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SELECTION OF SENSORS BY A NEW METHODOLOGY COUPLING A CLASSIFICATION TECHNIQUE AND ENTROPY CRITERIA

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Abstract: Complex industrial processes invest a lot of money in sensors and automation devices to monitor and supervise the process in order to guarantee the production quality and the plant and operators safety. Fault detection is one of the multiple tasks of process monitoring and it critically depends on the sensors that measure the significant process variables. Nevertheless, most of the work on fault detection and diagnosis found in literature place more emphasis on developing procedures to perform diagnosis given a set of sensors, and less on determining the actual location of sensors for efficient identification of faults. A methodology based on learning and classification techniques and on the information quantity measured by the Entropy concept, is proposed in order to address the problem of sensor location for fault identification. The proposed methodology has been applied to a continuous intensified reactor, the 'open plate reactor (OPR)', developed by Alfa Laval and studied at the Laboratory of Chemical Engineering of Toulouse. The different steps of the methodology are explained through its application to the carrying out of an exothermic reaction.

Keywords: fault detection; sensor location; learning; classification; information theory; intensified reactor.

INTRODUCTION

Undetected abnormal process behaviours have a serious impact on product quality, safety, productivity, pollution and economical levels. Hence, chemical industries need efficient automated supervision systems in order to detect, diagnose and correct such abnormal behaviours. In the past decades this area has considerably attracted the attention of researchers. A variety of approaches have been proposed for the development of improved supervisory systems. Most of the approaches for fault detection and diagnosis involve, in some way, the comparison of the observed process behaviour to a reference model. Thus, the efficiency of the diagnosis system depends on the number of process sensors and the selection of the important process variables to be monitored. Increasing the number of sensors will increase the information that can be obtained from the process,

but it will also increase the induced instrumentation cost associated with the process measurement system. Therefore, there is a need to design a reliable fault-monitoring system for the safe operation of typical industrial process, allowing a reduction of the instrumentation costs.

The problem of optimal sensor location is of crucial importance, as all the fault-diagnosis techniques depend on a given set of observed fault symptoms. Nevertheless, the emphasis of most of the work on fault diagnosis has been directed towards procedures to perform diagnosis given a set of sensors rather than on performing the actual selection of sensors for efficient fault identification. Some researchers have addressed the problem of sensor location for fault diagnosis. Fault-trees with given fault probabilities were used by (Lambert, 1977) to analyse the location of sensors depending on the effect of basic units (failure origins) on the process

variables. This work was the first based on a diagnosis observability criterion for the design of sensor location. Ali and Narasimhan (1993) extended the observability measurement for sensor network design considering the reliability of linear processes. Chang *et al.* (1993) developed an optimal strategy for the design of model-based fault-monitoring systems using the concepts of fault observability and fault resolution. They proposed a trial-and-error algorithm that uses a diagnosis efficiency table. Raghuraj *et al.* (1999) proposed algorithms to solve the problem of sensor location based on various fault diagnosis observability and reliability criteria. In their work use is made of a digraph that represents the cause-effect behaviour of the process to identify optimal sensor locations.

In the framework of nonlinear systems Watanabe *et al.* (1985) designed a reduced-order time-varying linear observer for full state estimation. Fault detection and diagnosis are achieved, without any statistical test, by inspection of the state estimates and/or several observer residuals. The optimum sensor location problem is then solved by an exhaustive search for minimizing the observation cost associated to each set of measurements. In the context of structural dynamics Worden and Burrows (2001) presented several methods such as: an heuristic method based on iterative insertion/deletion of sensors, genetic algorithms and simulated annealing, for determining sensor distributions for fault diagnosis. Recently, Yan (2004) presented a method of sensor placement based on diagnosability analysis and the use of analytical redundancy relations (ARR). The evoked approaches are in general either model-based approaches or depend on the mathematical equations in order to represent the process.

In this paper, we address the problem of sensor location for fault detection and diagnosis in complex industrial processes where a mathematical or structural model is not always available or suitable. We propose a methodology based on two principal steps. The first step consists of using classification techniques in order to identify all the observable faults with all the possible measurable process variables. Then, according to the characteristics of the identified classes, the information entropy criterion is used to select a minimum number of sensors which allows the resolution of a maximum number of faults under single-fault and multiple-fault assumptions. The overall methodology will be presented in the following section. Then, the obtained results of its application to a new concept of intensification reactors, the 'open plate reactor (OPR)', developed by Alfa Laval and studied at the Laboratory of Chemical Engineering of Toulouse (Prat *et al.*, 2005) will be detailed.

SENSOR PLACEMENT SUPPORT TOOL

The principal objective of this work is the design of an efficient monitoring system that helps process operators to identify faults in an efficient and fast manner. The basis of any fault detection and diagnosis technique relies on the generation of *a priori* knowledge about the process faults. That is, the characterization of all the known possible faults has to be defined clearly. Once the process faults are characterized, the next problem is the observation of these faults. For this, the *observability* and the *fault resolution* conditions can be introduced (Tanaka, 1989). The concept of observability refers to the condition that every fault identified on a process

must be observed by at least one sensor. This ensures that no fault (at least those known *a priori*) becomes unobserved (or undetected) given a set of sensors. The resolution concept refers to the ability of identifying the exact fault that has occurred. Given the constraints on measurement points, sensors must be placed in such a way that every fault is resolved to the maximum possible extent.

Learning and classification techniques have been used as a basis for the proposed sensor-location methodology. Indeed, these techniques allow the identification and the characterisation of all possible faults in order to establish which features (measurable process variables) provide the most relevant information to detect each fault. In this section some of the techniques most commonly used to define the process faults will be briefly reviewed. Some of the concepts of Shannon's information theory used in the algorithm for the selection of the most relevant sensors will also be described.

Learning and Classification Techniques

The principal aim of classification techniques when used for fault detection is to perform an automatic classification of elements, according to their resemblance to a reference class or prototype. That is, to decide to which class an observed element resembles the most. For this, a classifier must be elaborated allowing the assignment of an observed element to one of the existing classes. The classifier is generally designed using a training set made of the elements for which knowledge of the membership to the various classes may or may not be given. Each element is represented as a vector $x \in \Theta \subset \mathbf{R}^P$, $x^T = [x_1, x_2, \dots, x_P]$ where the dimension P of the space Θ (*description space*), is the number of attributes (available measurements) describing each element. These attributes are called *descriptors*.

The next section gives a brief presentation of the main approaches that we consider convenient for the attempted result.

Clustering methods endeavour to find natural groups of data, according to the similarities among the elements. Typically the *similarity* concept is defined as the distance between a data vector and the cluster prototype (centre). The characteristics of the prototypes are not usually known beforehand; they are chosen randomly and updated at the same time as the partitioning of the data is made. The *K-means* (Jain *et al.*, 1999) and *Fuzzy C-means (FCM)* (Bezdek, 1981) algorithms are based on an iterative optimisation of an objective function (e.g., variability within clusters).

$$J_{FCM}(X, U, V) = \sum_{k=1}^K \sum_{i=1}^N (\mu_{ki})^m D_{ki}^2 \quad (1)$$

Equation (1) represents the objective function for the *FCM* algorithm where: $X = [x_i^j]$ is the $N \times P$ matrix representing the set of elements, $U = [\mu_{ki}]$ is the fuzzy partition matrix with $K \times N$ dimensions which defines the membership degree of each element x_i to each class C_k , where $\mu_{ki} \in [0, 1]$ and $V = [v_1, v_2, \dots, v_K]$ is the matrix of cluster prototypes (centres). $m \in (1, \infty)$ is a weighting exponent that determines the *fuzziness* of the resulting clusters, commonly chosen to be $m = 2$. The only difference with the *K-means*

functional is the $(\mu_{kiA})^m$ term, since the *K-means* algorithm gives a crisp assignment of the elements.

D_{ki}^2 determines the distance measured between the element x_i and the prototype v_k . For the *K-means* and *FCM* algorithms the Euclidean distance is used leading to spherical clusters. The Gustafson and Kessel (1979) algorithm replaces the Euclidean distance by the Mahalanobis distance, which provides ellipsoidal clusters with different orientations and takes into account the correlations of the data points.

