

Process and Operator Performance Analysis in Process Operational Safety

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given where reference has been made to the work of others

*In memory of
My mother, father and brother Jassim
May Allah bestow his mercy upon them*

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Abstract

Abnormal operation of chemical processes caused by equipment and sensor faults, such as plugging of pipes, control system failure or improper operation by personnel can result in poor product quality, equipment damage, or a catastrophe process failure leading to loss of equipment and worker injury, as well as significant economic losses. It is estimated that the cost attributable to preventable losses in the petrochemical industry only is around several billion pounds per year. Independent studies of case histories by the Health and Safety Commission in the UK and by a Honeywell led industrial consortium in the US and world wide show that human errors represent the major cause of failures. In contrast to this discovery, the majority of pervious studies on computer aided systems for fault detection and diagnosis has focussed on the process side only. It is now widely acknowledged that there is only limited information on how human factors can be assessed and even less that is specific to chemical industry, therefore research is much needed in this area.

This study presents a methodology to involve human factors into the development of systems for automatic identification and diagnosis of abnormal operations and develops methods and techniques that can be used to simultaneously capture, characterise and assess the performance of operators as well as of the process. A joint process – operator simulation platform was developed which was used as a test-bed for carrying out the studies. The process part is a simulator, which emulates in high fidelity the dynamic behaviour of the process, which is subject to influence of various disturbances and operators intervention. The operator module was developed as a real-time expert system, which emulates operator's behaviour in interpretation of received signals, planning and executions of the decisions. The interaction between the two modules is managed through an interaction module, which handles the real-time exchange of data using DDE (Dynamic Data Exchange). The interaction module also contains the toolkits for analysing the dynamic behaviour of the joint process-operator system.

The operator simulation module was developed based on a theoretical model of human behaviour, which breaks operator's activities into perception of signals and

interpretation of the received information, planning for actions and execution of the decisions. The system was implemented as a real-time expert system using visual Prolog. Numerical models were also integrated into the expert system, e.g. stress models of operators. This flexible system allows studies on individual operators actions, stress, intervene time, the frequency of intervene and near-miss or near-hit in operation.

As part of the effort to use the platform to develop methods and tools for characterising and assessing the dynamic behaviour of the joint process-operator system, a digraph method for qualitative /quantitative modelling of the dynamic behaviour of the combined system was proposed. The method involves categorical characterisation of dynamic trends using principal component analysis and fuzzy *c*-means and sectioning of the clusters. An iterative method for determining the number of the clusters and sections based on the global performance was derived. Compared with pervious studies on qualitative process modelling, the proposed approach is more accurate and has higher resolution, and more importantly is able to deal with joint process-operator systems.

The methods and systems developed were illustrated and fully tested using simulated and industrial case studies.

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Chapter 1

Introduction

1.1 The Background

Operational safety of processes is of paramount importance and therefore should be the first objective of process control (Marlin, 2000). Problems caused by operational faults range from increased operational costs to forced shutdown of processes. In some cases, it can result in catastrophic fire and/or explosion. The complexity and the increased degree of integration of modern chemical plants means that the potential economic loss is greater when a fault occurs and the diagnosis of fault locations becomes more difficult.

Apart from alarms, modern computer control systems are not yet equipped with systems that can automatically predict and detect the abnormal operations and diagnose fault locations. The safety issue is addressed in three layers as depicted in Fig 1.1. The inner layers is the plant control system which consists of control loops that can reject common cause variations or disturbances and maintain steady state operation, as well as alarm systems and recovery options. The middle layer is comprised of prediction systems that require power supply. They include interlocks, energy shutdown systems, fire and gas detection systems and dual and backup systems. The outer layer provides the final protection, if everything including power supply fails. This is done through selection and design of inherently safe equipment and devices, for example, through minimisation of inventories, containment, selection of pressure devices and fail-safe design. It is the plant operators who play the crucial role of continuously assessing the operational status and diagnose abnormal situations that the inner control layer cannot cope with and take necessary actions to prevent process shutdown.

