root cause. Figure 3.13 shows an example. The variable number 13 (e.g. reactor level) presents the larger error contribution and the fault is localised in relation to it.

The use of external information, batch run specific or process specific information can improve the methodology of on-line MPCA. The objective is to increase the detection capability and/or the diagnostic capability (locating and finding the causes of the fault). This combination has been introduced by Smilde et al., 2000.

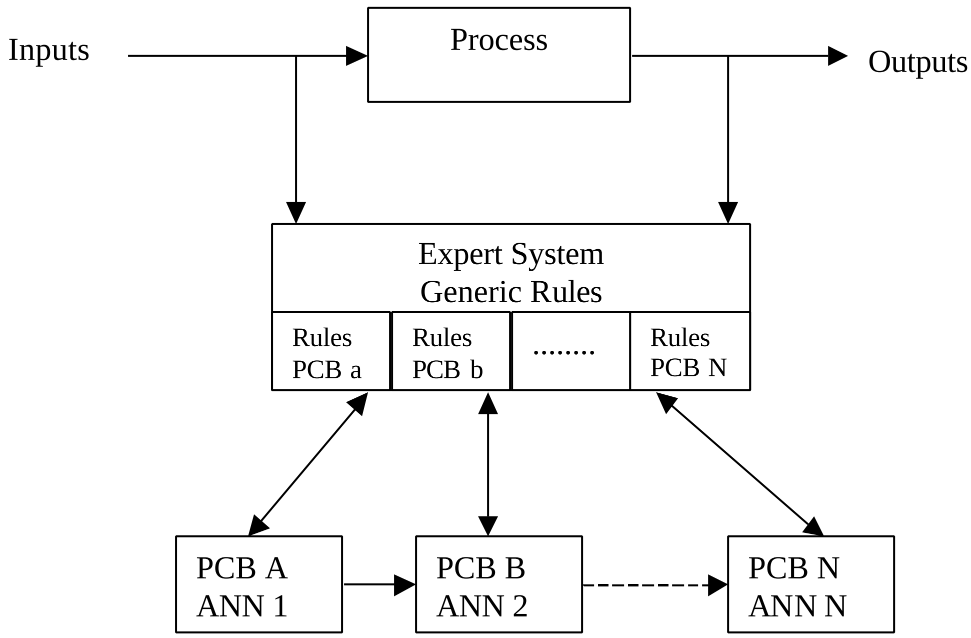

Figure 3.14. Hybrid modular hierarchical architecture for FD in batch plants

In relation to the already mentioned combination methods for FD, there are very few reports of their applications to batch processes.

Frameworks of integration of MPCA and knowledge based fault diagnosis is being tried at pilot plant scale (Leung and Romagnoli, 2000).

A hybrid modular hierarchical approach has been proposed for FD in batch plants (Scenna et al., 2000). By using such modular architecture the temporal evolution of the process is divided in a set of a temporal invariant modules (models). Each qualitative partition of the process is called Pseudo Continuous Block (PCB). Different temporal parts of the batch process are qualitative assimilated to continuous processes.

This system architecture has been implemented using a set of ANNs, that is a modular system, identifying each ANN with a portion of the temporal evolution of the process. Besides, the control unit includes an Expert System conforming a hybrid hierarchical system, which uses the outputs of the ANNs in addition to process variables for the FD (Figure 3.14). The developed approach has been successfully applied to a batch distillation column. The type of ANNs used in that work were the SOMs.

The necessities of the information support system for the plant includes the integration of different hierarchical levels as well as specific developments in the programming, monitoring, diagnosis and control (Reklaitis, 1996). The integration of FD and the scheduling and planning system in multipurpose batch chemical plants is matter of current research. In batch plants, it is difficult to predict the processing times of each unit. The variability is due to different deviations such as equipment faults, fluctuations in utilities availability and changes in the quality of raw materials. The modification of the schedule in the most effective way is called “reactive scheduling”. A scheme based on the heuristic of the least impact has been proposed by Kankamedala et al., 1994. Scheduling in multipurpose batch chemical plants in the presence of uncertainties has been considered recently (Sanmartí et al., 1997). Puigjaner and Espuña (1998) proposed a integrated system of management and control in the manufacturing batch industry.

In all the above cases, the main problem is the complex strategy of implementation that delays their application in real industrial plants. It is important to take into account that the information given by the FDS of a batch plant has to be used at different levels in the decision-making hierarchy structure, including the advanced control system and the scheduling system. While developing and implementing a FDS, this important aspect must be considered.

Acronyms

ABM	Assumption Based Method
AEGIS	Abnormal Events Guidance and Information System
ANN	Artificial Neural Network
ASM	Abnormal Situation Management
BPN	Backpropagation Artificial Neural Network
EKF	Extended Kalman Filter
FD	Fault Diagnosis
FDS	Fault Diagnosis System
FLS	Fuzzy Logic System
IFAC	International Federation of Automatic Control
KB	Knowledge Base
KBES	Knowledge Based Expert System
MPCA	Multiway Principal Component Analysis
NF	Neuro-Fuzzy
NLPCA	Nonlinear Principal Component Analysis
OBM	Observer Based Method
PCA	Principal Component Analysis
PCB	Pseudo Continuous Block
PCEG	Possible Cause-Effect Graph
PLS	Partial Least Squares
QTA	Qualitative Trend Analysis
RB	Rule Based
RBFN	Radial Basis Function Neural Network
SDG	Signed Directed Graphs
SOM	Self Organising Map
SPC	Statistical Process Control
SPE	Squared Prediction Error

Notation

E	Residual matrix for a new batch
$\underline{E}$	Residual matrix for historical database
i	Index for batches (or for samples)
I	Total number of batches
j	Index for measurements variables
J	Total number of measurements variables
k	Index for time intervals
K	Total number of time intervals
p	Principal components loading vector
P	Principal components loading matrix
P^T	Transpose of matrix P
Q	Sum of squares of the residuals
r	Index for principal components
t	Principal component scores vector
T	Principal component scores matrix
T^2	Overall measure of variability
X	Bidimensional matrix
$\underline{X}$	Tridimensional matrix