A drawback of these techniques is that they are sensitive to the selection of the initial partition since it is made in a random way. Moreover, the number of clusters must be given initially.

Artificial neural networks (ANN)

ANNs refer to a complex nonlinear modelling technique initially based on a human's neuron model. A neural net is used to predict outputs from a set of inputs by taking linear combinations of the inputs and then making nonlinear transformations of the linear combinations using an activation function. Before being used as classifier, a learning step consisting of the determination of the network parameters has to be performed. The most commonly used networks which perform with a supervised learning mode (i.e., when the measurements in the training data set are accompanied by labels indicating the target classes where they belong), are the Perceptron, the multi layer perceptron (MLP) (Mange and Tomassini, 1998), and the radial basis functions (Looney, 1997). In the case of unsupervised learning (i.e., when the measurements do not have explicitly known class labels), the network adapts itself purely in response to its inputs and the resulting classification is examined through global criteria. Some networks are able to model the partition space, usually in terms of a probability density function, or by representing the data in terms of cluster centres and widths. This type of network includes the Gaussian mixture models, the Kohonen networks and most recently the cluster detection and labelling (CDL) network (Eltoft and deFigueiredo, 1998; Lurette and Lecoeuche, 2003). After the learning phase, the network is ready and it can then be used to generate predictions or to classify new data into the existing classes.

Neural nets perform very well in complex, non-linear domains where it becomes more and more difficult to use classical techniques. They also perform well in noisy domains. One of the drawbacks in using ANNs is that the learning step process is generally very slow. Additionally, ANNs do not provide explicit knowledge representation in the form of rules, or in some other easily interpretable forms. The model is implicit, hidden in the network's structure and the optimised weights attached to the nodes.

Principal component analysis (PCA)

PCA is a commonly used multivariate statistical technique that acts in an unsupervised manner (Jackson, 1991; Jolliffe, 1986). They are powerful tools, able to compress data and to reduce their dimensionality so that the essential information is maintained and is easier to analyse than in the original dataset. PCA can be used to compute the principal directions of variability in data, finding an alternative set of axes from which these data can be represented. It indicates along which axis there is the most variation; axes are orthogonal

to each other. In this way the original set of correlated variables are transformed into a smaller set of uncorrelated variables. The new uncorrelated variables are linear combinations of the original variables. These principal components represent the most important directions of variability in a dataset. When plotted, the principal components may reveal natural clustering in the data samples.

PCA have been widely used in the process industries (continuous and batch) for process monitoring, fault detection and diagnosis (Ku *et al.*, 1995; Dunia and Qin, 1998; Singhal and Seborg, 2002).

LAMDA (learning algorithm for multivariate data analysis)

LAMDA is a fuzzy methodology of conceptual clustering and classification. It is based on finding the global membership degree of an individual to an existing class, considering all the contributions of each of its attributes. Attributes can be numeric, symbolic or mixed (it is a real advantage compared to other fuzzy classifiers which can only handle numeric descriptors). A numeric component of x is the normalized value of the attribute, on the contrary if the component is a symbolic descriptor its value is called a 'modality'. The contribution of each descriptor is called the *marginal adequacy degree (MAD)*. When the descriptor is a numerical type, the MAD is calculated by selecting one of the different possible functions (Aguado and Aguilar-Martin, 1999):

'Fuzzy' extension of the binomial function given by

$$MAD[x_j|\rho_{kj}] = \rho_{kj}^{\tilde{x}_j} (1 - \rho_{kj})^{(1-\tilde{x}_j)} \quad (2)$$

where $\tilde{x} = (x - \min x) / (\max x - \min x)$ and ρ_{kj} corresponds to the mean value for parameter (descriptor) j characterizing class k .

Centred functions: if a prototype $\tilde{x} = m$ has to be respected, then a parameter σ measuring the proximity to the prototype is introduced so that $\forall x \neq m: MAD[m|m, \sigma] \geq MAD[x|m, \sigma]$ and for $\sigma_1 \leq \sigma_2 \forall x \neq m$ we have the ordered adequacies $MAD[x|m, \sigma_2] \geq MAD[x|m, \sigma_1]$. A typical function satisfying this condition is the so called Gaussian membership:

$$MAD[x_j|m_{kj}, \sigma_{kj}] = e^{-(1/2)(\tilde{x}_j - m_{kj}/\sigma_{kj})^2} \quad (3)$$

When the descriptor is qualitative, the observed frequency of its attribute modality is used to evaluate the MAD. Marginal adequacies are combined using fuzzy logic connectives (Zadeh, 1978) as aggregation operators in order to obtain the global adequacy degree (GAD) of an individual to a class (Aguilar *et al.*, 1982).

Fuzzy logic connectives are fuzzy versions of the binary logic operators, particularly, intersection (*t-norm*) and union (*t-conorm*). The aggregation function (Piera and Aguilar, 1991) is a linear interpolation between *t-norm* (γ) and *t-conorm* (β) as shown in equation (4), where the parameter α , $0 \leq \alpha \leq 1$, is called *exigency*.

$$GAD(x|C) = \alpha \cdot \gamma[MAD(x_1|C), \dots, MAD(x_P|C)] + (1 - \alpha) \cdot \beta[MAD(x_1|C), \dots, MAD(x_P|C)] \quad (4)$$

The most commonly used fuzzy logic operators are:

$$\begin{aligned} \gamma(a, b) &= a.b \text{ (t-norm) and } \beta(a, b) \\ &= a + b - a.b \text{ (t-conorm)} \\ \gamma(a, b) &= \min(a, b) \text{ (t-norm) and } \beta(a, b) \\ &= \max(a, b) \text{ (t-conorm)} \end{aligned}$$

An element is assigned to the class with the maximum GAD (see Figure 1). To avoid the assignment of a not very representative element to a class, that is an element with a small membership, a minimum global adequacy threshold is employed, called the non-informative class (NIC).

If passive recognition is desired, whenever an element is assigned to the NIC, it is considered unrecognized, whereas if self-learning is allowed (Rakoto-Ravalontsalama and Aguilar-Martin, 1992), a new class is created and initialized with that element and the NIC parameters. On the contrary, if the element is assigned to an existing class and self-learning is selected, the parameters of this class are updated with the values of the element. For the Gaussian membership function, equations (5) and (6) illustrate how the new parameters for class k are calculated, where T corresponds to the number of assigned elements in the class.

$$\hat{m}_{kj} = m_{kj} + \frac{1}{T+1}(\tilde{x}_j - m_{kj}) \quad (5)$$

$$\hat{\sigma}_{kj}^2 = \sigma_{kj}^2 + \frac{1}{T+1}[(\tilde{x}_j - \hat{m}_{kj})^2 - \sigma_{kj}^2] \quad (6)$$

By this mechanism (self-learning) it is possible either to start a classification without any prior information, having only the NIC as an existing class when the first element is processed, or to initialize the procedure by introducing pre-assigned elements given by the process expert. Moreover it is also

possible to keep active the learning ability after a previous phase of directed learning (Kempowsky *et al.*, 2003). The general principle of the algorithm is illustrated in Figure 2.

A procedure has been added to map classes to states: one state can be associated to several classes (Kempowsky, 2004). This characteristic enables one to synthesise the information given to the operator. The number of generated classes can be modified through a variability criterion. As it will be seen subsequently the generation of numerous classes can be interesting when specific short behaviour has to be identified (for example the alarm state preceding the established fault).

Sensor Selection Criteria

The Shannon's information theory and entropy concept

Information theory was proposed by Claude E. Shannon in 1948 (Shannon, 1948), it belongs to the probability field in which a new mathematical model of communication systems is proposed. A postulate of this theory is that information can be treated as a measurable physical quantity, such as density or mass. In this theory, Shannon showed that it was possible to quantify the capacity of information introducing a numerical value via the 'entropy' concept.

The concept of entropy is referred within two fields: physics and information theory. In physics, the entropy is a measurement of the disorder of energy and it increases naturally. The disorder of a system is the number of states in which the system can be. In information theory, the entropy is the quantity that measures the information contained in a data flow. In this work, the concepts of the two approaches are used to calculate the entropy, i.e., the entropy depends on the number of states in the system, and of the probability with which an element of the system belongs to each state.