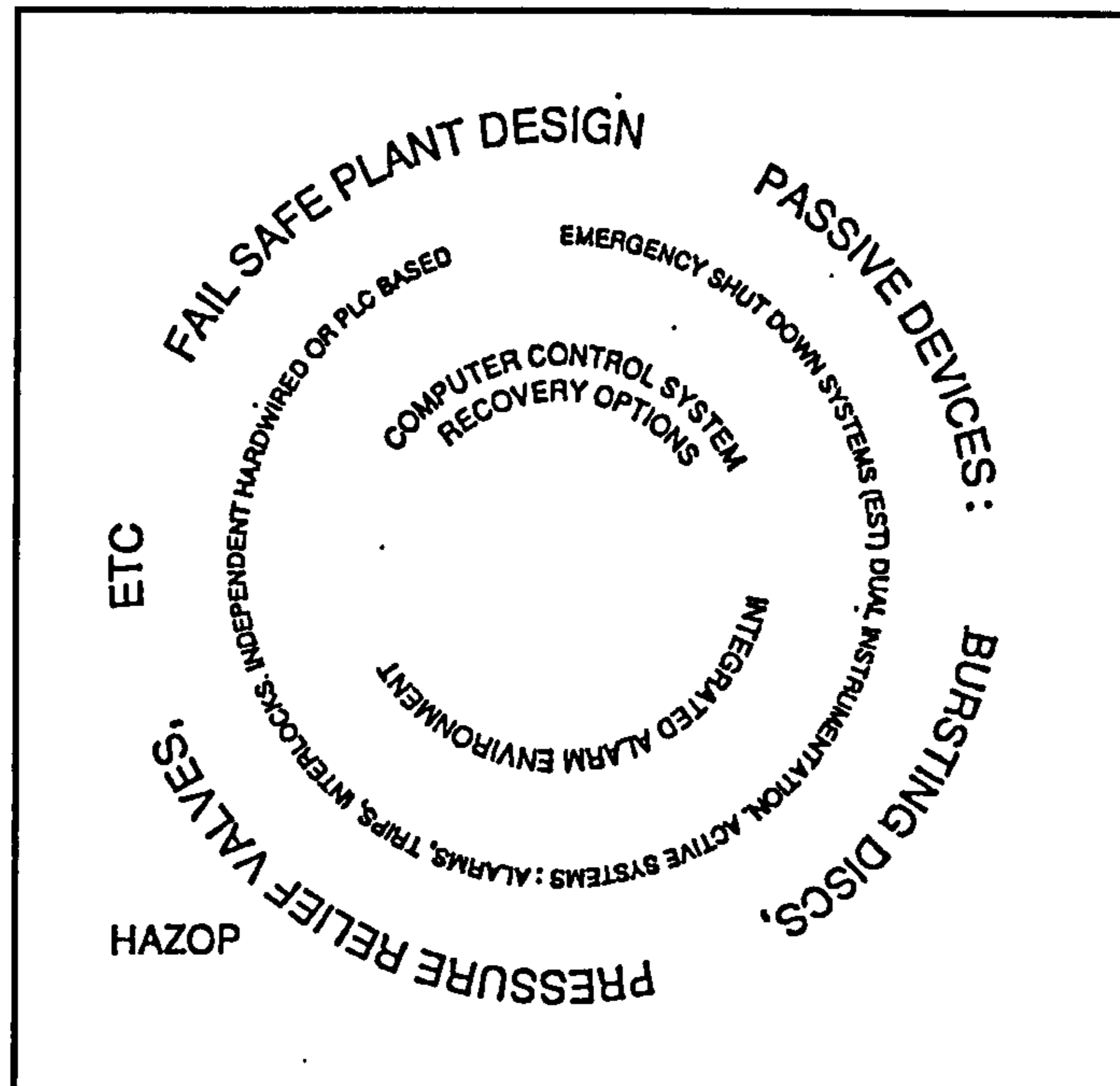


Fig 1.1. Layers of the operational process safety of computer control systems.

To help operators to assess operational status, computer control systems collect and display a large amount of information. The information, however is overloaded where critical decisions about process operation have to be made very quickly by plant personnel: in a chemical plant, a few hundred to over fifty-thousand variables may be measured and sampled as frequently as every minute or less. During the periods of abnormal operation, often too many alarms are issued and too many variables are evolving irregularly. Case histories show that operators do not always make correct decisions.

As a result, there have been tremendous interests in developing methods and techniques for automatic interpretation of operational data, and for fault detection and diagnosis. These include investigation into real time expert systems, supervised and unsupervised neural networks, statistical process control, fuzzy logic, qualitative reasoning and wavelets. The most important progress has been made in the last ten to fifteen years and the work has been reviewed by numerous researchers such as Dash and Venkatasubramanian (2000), Himmelblau (2000), and Wang (1999) from different perspectives and a more comprehensive review will be made in chapter 2 of this thesis.

1.2 Motivations of the Research

Case histories of failure revealed a very important discovery that human errors represent the major factor of failures. According to a survey conducted by a consortium led by Honeywell around the world including USA, UK, Canada, Europe and Japan about 40% of abnormal operations were caused by human errors (Nimmo, 1995). In a parallel study by the Health and Safety Commission (Lardner and Fleming, 1996), it was found that 80% of accidents that involve a factor of human errors. Previous work on automatic process fault detection and diagnostic systems will no doubt help reduce the load of operators by providing them with quick solutions. However they have not fully addressed the issue of human factors or human errors in process operational safety. Firstly, most previous studies have assumed that after a fault occurring the process will evolve without operator intervention, this is clearly an ideal situation. In addition almost all of the previous efforts have focused on automatic assessment of the process behaviour. No effort has been made on automatic monitoring and assessment of operators performance. A good example of human factor is 'near-miss' or 'near-hit' operations. It can be useful if such operations can be captured automatically and fed back to the operators. As indicated by the Health and Safety Executive (UK), there is only limited information on how human factors can be assessed and even less that is specific to chemical industry. Studies on human factors in operational process safety have mainly been conducted by human behaviour and ergonomic scientists, psychologist and statisticians using various approaches such as statistical analysis of past incidents, interview and questionnaires, and tests of operators at certain conditions. The work has been aimed at discovering common human factors so that better computer displays and improved management and company culture can be developed. However, chemical engineers interest in process safety has mainly focused on the plant and its monitoring and control systems, probably because human factors are often regarded as a management and culture issue. It is often considered difficult to capture and assess information on human factors more scientifically, rigorously and faithfully, especially for information, which is specific to individuals (Johnson, 1999). It is well known that operators vary in skill (Juespert and McAvoy, 1994). One operator may exhibit better control than the others. The resulting fluctuations in control quality cause corresponding fluctuations in process conditions, creating unprofitable or even unsafe situations. If the skills of experienced and inexperienced operators were continuously monitored, captured, characterised and analysed, the knowledge can be used to improve the operators skills and develop better abnormal management strategies and even improve process design. An

important progress in addressing operators skills is the use of dynamic training simulators. It is estimated that using a training simulator, an operator can experience more scenarios in weeks than operating in the real plant for months even years. However, based on the several years of experience of developing dynamic training simulators for refining and petrochemical industries, it is our belief that it is an unrealistic expectation that operators can experience all scenarios on a simulator that they may meet later.

1.3 Objectives

The overall aims of the research were to develop a methodology and system to involve human factors into the development of systems for automatic identification and diagnosis of abnormal operations, and to investigate methods and techniques that can be used to capture, characterise and assess the performance of the operators, as well as that of the process. More specifically the research objectives are described below:

- (1) Developing a joint process-operator platform for carrying out the study. The joint process-operator platform will be a dynamic environment, consisting of a dynamic simulator of the process, system that models the operators behaviour in supervising and controlling the process, as well as an interaction module which manages the data transformation and real-time exchange of data between the process and the operator evaluation system. The interaction module also serves as an interface for monitoring the joint system behaviour.
- (2) Study the theoretical models for modelling operators cognitive behaviour and action in process operation and develop a high fidelity and easy to modify system to reflect varied scenarios of operators behaviour.
- (3) Develop methodologies and techniques that can be used to capture, characterise and assess the dynamic behaviour of the joint process operator system as well as the performance of operators.
- (4) Validate the above methods and systems using case studies.

1.4 Organization of the Thesis

The thesis is organized as follows:

Chapter 2 provides a critical review of the literature for the topics of this research, focusing and integrating the areas selected for development. It also sets the context in which the problem will be approached. It involves the critique of real-time expert systems univariate and multivariate statistical process control, supervised and unsupervised neural networks as well as data processing technique, hybrid systems, and digraphs. The purpose is not to exhaust the literature; rather it is aimed at comparing the methods and highlight areas that need further research.

Chapter 3 describes the role and implementation issues of the process-operator interaction system. This is a platform consisting of three components: the process simulator, the operator module and the interaction system. The process simulator simulates dynamically the behaviour of the process under the influence of disturbance. The operator module emulates the behaviour of the operators, while the interaction module manages data exchange and serves as an interface.

Chapter 4 describes the theoretical models of human behaviour and develops a system of operator behaviour. The system is implemented as a real-time expert system, which emulates operator's behaviour in perception and interpretation of signals, and planning and execution of actions.

Chapter 5 describes the role and the implementation issues of the process operator interaction module, reviews other modules and discusses the proposed interaction module with the aid of process operator condition monitoring examples.

In chapter 6, a new digraph method for qualitatively modelling process dynamic behaviour is proposed. The chapter also reviews a number of digraph methods, discusses the problem of clustering the principal components, proposes an optimisation method for clustering and sectioning and propose a number of sectioning methods.

Chapter 7 examines the methodology proposed in chapter six using application to the CSTR case study. A number of qualitative models will be developed from the process variables trends, such as product temperature and concentration output trends. It also discusses and uses the ANOVA analysis during the evaluation of the models developed.

Finally chapter 8 summarises the findings and gives suggestions for future work.

Chapter 2

Literature Review

2.1 Introduction

This chapter provides a critical review of the literature for the topics of this research, focusing and integrating the areas selected for development. It also sets the context in which the problem will be approached.

In section 2.2, we will analyse the challenges facing on-line monitoring and fault diagnosis of chemical processes, and present some classification schemes of computer-based techniques for process monitoring and fault diagnosis. We will then make a review of the techniques which have been studied in the last ten to fifteen years, including real-time expert systems (section 2.3), univariate and multivariate statistical process control (SPC and MSPC) (section 2.4), supervised and unsupervised neural networks (section 2.5), as well as data pre-processing techniques, hybrid systems, and graph theory based signed digraphs (SDG) (section 2.6). The techniques that will be used in this work, for example MSPC will be reviewed in more detail than others. Some methods will be only very briefly mentioned because they will be described in more detail in later chapters, for instance, the graph theory based SDG. Section 2.7 is dedicated to reviewing the work on how human factors can be considered in developing monitoring and fault diagnosis systems. A brief summary of this chapter will be made in section 2.8.

2.2 Computer Based Systems for Process Monitoring and Fault Diagnosis

2.2.1 Computer Based Process Control Systems

Traditional computer based process control systems do not have fault detection and diagnosis functions. Process operational safety is addressed at three levels in equipment and control system design. At the center it is the automatic control loops, which are responsible for steady state and normal operation, and therefore the disturbances should be handled at

this layer. The middle layer is called the active safety layer, which includes hardware and software protection. The layer represents an extra safety protection system but needs power in order to act. The outer layer is called passive safety layer. It means that when every thing else fails, such as failure in power supply, the inherent safety equipment design will provide the final protection.

Clearly the three layered control and protection design does not include tools that can help operators to carry out the task of analysing the data collected and assessing the operational status. It has long been recognised that the information collected by computer control systems tends to overwhelm operators and makes it difficult to take quick and correct decisions, especially in critical circumstances. There is a clear need to develop methodologies and tools to automate data interpretation and analysis's in order to provide operators with assessment of states of operation and guidance in how to make adjustments. The methodologies and tools should become part of a computer control system configuration.

Many methods on computer aided operational decision support systems have been developed over the last ten to fifteen years, but little information is available on benchmarking these methods. Dash and Venkatasubramanian (2000) summarised some issues that need to be considered in benchmarking the techniques. These include,

- (1) The ability to give early detection and diagnosis of faults.
- (2) Isolation, to be able to discriminate between faults. Some faults may give similar responses therefore isolation refers to the resolution of a method.
- (3) Robustness in the presence of noise and uncertainties in measurements.
- (4) Novelty of identification, referring to the capability to be able to diagnose faults, which were not experienced before.
- (5) Multiple fault identification.
- (6) Explanation facility. Some methods do not have explanation facilities, reducing the confidence of users.
- (7) Adaptability to changes in processes.
- (8) Speed.

Some other researchers have addressed these issues in more specific terms, for example, whether a method is recursive or not recursive. The former allows on-line learning using data continuously collected and the existing knowledge that has been learned will not be corrupted. In contrast, the later always needs a batch of new data to be mixed with previous data. The consideration is clearly related to adaptability of a method but is more rigorous and specific.

2.2.2 Classification of Computer Based Techniques for Fault Detection and Diagnosis

The work on computer aided fault detection and diagnosis has been recently reviewed by a number of researchers such as Dash and Venkatasubramanian (2000), Himmelblau (2000) and Wang (1999) from different perspectives.

Dash and Venkatasubramanian (2000) broadly classified the methods into process model based and process historical data based, as depicted in Figure 2.1.