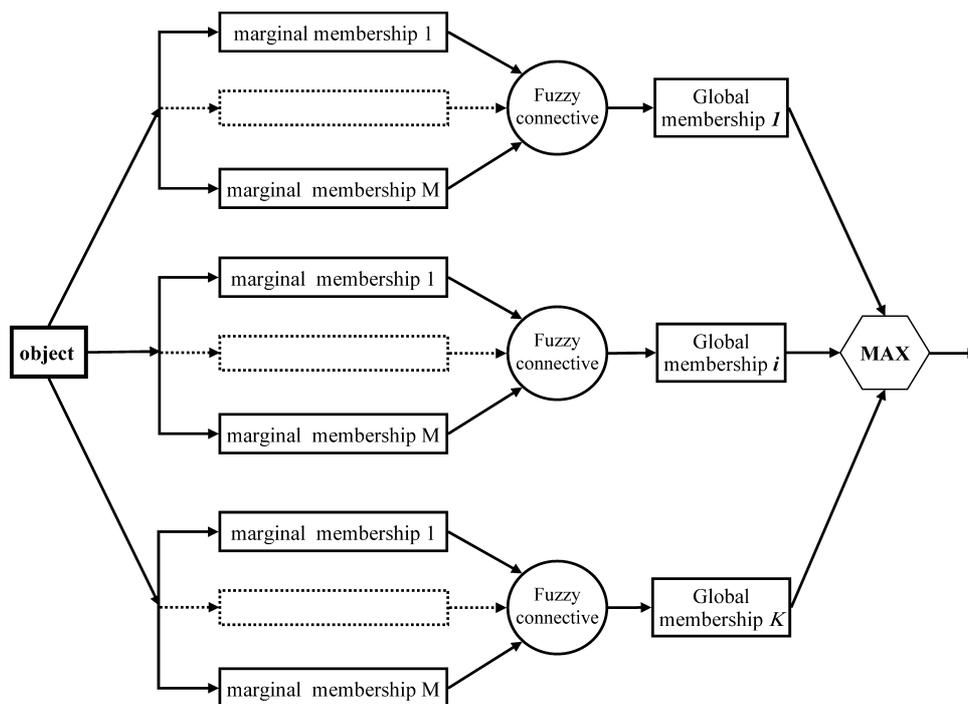


Figure 1. LAMDA algorithm: marginal and adequacies.

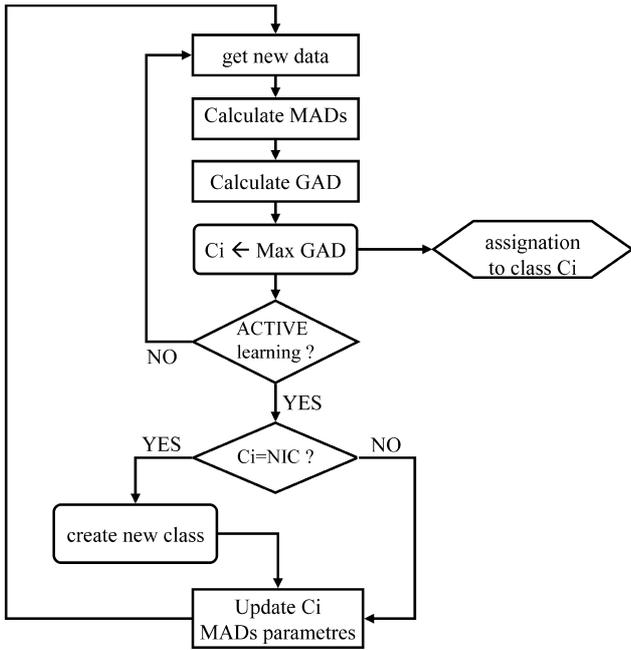


Figure 2. LAMDA algorithm principle: learning and recognition.

Shannon derived his definition of entropy (H) from the following assumptions:

- (1) H should be continuous (proportional) in p_i , i.e., changing the value of one of the probabilities by a very small amount should only change the value of H by a small amount.
- (2) If all p_i are equal, $p_i = 1/n$, then H should be a monotonic increasing function of n . With equally likely events there is more choice, or uncertainty, than when one event is more probable.
- (3) If a choice has to be made in two successive steps, then, the final H should be the weighted sum of the entropies of the two steps.

The only H satisfying the three above assumptions is of the form:

$$H = -K \sum_{i=1}^n p_i \log p_i \quad (7)$$

where K is a constant chosen according to measurement units. Quantities of the form $H = -\sum_{i=1}^n p_i \log p_i$ play a central role in information theory as measures of information, choice and uncertainty and H is named the entropy of the set of probabilities p_1, \dots, p_n .

The entropy in the case of two events with probabilities p and $q = 1-p$, is plotted in Figure 3 as a function of p .

The quantity H has a number of interesting properties which substantiate it as a reasonable measure of choices or information.

- (1) $H = 0$ if all the p_i but one are zero, this one having the value unity. Thus only when we are certain of the outcome does H vanish. Otherwise H is positive.

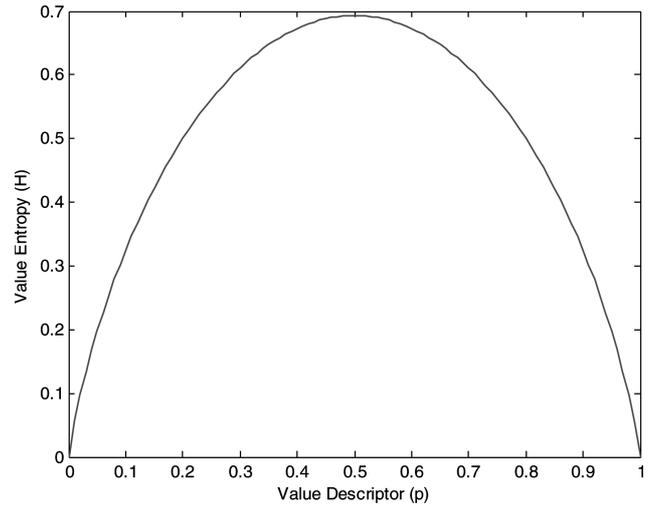


Figure 3. Entropy in the case of two possible events with probabilities p and $(1-p)$.

- (2) For a given n , H is maximum and equal to $\log n$ when all p_i are equal (i.e., $1/n$). This is also intuitively the most uncertain situation.

Information gain

The information gain in the context of diagnosis can be seen as a measurement of the quality of the descriptor for fault discrimination. According to the work of Fernandez Pellon-Zambrano (2002), information gain is the measure which makes possible the quantification of information provided by a descriptor d_j allowing, therefore, the solution of the problem of selecting the most representative features. As presented in equation (8), the information gain is defined as the difference between Shannon's maximum entropy (H_{\max}) and the value of the entropy for the descriptor [$H(C/d_j)$]. The maximum entropy corresponds indeed to the case where the element has the same probability of belonging to any class ($p_i = (1/K) \Rightarrow H_{\max} = \log K$; $K =$ number of classes). The entropy is then interpreted as the classification error of an element to the class. The information gain can be then considered as the inverse of the entropy, i.e., the maximum entropy corresponds to the minimum of information (total uncertainty) and the smaller the entropy is the greater the information will be

$$I_G = H_{\max} - H(C|d_j) \quad (8)$$

where $I_G \geq 0$, $H_{\max} = \log K$, $H(C|d_j) = -\sum_{k=1}^K (p_k) \log (p_k)$ and p_k is the probability that an element belongs to the class C_k (see Figure 4).

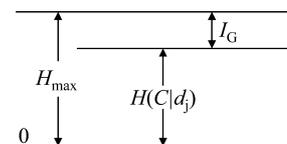


Figure 4. Information gain.

A relative information gain may also be defined as

$$I_G R = \frac{I_G}{H_{\max}} \times 100\% \quad (9)$$

The role of a pertinent descriptor is to maximize the gain to get a better contribution in the detection of the fault.