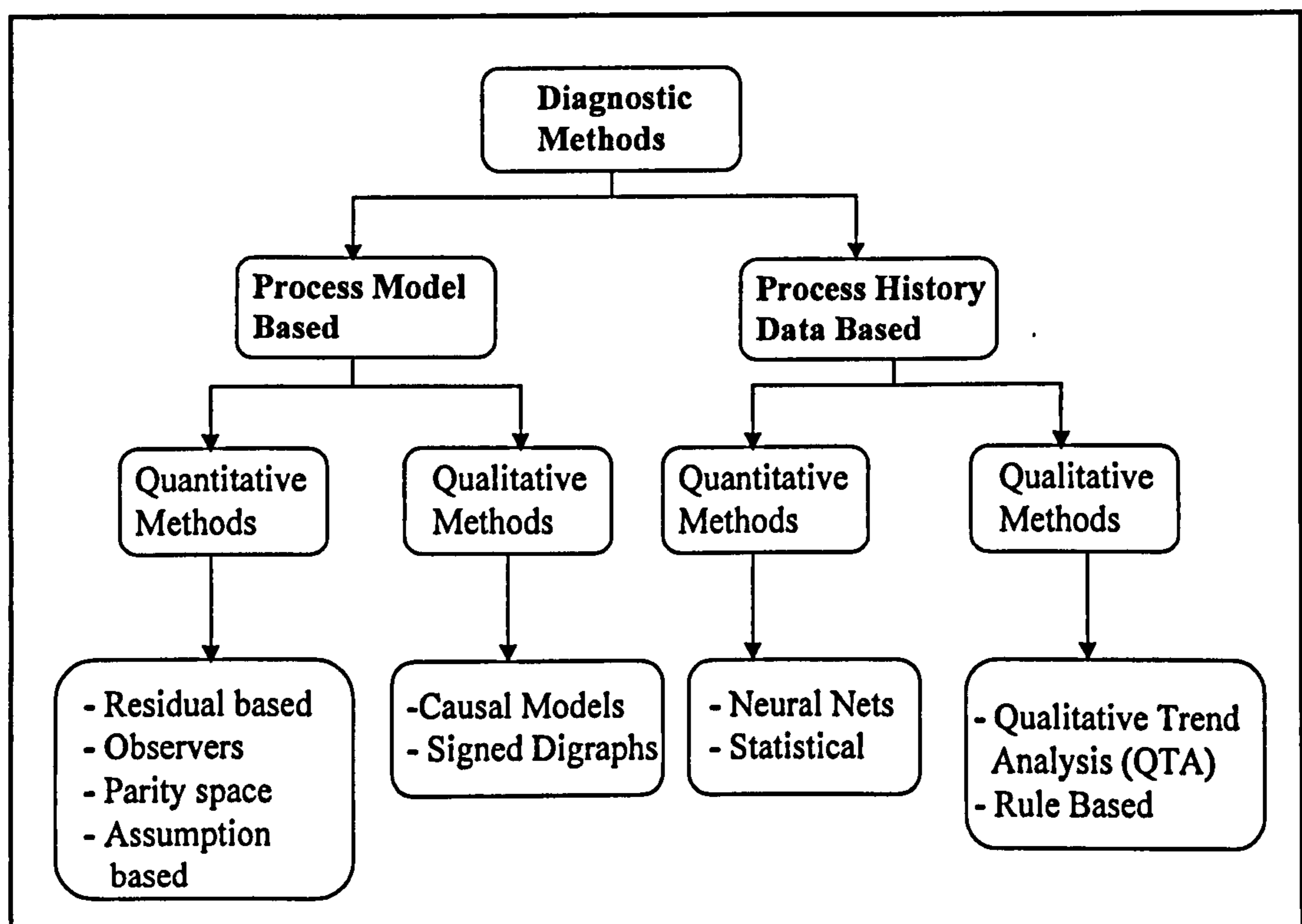


Fig. 2.1. Classification of fault diagnostic methods (Dash and Venkatasubramanian, 2000).

2.2.2.1 Process Model Based Methods

Process model based methods use qualitative knowledge and quantitative models extracted from process principles. The model represents the interacting relationships between various process variables. The philosophy of the approaches are founded upon the assumption that a fault will cause changes to certain physical parameters which in turn will lead changes in some of the model parameters or states. It is then possible to detect and diagnose these faults by monitoring the estimated model parameters or states.

The methods based on process models can further be sub-divided into qualitative causal models and quantitative methods. The strategy employed in qualitative models is the cause-effect reasoning about system behaviour. The most popular methods are *fault-trees* and *signed digraphs* (SDG). Fault trees (Lapp and Powers, 1977) use backward chaining until a primary event is found that presents a possible root cause for observed process deviation. Signed digraphs (Iri et al., 1979) is another representation of the causal information in which the process variables are represented as graph nodes and causal relations by directed arcs. Causal model-based methods mimic human reasoning and so explanation generation is relatively straightforward making them more interactive.

Quantitative methods for fault detection and diagnosis based on process models can be accurate since process models come from underlying first principles. However, comprehensive theoretical models for complex processes can be very difficult to develop. This is because fault identification and diagnosis is the inverse of dynamic process simulation. In the dynamic process simulation, the purpose is to model the dynamic behaviour of the process subject to disturbances, while the task of fault detection and diagnosis is to find the cause of disturbance or faults for observed process dynamic response.

2.2.2.2 Process History Data Based Methods

Process history data based methods make use of the history data of process operation. Data and knowledge for fault identification and diagnosis can be extracted. The knowledge can be rules and formulations. The methods also can be further divided into qualitative methods, such as rule-based, and quantitative methods, such as neural networks and statistical approaches.

One of the most popular data based methods is the neural network. Neural networks can learn from data the relationship between the symptoms of faults and their causes and

store them as network weights. The trained network can then be used to diagnose subsequent faults by associating the observed malfunction with the corresponding previously identified fault.

Another data driven method, which has received much attention is statistical process control (SPC). The traditional SPC based on Shewhart and CUSUM charts are well established for monitoring univariate processes, but they do not function well for multivariable processes with highly correlated variables. A notable recent development is on multivariate statistical process control (MSPC), which proves to be an effective diagnostic tool for monitoring and detection of process faults for both continuous and batch processes (e.g., MacGregor and Kourti, 1995; Neogi and Schlags, 1998; Dunia et al., 1996; Chen et al., 1996; Negiz and Cinar 1997; Dong and McAvoy, 1996a).

Wang (1999) classified fault detection and diagnosis techniques based on learning from previous process history data according to the following scheme: (1) data pre-processing techniques for noise removal, dimension reduction and feature extraction, such as wavelets and qualitative interpretation of dynamic trends; (2) supervised and unsupervised clustering algorithms, i.e. training based classification such as back propagation neural networks and automatic clustering using neural and statistical algorithms; (3) numerical and conceptual clustering approaches; as well as (4) decision tree and rule based methods. Another consideration in examining a learning method is recursive (or incremental) or not recursive (non-incremental). The former learns from one data set at one time, i.e. updating the knowledge, which was learned using previous data every time a new data set is presented. In this case the existing knowledge is updated without any corruptions. The latter needs to learn on a mass of training examples, i.e. when a new data set is present, it has to be combined with the previous data. Recursive methods are particularly useful for online use, because in online applications, data is continuously received. These conditions provide a useful scheme for analysis of the advantages and disadvantages of various techniques.

There are many other new techniques being investigated for process monitoring and diagnosis, such as *wavelets* (Kosanovich and Piovoso, 1997; Bakshi, 1998; Chen et al., 1999, Wang et al., 1999), and image analysis techniques (Bharati and MacGregor, 1998).

2.3 Real-Time Expert Systems

An expert system (ES) is a knowledge-based system that makes use of knowledge acquired from one or more human experts. It often includes a knowledge base, an inference

engine and a database. ESs are designed to advise on a solution method, offer objective advice, make available the best experiences to others, evolve as knowledge and heuristics are added, and be capable of explaining decisions or recommendations and be a repository of experience which can evolve continuously. ES was one of the first few artificial intelligence techniques studied for on-line process fault detection and diagnosis (e.g., Moore and Kramer, 1986). The success of the object-oriented real-time expert system G2 of Gensym was a clear indication of its attraction. Early real-time ESs used rules summarised by domain experts and the capability in describing process dynamic behavior was limited. For example, G2 used simple descriptors to describe the dynamic transient behaviour, such as *increase* and *decrease*.

The advantages of knowledge based systems are that the knowledge used for fault diagnosis is causal and transparent; heuristic rules can be easily added to and removed from the rule base and rigorous process model is not needed; and human experts knowledge and experience can be easily stored and used. However, ESs are known to have the following limitations:

- (1) Rules are often obtained from human experts, therefore are often subjective. If the rules are not sufficient and do not describe all the operation and possible faults, then the ES developed may not be very useful and need continuous upgrading to include information about the newly developed faults, which were not included in the initial stages of the development.
- (2) ESs often does not have learning capability and therefore cannot dynamically improve its performance.
- (3) Qualitative interpretation of plant measurement inevitably leads to loss of information.
- (4) Because of the complexity of the dynamic behaviour and the interactions between the variables of a process under fault conditions, the experienced human experts may not have the necessary expertise to describe the causal relationships, therefore knowledge acquisition represents the bottleneck in developing real-time expert systems for process fault detection and diagnosis (i.e. knowledge about the process faults and abnormal operations rarely happen and hence they are very hard to obtain because during the real time process operation fewer abnormal operations can be experienced).
- (5) Rules can be in conflicting when the size of the knowledge base is large.

- (6) The overall causal relationships of all process variables may be buried in a large rule base, making it far more complex to be viewed clearly by decision makers.

There has been some progress in addressing some limitations of expert systems, for instance, the use of inductive learning to automatically extract knowledge rules from data (Wang et al., 1997; Wang, 1999). Progress in qualitative interpretation of dynamic trends (Janusz and Venkatasubramanian, 1991, Bakshi and Stephanopoulos, 1994 a&b) also makes it possible for using expert systems to describe complex dynamic behaviour of processes under fault conditions, with minimum loss of information.

Despite the rapid development of other techniques such as neural networks and statistical methods, the interests in expert systems remain, especially in its combined use with other techniques to develop hybrid systems. McGuin and Tolman (1996) coupled the real-time expert system G2 of Gensym with dynamic simulation system SpeedUp of Aspen Tech for use in on-line process monitoring, supervisory control and fault diagnosis. The G2 real time ES was interfaced with SpeedUp simulation model to exploit the various advantages associated with shallow, deep, compiled and rule-based knowledge. Leung and Romagnoli (2000) developed a real time ES, also using G2, which comprises of three major elements, monitoring and assessment for control state monitoring and classification, decision support for providing operator guidance and a heuristic-based adaptation mechanism to intelligently response to any change in control scenarios. Jong and Poong (2000) studied the dynamic aspects of fault diagnostic systems in nuclear power plants. They developed an operator decision support system, which was aimed at increasing the efficiency of the plant and to reduce the human error and cognitive workload that may cause accidents. The system consists of a knowledge base, an inference engine and a user interface.

2.4 Univariate and Multivariate Statistical Process Control (SPC and MSPC)

SPC and MSPC have been widely studied in the last several years. Reviews can be found in Russell et al., (2000), Kourti and MacGregor (1995), MacGregor and Kourti (1995), Li (2000), Wise and Gallagher (1996), Cinar and Undey (1999), Wang (1999), and Martin and Morris (1996).

2.4.1 MSPC Based on Principal Component Analysis (PCA)

MSPC is an extension of univariate SPC using PCA. PCA is a dimension reduction technique, which reduces the dimensionality of a data set consisting of a large number of interrelated variables, while retaining as much as possible of the variation present in the data. PCA uses all the original variables to obtain a smaller set of new variables, i.e. principal components (PCs) that can be used to approximate the original variables. The PCs represent a new set of co-ordinates that are orthogonal to each other. The first PC is the linear combination of the original variables and indicates the direction of the greatest variation in data. The second PC is also a linear combination of the original variables and describes the next dominant direction of variation, but is orthogonal to the first PC. The same number of PCs as the original variables can be calculated but only the first few PCs are used to represent the feature of the data, because the remaining PCs are often considered as representing noise.

Univariate SPC uses control charts, most noticeably the Shewhart charts. An example of univariate Shewhart charts is given in Fig. 2.2. At common cause variation, e.g., random disturbances, the values of variables should satisfy a normal distribution centred on the mean μ with a standard deviation σ . The upper and lower control limits (UCL and LCL) can be set as $+\sigma$ and $-\sigma$, then the probability that the value of the variable goes outside UCL and LCL is less than 5%. Higher than 5% is an indication of potential occurrence of special cause variation, or faults. The UCL and LCL can also be set as $+2\sigma$ and -2σ , and $+3\sigma$ and -3σ , then the probability limits become 4%, 3% or less.

Because of the multivariate nature of process operational states, monitoring of operation based on univariate SPC is some times not sufficient: even all the variables are within the UCL and LCL, it does not mean that the process is definitely within the normal zone of the multidimensional space. Hotelling's (1947) developed the multivariate Shewhart charts, the T^2 charts. The 95%, 98% and 99% on a T^2 chart can also be calculated.