Design Steps of the Sensor Placement Support Tool

Figure 5 shows a flowchart with the different stages proceeded by the sensor placement support tool. The four main stages are described next.

Fault identification using learning and classification techniques

The first stage enables to identify and characterize all the known process faults or those that can be simulated. In this work, the classification technique used was LAMDA (software tool SALSAs) but the developed methodology is generic and can thus implement any classification technique that gives as a result a matrix binding the classes to the various descriptors and therefore providing information of each class characterizing a process situation. In this 'profile' matrix each row represents a failure of the process and the columns represent all the available descriptors. From the class profile, the contribution of each descriptor to a given situation (class) can then be determined.

Sensor selection

In this step, the entropy and the information gain concepts have been used as means of information measures to determine the quality of each descriptor for the discrimination of faults, i.e., to choose consequently those enabling the detection of all the failures and providing thereafter, relevant

information to establish a diagnosis. The proposed approach consists of calculating the 'probabilistic entropy' and the resulting information gain of each descriptor using a procedure by pairs of classes based on the class profile matrix. Each pair is made up of the normal operation class and a failure or abnormal situation class. The descriptor with the greatest relative information gain will be selected as the most relevant to identify the given process fault.

The total number of formed pairs (Z) is equal to the number of process failures present in the learning dataset. Each pair is described by taking the normal operation class parameters as well as those of a given fault from the profile matrix. Table 1 shows the representation of each pair of classes, where A_{kj} indicates the normalized mean value for descriptor j characterizing class k . In the case of LAMDA algorithm A_{kj} is represented by ρ_{kj} for the fuzzy binomial function or by m_{kj} for the Gaussian function. To better understand this procedure, the estimation of the probabilistic entropy for a descriptor in each pair of classes will be detailed:

If a descriptor d_j has the same value (or more generally a MAD) for the normal class and the failure class (i.e., there is no change in the class profile following the occurrence of a failure for this descriptor), then, since a probabilistic space is considered it will have a normalized value of 0.5, which implies that it will have a maximum entropy value ($\text{Log}2$) (see Figure 3) and a null information gain. On the other hand, if a given descriptor has very different values for the normal class and the failure class (ex. 0 or 1), it will have a value of minimal entropy and in consequence a maximum gain of information. This means that with this descriptor the failure can be observed. Indeed, this descriptor will make it possible to more easily discriminate between the normal operation and the failure.

The procedure by pairs is carried out according to the following steps:

Step 1: To apply the concept of entropy, we must handle a probabilistic space because the sum of the columns on

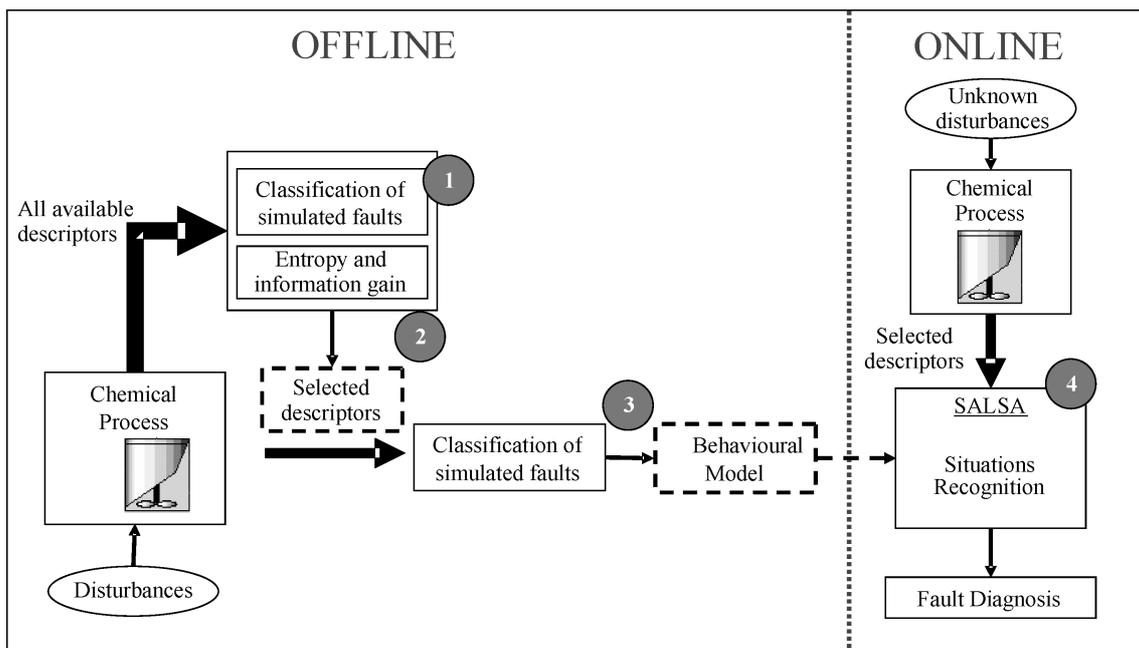


Figure 5. Stages of the methodology for sensor location and fault diagnosis of chemical processes.

Table 1. Description of a normal-fault pair of classes.

Class name	Descriptor 1	Descriptor 2	...	Descriptor P
Class 1: normal state	A_{11}	A_{12}	...	A_{1P}
Class 2: fault	A_{21}	A_{22}	...	A_{2P}

Table 1: $\sum_{k=1}^2 A_{kj}$ is generally different from unity. In order to fit the probabilistic case, each element A_{kj} is normalized with respect to the total sum of the considered descriptor mean values on all the classes:

$$\tilde{A}_{kj} = \frac{A_{kj}}{\sum_{k=1}^2 A_{kj}} \quad (10)$$

where j identifies the descriptor and k the class.

Step 2: The maximum entropy (H_{\max}) of the resulting classification (with two classes) is

$$H_{\max} = \log K; K = 2 \Rightarrow H_{\max} = \log 2 \quad (11)$$

Step 3: The probabilistic entropy to each descriptor is then calculated in the following way:

$$H(\tilde{A}_j) = - \sum_{k=1}^2 \tilde{A}_{kj} \log \tilde{A}_{kj} \quad (12)$$

Step 4: The information gain is evaluated for each descriptor. In this way, it is possible to quantify the information provided by a specific descriptor.

$$I_G = H_{\max} - H(\tilde{A}_j) \quad (13)$$

Step 5: Finally, the relative gain of a descriptor is obtained using the following relation:

$$I_{G \text{ rel}} = \frac{I_G}{H_{\max}} \times 100\%$$

The most relevant or representative descriptor (sensor) for a given fault is that which offers the highest relative gain. This procedure is repeated for all the 'normal-fault' pairs. A flow chart of the procedure by pairs of classes is given in Figure 6. The advantage of this procedure is that the most relevant descriptors for each failure can be directly obtained, since the analysis for each pair is made independently.

Generation of a behavioural pattern of the process

The finality of this section is to obtain a behavioural model of the process that will be used as a reference for the detection of abnormal situations. The aim is to design a classifier characterized by a set of classes which allows the identification of the different process situations (normal operation and failures). The behavioural model is built up offline using the dataset from the previously selected descriptors (process variables) and the LAMDA learning and classification algorithm through the SALSA software tool. The historical dataset for the design of the behavioural model is obtained from all the known available scenarios. Nevertheless, it should be remarked that the behavioural model is far from being complete because of the difficulty in apprehending the exhaustiveness of the faults in a complex process. Moreover,

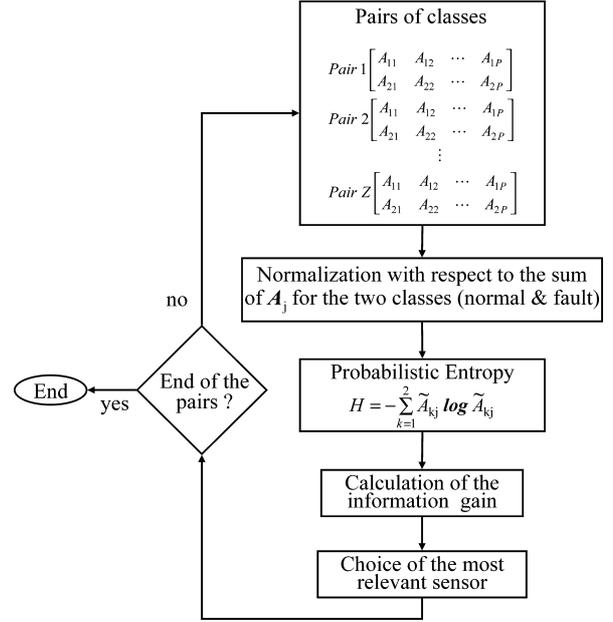


Figure 6. Sensor selection: probabilistic procedure by pairs of classes.

two or more combined faults may induce symptoms that none of them, taken separately could produce (synergy). In addition, progressively with the arrival of new observations, new situations can appear in the initial structure. For this reason, it is necessary that the monitoring system presents an adaptive character at the moment of identifying new situations. A proposition of how these new situations, presented as unrecognised observations, could be considered to complete the behavioural model has been described in Kempowsky *et al.* (2004). Briefly, the principle is to perform a new learning stage considering only the unrecognised observations and preserving the previously validated classes. This has been called 'active supervised learning'.

Online recognition and validation

This last part is devoted to the online recognition of faults whose appearance and amplitude are not previously known. This is done to validate the behavioural model as well as the relevance of the choice of the selected sensors.

Once the behavioural model is built, online situation assessment can be performed. This consists of a process tracking phase, which aim is to associate every new observation to one of the possible process situations recorded in the behavioural model.

PROCESS DESCRIPTION: 'OPEN PLATE REACTOR—OPR'

The methodology of sensor placement has been applied to an intensified reactor developed by Alfa Laval. It is based on heat exchangers technology and combines intensified mixing and reaction with enhanced heat transfer into a single device. This enables the heat of reaction to be removed as rapidly as it is generated. Consequently such a reactor offers many benefits, including improved safety, better product quality, faster throughput and improved energy-efficiency. This allows

performing complex chemical reactions with a very accurate thermal control (Haugwitz and Hagander, 2004, 2005).

The OPR is a plate heat exchanger of new design, where one side is used as a chemical continuous reactor and through the other side a cooling/heating thermal fluid flows, the so called 'utility flow'. The primary reactant $R1$ flows from the inlet to the outlet of the reactor. The secondary reactant $R2$ can then be injected along the reactor side with $R1$ [Figure 7(a)]. Depending on the reaction, there is a need for the utility flow to cool (exothermic reaction) or heat (endothermic reaction) the reactor side. Figure 7(b) displays the schematic representation of the pilot plant; two feeding loops ensure the introduction of the reactants in the reactor at ambient temperature. Each loop is composed of a pump, a valve (V) and a flow rate measurement system (F).

Since the simulated faults will concern the feed (composition, temperature and flow of the primary and the secondary reactant) it is considered that these information are not measured online (otherwise the diagnosis of these faults would be trivial). Similarly, it is considered that measurements of flow and temperature of the utility are not available for the same reason. Most of the available sensors are internal temperature sensors at different locations of the

reactor (Table 2). It is important to indicate that no online composition measurement is available. The absence of concentration measurement is typical in industry especially on chemical units involving more than a binary mixture. The cost of online multi-component composition analysis (when it exists) is still really prohibitive. One of the main objectives of this work is to evaluate how a good placement of rustic sensors (such as temperature sensors) can help to diagnose a drift in the reactant inlet compositions affecting the production quality without performing any direct concentration measurement.

A simulation framework has been developed in order to assess the feasibility and potentialities of new reactions carried out in this reactor (Elgue *et al.*, 2005). The dynamic formulation of the model leads to a hybrid differential and algebraic equations (DAE) system. The solution of this system is obtained by means of a differential and algebraic equation solver: DISCo. The peculiar characteristics of DISCo (operator sparse option, event management procedure, automatic initialization procedure) allow the large dynamic model (integrating up to more than 10 000 equations) to be fast and reliably solved, but also dynamics such as start-up procedures or disturbances to be taken into account.

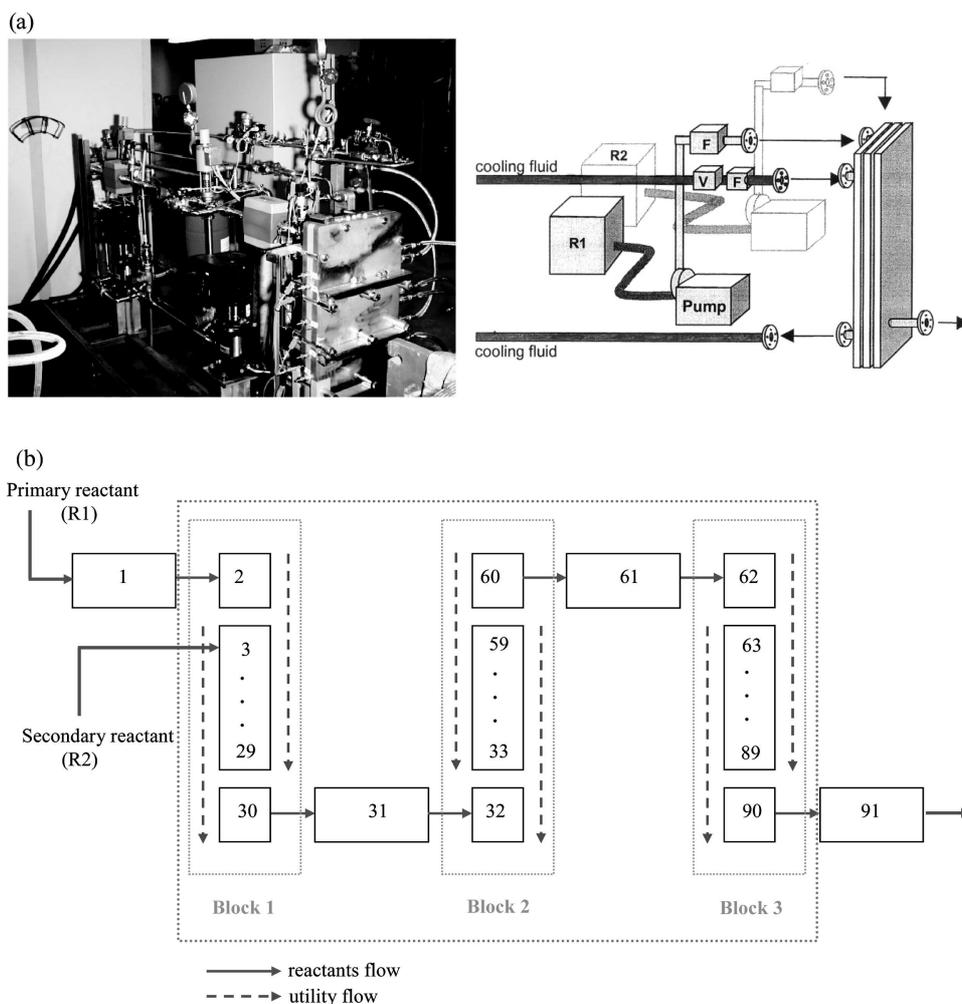


Figure 7. Open plate reactor: (a) Experimental setup: the OPR (right side) and the utility system (left side), (b) Schematic representation with the cells index.

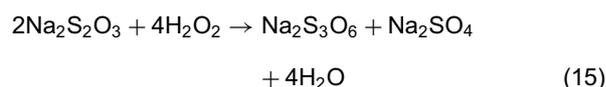
Table 2. Available sensor measurements on the OPR considered for the selection procedure.