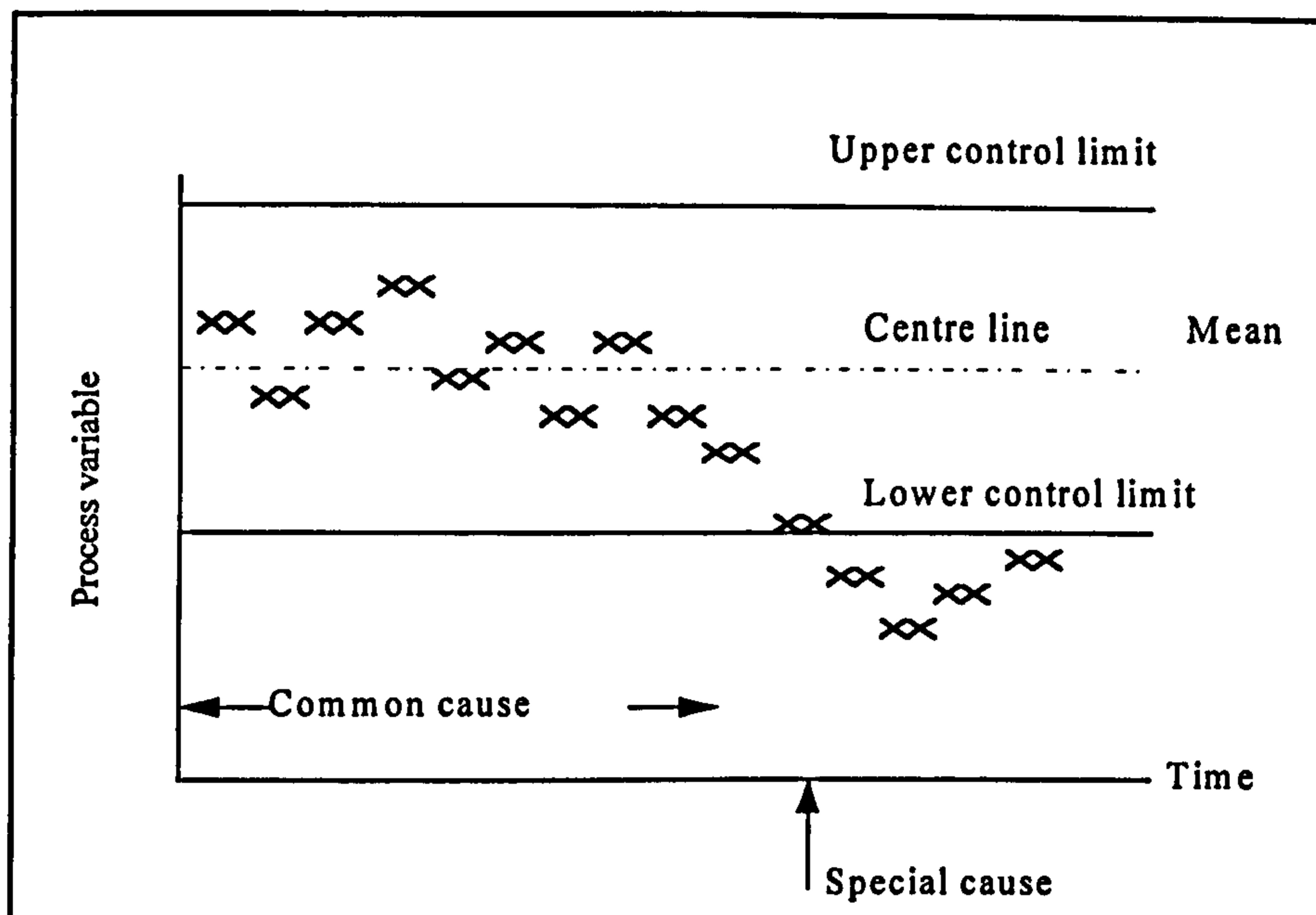


Fig. 2.2. Univariate Shewhart chart.

PCA based MSPC is based on the observation that many of the process variables are auto-correlated, only a few underlying events are driving a process at any time, and all these measurements are simply different reflections of these same underlying events. It means that only the first PCs can be used, rather than all the original variables. If A PCs are used, the Hotelling's T^2 can be calculated by,

$$(1) \quad T^2_A = \sum_{i=1}^A \frac{t_i^2}{S_{t_i}^2} \quad (2.1)$$

Where t_i is the principal components and $S_{t_i}^2$ is the estimated variance of t_i .

However T^2 will only detect whether or not the variation in the original variables in the plane of the first A PCs is greater than can be explained by common cause. If a totally new type of special event occurs, it can be detected by computing the squared prediction error (SPE) of the residual of a new observation,

$$SPE = \sum_{i=1}^k (y_{new,i} - \hat{y}_{new,i})^2 \quad (2.2)$$

where $y_{new,l}$ is computed from the reference PCA model. SPE is also referred to the distance to the PCA model. It represents the squared perpendicular distance of a new multivariate observation from the projection space.

To find out the original variables that are responsible for the observed T^2 and SPE exceeding the control limits, contribution plots are used. Fig. 2.3 shows that the variable that has the most important impact on SPE is variable 7. Fig. 2.4 indicates that the main variable that contributes to the first principal component t_1 is variable 9.

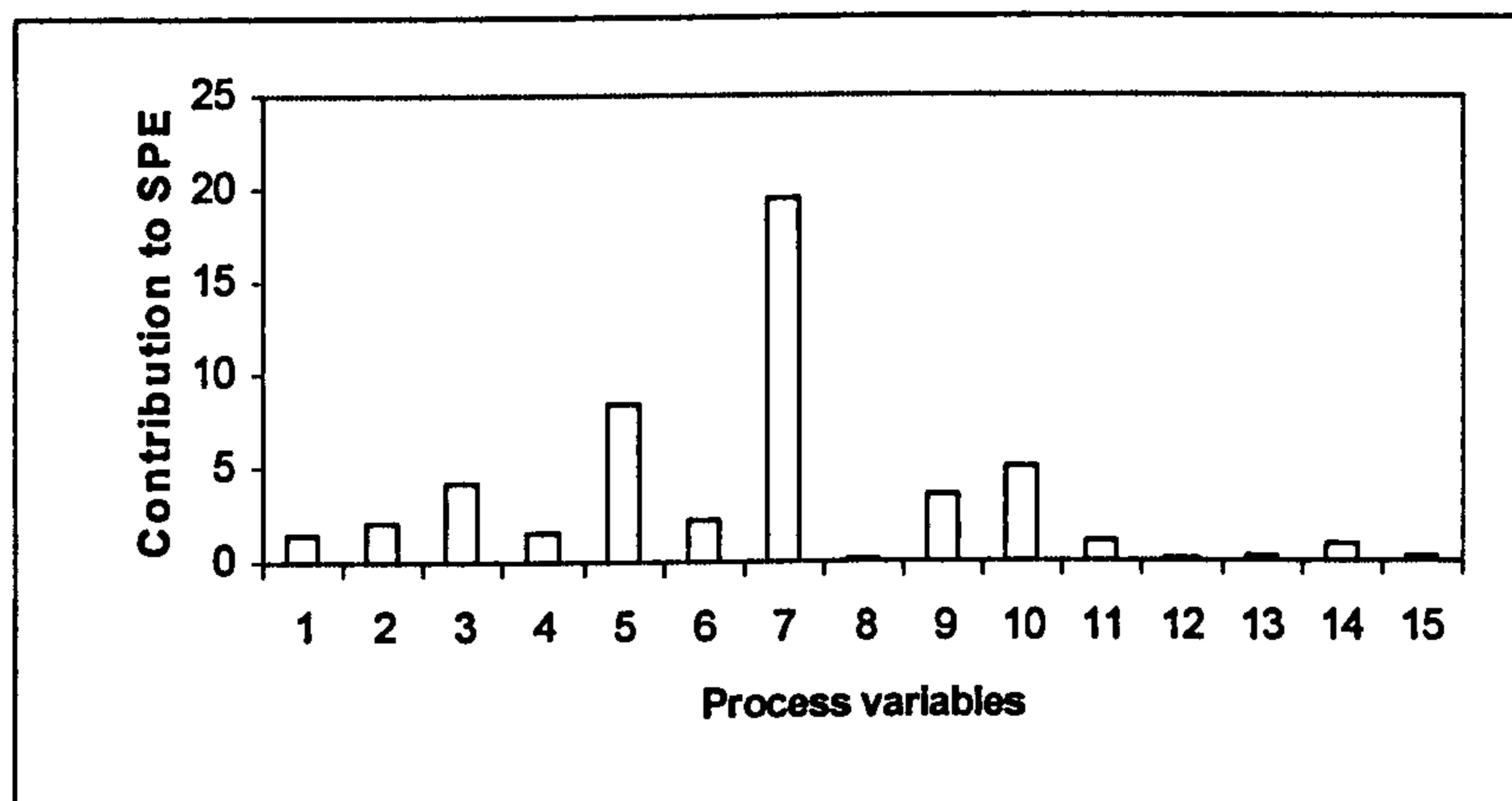


Fig. 2.3. Contribution plot of a process at a sampling point.