Sensor name	Variable description	Position	Sensor name	Variable description	Position
TP_B1_1	proc. fluid temp. block 1 cell 1	3	TP_B2_7	proc. fluid temp. block 2 cell 27	59
TP_B1_2	proc. fluid temp. block 1 cell 2	4	TP_B3_1	proc. fluid temp. block 3 cell 1	63
TP_B1_3	proc. fluid temp. block 1 cell 3	5	TP_B3_5	proc. fluid temp. block 3 cell 5	67
TP_B1_4	proc. fluid temp. block 1 cell 4	6	TP_B3_10	proc. fluid temp. block 3 cell 10	72
TP_B1_5	proc. fluid temp. block 1 cell 5	7	TP_B3_15	proc. fluid temp. block 3 cell 15	77
TP_B1_10	proc. fluid temp. block 1 cell 10	8	TP_B3_20	proc. fluid temp. block 3 cell 20	82
TP_B1_15	proc. fluid temp. block 1 cell 15	17	TP_B3_27	proc. fluid temp. block 3 cell 27	89
TP_B1_20	proc. fluid temp. block 1 cell 20	22	FP_OUT	Process fluid output flow	91
TP_B1_27	proc. fluid temp. block 1 cell 27	29	PP_IN_1	primary reactant pressure (inlet)	1
TP_B2_1	proc. fluid temp. block 2 cell 1	33	PP_IN_2	secondary reactant pressure (inlet)	3
TP_B2_5	proc. fluid temp. block 2 cell 5	37	PP_OUT	Process fluid output pressure	91
TP_B2_10	proc. fluid temp. block 2 cell 10	42	TU_B1_OU	Utility fluid temp. block 1	30
TP_B2_15	proc. fluid temp. block 2 cell 15	47	TU_OUT	Utility fluid temp. (outlet)	90
TP_B2_20	proc. fluid temp. block 2 cell 20	52			

Case Study: The Thiosulphate Reaction

Very interesting results have been obtained from the study of the oxidation of sodium thiosulphate $\text{Na}_2\text{S}_2\text{O}_3$ (R1) by hydrogen peroxide H_2O_2 (R2). In a homogeneous medium, this reaction presents the following characteristics: its stoichiometry and kinetic are known, it is irreversible, fast and highly exothermic.

The reaction scheme is as follows:



where H_2O_2 is used in excess to restrain any possible side reaction.

The strong exothermicity of the thiosulphate reaction produces many safety constraints and therefore it requires a permanent cooling by the utility system.

Results

Failures in the OPR for the thiosulphate reaction were simulated in the form of disturbances on the main variables:

temperatures and flows of the primary and secondary reactants and of the utility system, as well as on the compositions of the primary and secondary reactants. A shutdown of the utility system was also included in the training dataset. Figure 8 illustrates the eight process variables on which the 17 faults were induced.

One can notice that among the simulated disturbances and faults, the major part concerns faults on the feed (composition, flow and temperature). Among the possible sensors (Table 2) let us recall that none of them give an information on the feed or on the utility inlet and there is no product composition measurement. So, one of the objectives of the sensor selection procedure is to determine the best place of common sensors (mainly temperature sensors) to diagnose a fault in the feed composition, which means also a fault in the product quality without composition measurement.

Selected sensors

The identification and characterization of the 17 faults was carried out using the self-learning procedure proposed by the classification technique LAMDA. From the profile of the resulting classes the entropy and information gain of each descriptor for each fault were calculated. In Table 3 the

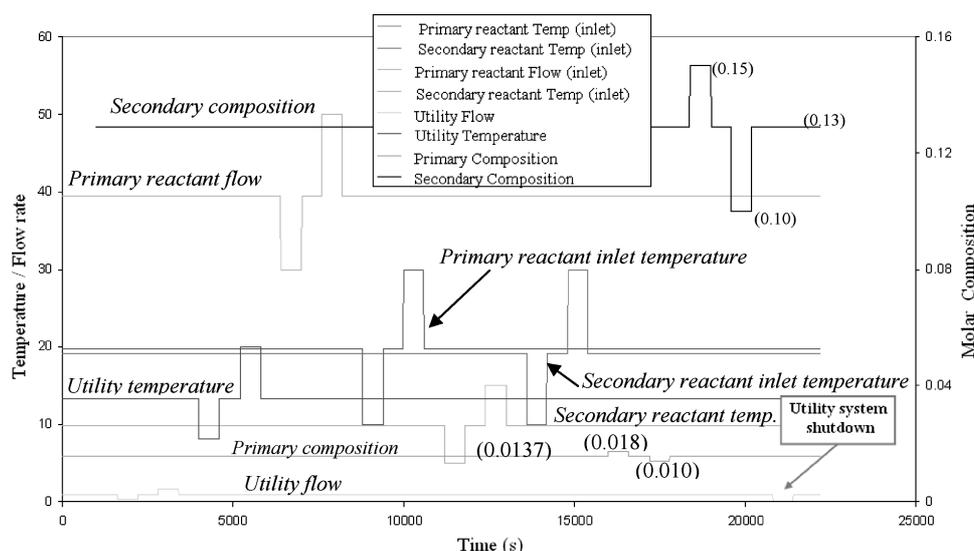


Figure 8. Simulated disturbances for the thiosulphate reaction.

Table 3. Thiosulphate reaction: selected sensors.

Class pairs	Selected sensors (descriptor label)	Sensor description
Normal-↓ Utility_Flow (inlet)	TP_B2_10	Proc. fluid temperature block 2 cell 10
Normal-↑ Utility_Flow (inlet)	TP_B2_10	Proc. fluid temperature block 2 cell 10
Normal-↓ Utility_Temp (inlet)	TU_B1_OU	Utility fluid temperature block 1
Normal-↑ Secondary_Composition	TP_B1_10	Proc. fluid temperature block 1 cell 10
Normal-↑ Utility_Temp (inlet)	TP_B2_20	Proc. fluid temperature block 2 cell 20
Normal-↓ Primary_React_Flow	FP_OUT	Process fluid output flow
Normal-↑ Primary_Composition	TP_B1_10	Proc. fluid temperature block 1 cell 10
Normal-↑ Primary_React_Flow	PP_OUT	Process fluid output pressure
Normal-↓ Primary_Composition	TP_B1_10	Proc. fluid temperature block 1 cell 10
Normal-↓ Primary_React_Temp	TP_B1_1	Proc. fluid temperature block 1 cell 1
Normal-↑ Primary_React_Temp	TP_B1_4	Proc. fluid temperature block 1 cell 4
Normal-↓ Secondary_React_Flow	TP_B1_10	Proc. fluid temperature block 1 cell 10
Normal-↑ Secondary_React_Flow	TP_B1_10	Proc. fluid temperature block 1 cell 10
Normal-↑ Secondary_React_Temp	TP_B1_5	Proc. fluid temperature block 1 cell 5
Normal-Utility_Flow_Stop	TP_B1_4	Proc. fluid temperature block 1 cell 4
Normal-↓ Secondary_React_Temp	TP_B1_10	Proc. fluid temperature block 1 cell 10
Normal-↓ Secondary_Composition	TP_B1_5	Proc. fluid temperature block 1 cell 5

sensors issued from the probabilistic entropy procedure are presented. The selection criterion was to choose the descriptor with the greatest information gain, as the most significant for the detection of a given fault. According to the results, nine different descriptors were selected as the most relevant ones. The internal temperature sensors in the first two blocks are the most pertinent measurements. Indeed, the reaction is highly exothermic and since there is no temperature control within the reactor, the evolutions of the internal temperatures distributed along the reactor provide significant information: the faster the reaction is, more heat is produced, and consequently resulting to an increase of the temperature of the process fluid which will in return accelerate the reaction. Moreover, finding process fluid temperature measurements at the outlet of blocks 1 and 2 in addition to temperature sensors in the first blocks is coherent with this exothermicity phenomenon. It should be noted also that the first block contains four of the nine selected sensors.

Design of the behavioural model for the thiosulphate reaction

The next stage is to build the behaviour pattern for the thiosulphate reaction using as a basis the selected sensors. This behavioural model must include the classes which define the faults and also classes corresponding to alarm situations so that it is able to anticipate the detection of faults. Figure 9 shows the results for the identification of the faults and alarms with nine descriptors. A great number of classes were generated (61 in total) since an unsupervised learning step has been deliberately performed with the objective to identify all the alarm states, i.e., the state preceding an established fault. Nevertheless, as previously mentioned a procedure has been developed which enables the mapping of several classes into a single state [from the representation given in Figure 9(b) to the representation given in Figure 9(c)]. The nine selected sensors allow the observation of all the simulated disturbances, even though there are some false alarms with respect to the observation of a change in the composition of the secondary reactant (states 5 and 19). This is not surprising since a change on the composition of the secondary reactant does not induce

a very significant variation on the observed variables [see Figure 9(a) interval [1700, 1900]].

In Table 4 the description of the behavioural model is presented. The table includes the name of the process situation (normal or fault), the set of classes associated to each functional state and the number of the associated state shown in Figure 9(c). For every set of classes related to a failure, pre-fault and post-fault situations were identified; they represent the states of alarm before and after the fault. For example, for the fault associated with a decrease in the utility feeding flow '↓Utility_Flow (inlet)', class 2 corresponds to the failure when it is perfectly established, while, class 39 represents the instant when the fault starts to manifest, and classes 19 and 55 correspond to the recovery of the process towards the normal state. Nevertheless, for some faults it was not possible to identify a pre-fault situation since the disturbances were not induced progressively. Another characteristic in this model is the existence of state 16 which represents a recovery from a decrease in the utility flow (↓Utility_Flow_Recovery) and is constituted of classes 19 and 55.

Validation of the behavioural model: recognition of unknown faults

The validation of this methodology was carried out by applying a recognition procedure to the elements of a new dataset. The objective is to assign each new element to one of the significant states of the behavioural model previously designed. The type of simulated faults constituting the new dataset were not specified, the only information available was the number of disturbances and their duration (starting and ending time) see Table 5.

Figure 10 displays the results obtained during the recognition phase for the unknown faults. Using the process description given in Table 4 the new scenario was interpreted. For example, *Fault 2* was assigned to class 8 (state 7) which corresponds to an increase of the primary reactant composition. *Faults 1* and *4* were identified as the alarm-state of a decrease in the utility flow (class 39–state 1). A similar case can be noticed for *Faults 3* and *6* which correspond to the alarm of an increase of the utility temperature (class 58–state 2). The classifier has also assigned class

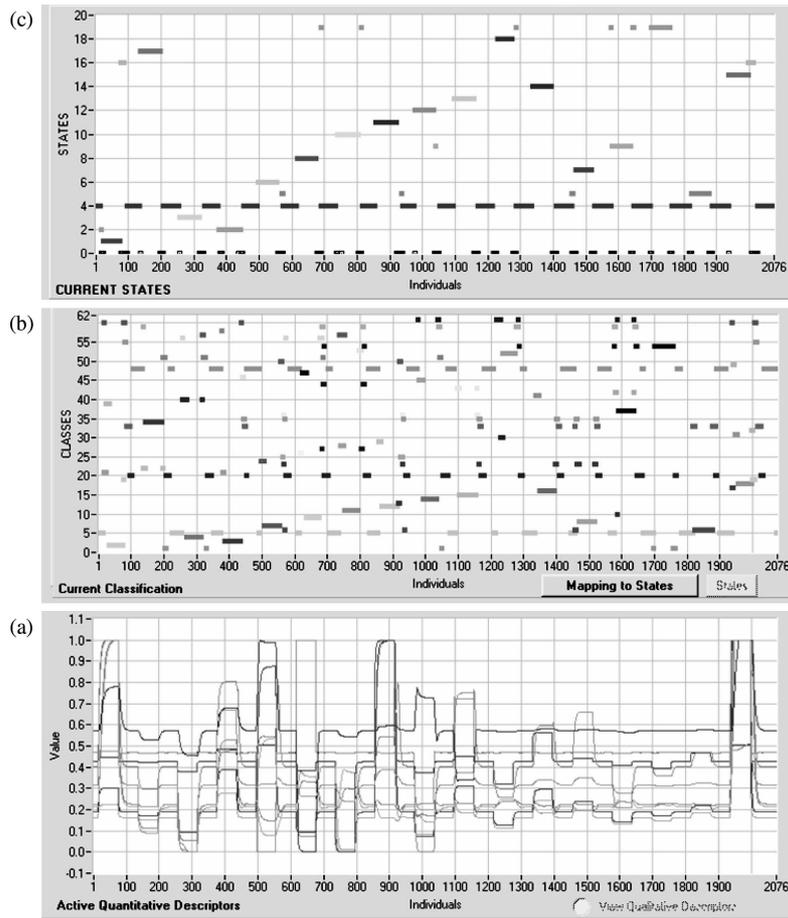


Figure 9. Thiosulphate reaction—fault and alarm identification with nine descriptors: (a) training dataset with only nine descriptors, (b) class generation for the identification of the different situations, (c) mapping classes into significant functional states.

58 at the beginning of *Fault 1*, this can be considered as a *false alarm*. However, the process behaviour at interval [25, 45] is similar to the behaviour for *Faults 3* and *6*. On the other hand, *Fault 5* is associated to class 61, which was

Table 4. Thiosulphate reaction: mapping classes into significant functional states.

Situation (functional state)	Class number	State number
Normal	5, 20, 48	4
↓ Utility_Flow (inlet)	2, 39*, 19+, 55+	1
↑ Utility_Flow (inlet)	34, 22*+	17
↓ Utility_Temp (inlet)	4, 40*+	3
↑ Utility_Temp (inlet)	3, 58*, 46+	2
↓ Primary_Reactant_Flow	7, 24*	6
↑ Primary_Reactant_Flow	9, 26*, 47*	8
↓ Primary_Reactant_Temp	11, 28*, 53+	10
↑ Primary_Reactant_Temp	12, 29*, 13+	11
↓ Secondary_Reactant_Flow	14, 45*	12
↑ Secondary_Reactant_Flow	15, 43*+	13
↓ S/Secondary_Reactant_Temp	52, 30*	18
↑ Secondary_Reactant_Temp	16, 41*	14
↑ Primary_Composition	8	7
↓ Primary_Composition	37, 10*, 42*+	9
↑ Secondary_Composition	54	19
↓ Secondary_Composition	6	5
Utility_Flow_Shutdown	18, 17*, 31*, 49*, 32+	15
↓ Utility_Flow_Recovery	19, 55	16

*Alarm, +Recovery.

not identified as a significant class in the model (state 0). This disturbance could represent a new situation not taken into account during the design of the behavioural model or a multiple-fault situation.

Consideration is now given to Table 6, which gives the real simulated faults. According to the description given for the unknown faults, the classifier correctly recognized three known situations, those corresponding to *Faults 1, 2* and *3*. In cases *1* and *3*, two alarms were detected, since for the two disturbances, the variations of the utility flow and the utility temperature are smaller than those presented in the design of the behavioural model (learning stage). This result is very important since it proves that it is possible to diagnose fault of smaller magnitude than those during the learning phase. Fault 2 corresponds to a fault on the feed composition: this fault has been correctly diagnosed even if

Table 5. Thiosulphate reaction: dataset of unknown situations.

Faults	Start	End
Fault 1	15	75
Fault 2	135	195
Fault 3	255	315
Fault 4	375	435
Fault 5	495	555
Fault 6	615	675