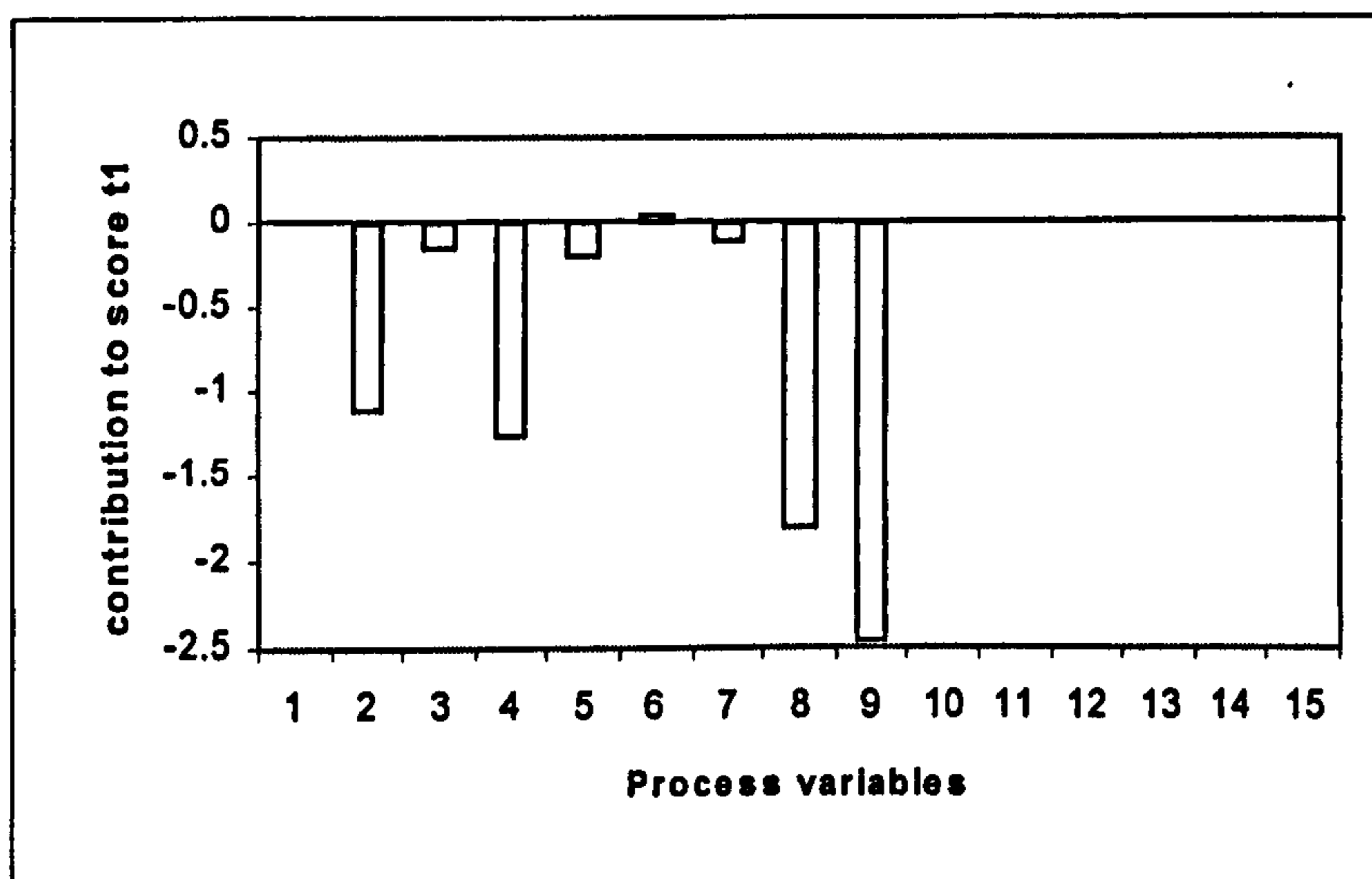


Fig. 2.4. Contribution plot to score of a process at a sampling point.

2.4.2 Application of MSPC Based on Principal Component Analysis (PCA)

Many researchers have successfully used multivariate statistical techniques based on PCA and PLS (Partial Least Square) in process monitoring, product design, fault detection, disturbance diagnosis and data analysis and on-line monitoring of batch processes. A comprehensive reviews have been made by MacGregor and Kourti (1995), Wise and Gallagher (1996), Cinar and Undey (1999), Wang (1999), Martin and Morris (1996), and Russell et al. (2000).

2.4.2.1 MSPC for Continuous Process Monitoring

Kresta et al. first studied PCA based on MSPC in 1991 but most of the progress was made in the last five years. Table 2.1 summarises the major publications on MSPC for monitoring and diagnosis of continuous processes. These studies have focused on the following issues:

- (1) Application of the methods, which were initially developed based on simulation studies to industrial processes (Kosanovich and Piovoso, 1997, Santen et al., 1997, Bakshi, 1998, Vedam and Venkatasubramanian, 1999, Jaeckle and MacGregor, 2000, Chen and Wang, 2000).
- (2) Application of the methods to more complex processes (Raich and Cinar, 1996, Kosanovich and Piovoso, 1997, Santen et al., 1997, Bakshi, 1998, Chen and McAvoy, 1998, Chen and Wang, 2000).
- (3) Study on fundamental issues of MSPC such as detectability, reconstruction and isolation ability (Dunia and Qin, 1998).
- (4) Integration of MSPC with other techniques such as wavelets (Bakshi, 1998).
- (5) Detailed examination on contribution plots.
- (6) Product design (Jaeckle and MacGregor, 1998; Chen and Wang, 2000).

Table 2.1. Summary of the publications on PCA-based MSPC for monitoring and diagnosis of continuous processes (Continued on next page.)