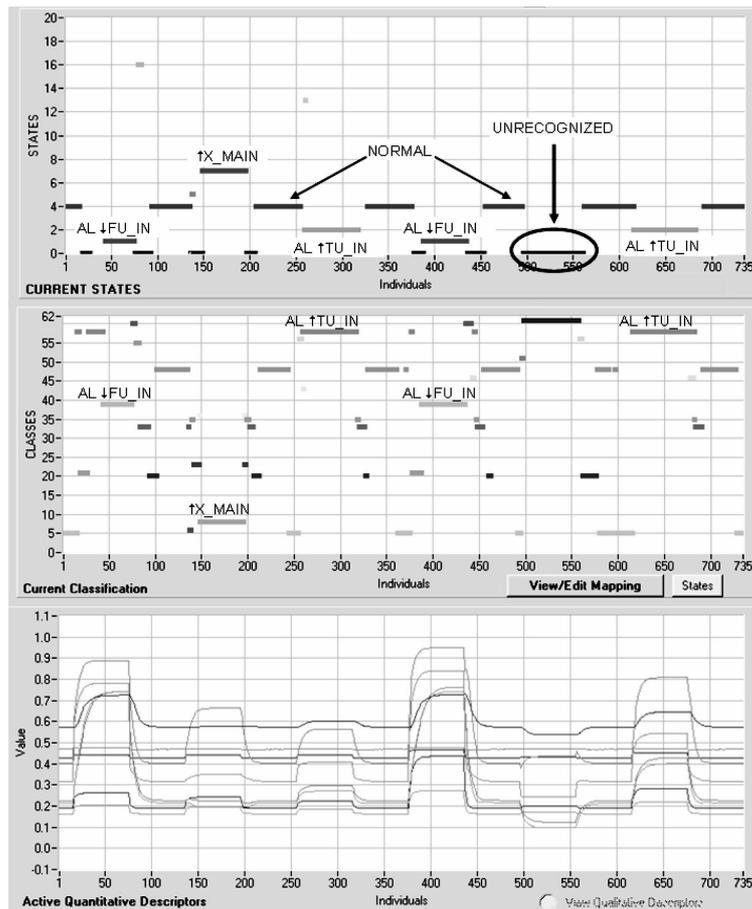


Figure 10. Thiosulphate reaction: recognition of unknown faults.

the magnitude was smaller than the one used in the learning step (Figure 8).

In the case of simultaneous faults, only one of them is recognised: for *Fault 4* the decrease in the utility flow and in *Fault 6* the rise in temperature of the utility fluid. The multi-fault situation was not included in the learning data base since it would be impossible to consider all the cases. Nevertheless, the results show that it is possible to identify one of the two faults occurring simultaneously. *Fault 5* is not identified as a failure state, in fact the combined effects

Table 6. Thiosulphate reaction: description of simulated faults for recognition.

Fault	Description
Fault 1:	Utility flow: $0.916 \text{ m}^3/\text{h} \rightarrow 0.3 \text{ m}^3/\text{h}$ ($\downarrow \text{FU_IN}$).
Fault 2:	Mass fraction of thiosulphate: $0.0137 \rightarrow 0.017$ ($\uparrow \text{X_MAIN}$).
Fault 3:	Utility temperature: $13.37^\circ\text{C} \rightarrow 15^\circ\text{C}$ ($\uparrow \text{TU_B1_IN}$).
Fault 4:	Simultaneous faults: mass fraction of thiosulphate: $0.0137 \rightarrow 0.0175$ and utility flow: $0.916 \text{ m}^3/\text{h} \rightarrow 0.3 \text{ m}^3/\text{h}$ ($\uparrow \text{X_MAIN} + \downarrow \text{FU_IN}$).
Fault 5:	Simultaneous faults: mass fraction of thiosulphate: $0.0137 \rightarrow 0.0165$ and utility flow: $0.916 \text{ m}^3/\text{h} \rightarrow 1.5 \text{ m}^3/\text{h}$ ($\uparrow \text{X_MAIN} + \downarrow \text{FU_IN}$).
Fault 6:	3 Simultaneous faults: mass fraction of thiosulphate: $0.0137 \rightarrow 0.0165$, utility flow: $0.916 \text{ m}^3/\text{h} \rightarrow 0.6 \text{ m}^3/\text{h}$ and utility temperature: $13.37^\circ\text{C} \rightarrow 14.8^\circ\text{C}$ ($\uparrow \text{X_MAIN} + \downarrow \text{FU_IN} + \uparrow \text{TU_B1_IN}$).

of the two disturbances cancel each other: the reactor is fed with a more concentrated reactant but the utility system cools more, which corresponds well to a normal operation (e.g., if there was a controller to maintain the temperature at the output of block 1, consecutively, to an increase of the mass fraction of a reactant, the utility flow will be increased by the controller).

In a diagnosis procedure the possibility to establish that an element (here the current state) is not recognised is of primordial importance. It is therefore much more interesting for the user or the operator to have the message: 'the process behaviour does not look like a normal state behaviour but it has not been recognised as a known fault' than to have a wrong affectation of this state to a fault (what is the case when an element is assigned to a wrong class). Moreover, the unrecognized elements will enable an evolution of the model. New classes corresponding to new faults can be created from these only elements without modifying the existing classes associated to the previously established faults. For this, the 'active supervised learning' procedure proposed in (Kempowsky *et al.*, 2004) can be applied. Hence, when a significant number of consecutive elements are assigned to the NIC, the aim is to identify and characterize this new situation by launching a new learning procedure. New classes are generated from the characteristics of the alone unrecognized elements, keeping unmodified the existing classes. The expert will next interpret the new classes in order to characterize the new behaviour.

Concerning the sensor selection procedure, one of its advantages is that it provides to the user an overview of the information gains for all the descriptors. So the user can choose to restrict the set of descriptor to its minimum set (adopted in this study) or to add supplementary descriptors or to replace a descriptor by a 'close one' (in term of information gain). The final selection criterion could include a priori knowledge related to the sensor nature such as: price, reliability, maintenance easiness, installation facility, and so on, so the final selection criterion could be a multi-objective criterion including not only the information gain but also these different practical elements. The user could easily extract a set of sensors yielding close information gains and choose among them the one leading to a best exploitation cost.

It is also possible from the knowledge of the information gains to choose supplementary sensors and not to restrict to those offering the highest gains. This possibility will be of great importance to treat properly the case of sensor failures, since there will have a redundancy of information but contrary to what is done most often, this redundancy will be based on the capacity of these supplementary sensors to produce an information of close quality.

CONCLUSIONS

In this work, a new methodology to identify the better location of sensors has been developed. These sensors are chosen into a set of possible sensors including only classical sensors such as temperatures, flows and pressures. Once the different process situations (normal and faults) have been identified and characterized by a learning procedure performed with a classification technique, the concepts of entropy and of information gain can be applied to determine the most relevant sensors. Let us remark that the proposed methodology is generic and can be performed with any classification technique. This methodology has been applied to a continuous intensified reactor: the open plate reactor (OPR). A reaction with a highly exothermic behaviour carried out in the OPR was used to illustrate and explain the different steps of the proposed methodology. The results from this example demonstrate the utility of the methodology for processes when a mathematical or structural model is not available or the mathematical model is too complex. This methodology can be applied either in the design stage of the plant as it was the case in the proposed example, or to reduce the quantity and synthesize the information given to the process operators, considering only the essential. Moreover, the resulting behavioural model can be used as a base for training new operators or to analyse scenarios of faults which have been observed on existing plants but which have not been detected (return on experience). This methodology can be applied easily in the design stage of the plant. Process designers are used to run simulations during the design stage. They have already all the needed information in the simulation results to apply this methodology. The determination of sensor location has to be done at this stage; after, during the production stage, it is generally too late to add a sensor. Moreover, this methodology leads to a behavioural model which can be easily updated by adding new states with the procedure of 'active supervised learning'. This is a very important result since the exhaustiveness of the

faults would never be guaranteed in particular in a complex process.

Concerning the classification technique itself, as it has been shown, the results mainly rely on the quality of the classification first obtained using all the possible sensors. Most often at this stage, the user should prefer to get a less sparse representation space (i.e., with less classes). Until now, this quality of the classification was let to the appreciation of the expert. In recent and actual works (Isaza *et al.*, 2006) studies have been devoted firstly to the definition of indexes for analysing the quality of the obtained partition and then to the optimization of the partition by acting on classification design parameter such as the exigency or the function used for the computation of the MAD. This approach includes the two steps: the partition validation and the clusters update. The partition quality is measured by a validation index, from which it is decided if it is necessary or not to modify the partition. In the second step concerning the clusters updating, the fuzzy similarity of classes is calculated and the merging of the two similar classes is thus performed. At final state, this partition validation will be coupled with the sensor selection procedure by the integration of the quality of the partition in the selection procedure: the 'best' sensors should be the ones yielding the 'best' information with the 'best' partition.

The future works will be devoted to an experimental validation of the sensor selection procedure. A special care will also be devoted to study sensor failures and specially how to take advantage of the sensor selection results to add accurate information redundancy by a good choice of supplementary sensors.

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