Continuous Processes					
References	Title	Purposes	Case Studies	Features	
Kresta, MacGregor, Marlin, 1991	Multivariate statistical monitoring of process operating performance	Process monitoring	Simulated processes: fluidised bed reactor and an extractive distillation	This is probably the first effort to use multivariate statistical methods such as PLS and PCA for process monitoring.	
MacGregor, Jaeckle, Kiparissides, Koutoudi, 1994	Process monitoring and diagnosis by multi-block PLS methods	Process Monitoring Fault diagnosis	A simulated tubular reactor	Proposed multi-block PCA/PLS method to monitor large scale continuous processes, however the number of process variables is only 6	
MacGregor, Kourti, 1995	Statistical process control of multivariate processes	Review		Review and tutorial on SPC based on PCA and PLS.	
Martin, Morris, 1996	An overview of multivariate statistical process control in continuous and batch process performance monitoring	Review		Review	
Wise, Gallagher, 1996	The process Chemometrics approach to process monitoring and fault detection	Review		Review	
Zhang, Martin, Morris, 1996	Fault detection and diagnosis using multivariate statistical techniques	Fault detection, Fault diagnosis	A continuous stirred tank reactor (CSTR)	Fault diagnosis can be performed by comparing the direction of the first loading vector of current observations with the directions of various faults in library.	
Raich, Clinar, 1996	Statistical process monitoring and disturbance diagnosis in multivariate continuous processes	Process monitoring Disturbance diagnosis	Simulation of Tennessee Eastman Plant	This paper provides a detail description of statistical process control to continuous process, and explores the discrimination and diagnosis of multiple disturbances.	
Kosanovich, Piovoso, 1997	PCA of wavelet transformed process data for monitoring	Process monitoring	<i>An industrial chemical process</i> (including reactors and flash drum)	Pre-filtering, then decompose the filtered signals with Haar wavelets and PCA is applied.	
Santen, Koot, Zullo, 1997	Statistical data analysis of a chemical plant	Fault detection	<i>Reactors in a shell petrochemical process</i>	Extract information through analysis of data from actual process using PCA	

Table 2.1. Summary of the publications on PCA-based MSPC for monitoring and diagnosis of continuous processes (Continued from last page).

Dunia and Qin, 1998	Subspace approach to multidimensional fault identification and reconstruction	Fault detection	A simulated process	The fundamental issues of detectability, reconstructability and isolate-ability were studied in this paper.
Bakshi, 1998	Multiscale PCA with application to multivariate statistical process monitoring.	Process monitoring Fault detection	<i>Industrial fluidised catalytic cracker unit (FCCU)</i>	Combining PCA and wavelet analysis.
Jaekle, MacGregor, 1998	Product design through multivariate statistical analysis of process data	Product design	<i>A simulated high-pressure tubular reactor process</i>	Using PLS to determine the new operating conditions to produce new product with desired quality specifications.
Chen, McAvoy, 1998	Predictive on-line monitoring of continuous processes	On-line process monitoring	Simulated Tennessee Eastman Process	Using Multi-way PCA to monitor a continuous process was reported in this paper.
Zhang, Tangirala, Shah, 1999	Dynamic process monitoring using multiscale PCA	Process monitoring	Simulator	Further discuss the advantages of combining PCA and wavelet analysis.
Vedam, Venkatasubramanian 1999	PCA-SDG based process monitoring and fault diagnosis	Process monitoring Fault diagnosis	Amoco Model IV FCCU	This paper first combines PCA and SDG. it uses PCA to monitor process and detect fault. Then SDG was applied to look for the root cause of the fault.
Cinar, Undey 1999	Statistical process and controller performance monitoring. A tutorial on current methods and future directions	Process monitoring		This is a tutorial paper.
Wang, Li, 1999	Combining Conceptual Clustering and Principal Component Analysis for State Space Based Process Monitoring	Proposed a conceptual clustering method For monitoring	A simulated CSTR and A simulated MTBE process	PCA was used for qualitative interpretation dynamic trend signals
Jaekle, MacGregor, 2000	Industrial applications of product design through the inversion of latent variable models	Product design	<i>An industrial semi-batch emulsion polymerisation process, and an industrial solution polymerisation process</i>	This work reported the two industrial examples of their proposed method (Jaekle and MacGregor, 1998)
Chen, Wang, 2000	Discovery of operational spaces from process data for production of multiple grades of products	Product design	<i>Industrial FCC distillation</i>	Industrial data

Table 2.2. Summary of the publications on PCA-based MSPC for monitoring and diagnosis of batch processes.

Batch Processes					
References	Title	Purposes	Case Studies	Features	
Wold, Geladi, Esbensen, Ohman, 1987	Multi-way principal component- and PLS-analysis	Propose a PCA method for dealing with three-way data	This was to propose a mathematical method, not specific to process industry	A mathematical method to analyse three-way data using PCA	
Nomikos, MacGregor, 1994	Monitoring batch processes using multi-way principal component analysis	Process monitoring	Simulated semi-batch reactor	Propose of multi-way PCA for monitoring batch processes	
Martin, Morris, Papazoglou, Kiparissides, 1996	Batch process monitoring for consistent production	Process monitoring	A batch polymerisation reactor	Based on Multi-way PCA, proposed using M^2 statistics as control index.	
Nomikos, 1996	Detection and diagnosis of abnormal batch operations based on multi-way principal component analysis	Fault detection Fault diagnosis	An industrial polymerisation reactor	An industrial application of using SPC and contribution plot to detect abnormal operation was presented in this work.	
Kosanovich, Dahl, Piovoso, 1996	Improved process understanding using multi-way principal component analysis	Fault diagnosis, Improve process understanding	A commercial batch reactor	Multi-way PCA was used to analyse historical data, leading to improved process understanding.	
Rännar, MacGregor, Wold, 1998	Adaptive batch monitoring using hierarchical PCA	Process monitoring	Industrial batch polymerisation process	A new approach was presented, which overcome the need of estimating or filling data from the current time to the end of batch. It is based on a recursive multi-block PCA/PLS method, which processes the data in a sequential and adaptive manner.	
Tates, Louwerse, Smilde, Koot, Berndt, 1999	Monitoring a PVC batch process with multivariate statistical process control charts	Process monitoring Fault diagnosis	An industrial PVC batch process	This work reported an industrial example of monitoring batch process using multivariate statistical process control charts.	
Louwerse, Smilde, 2000	Multivariate statistical process control of batch processes based on three-way models	Process monitoring	A simulated semi-batch emulsion polymerisation process	Unfold-PCA, PARAFAC, and Tucker3 models are discussed and compared.	
Yuan, Wang, 2000	Multilevel PCA and inductive learning for knowledge extraction from operational data of batch processes	Process monitoring	Simulated polymerisation reactor	wavelet was used for automatic determination of stages rules can be extracted from data for monitoring	

2.4.2.2 MSPC for Batch Process Monitoring

In continuous processes, the data to be processed is a two-way array, $X(I \times J)$, where J is the number of variables and I the observations. In batch processes, for each variable at each observation, since its values correspond to a trajectory spanning the whole batch run (or campaign), the data to be analysed is a three-way array $X(I \times J \times K)$, where J is the number of variables measured at K time intervals throughout a batch, and I is the number of batch runs. The MSPC was adapted to such three-way data by Nomikos and MacGregor (1994, 1995) using the multi-way PCA technique developed by Wold et al. (1987). Figure 2.5 depicts the procedure. Table 2.2 gives a summary of the publications on multi-way PCA for batch process studies.

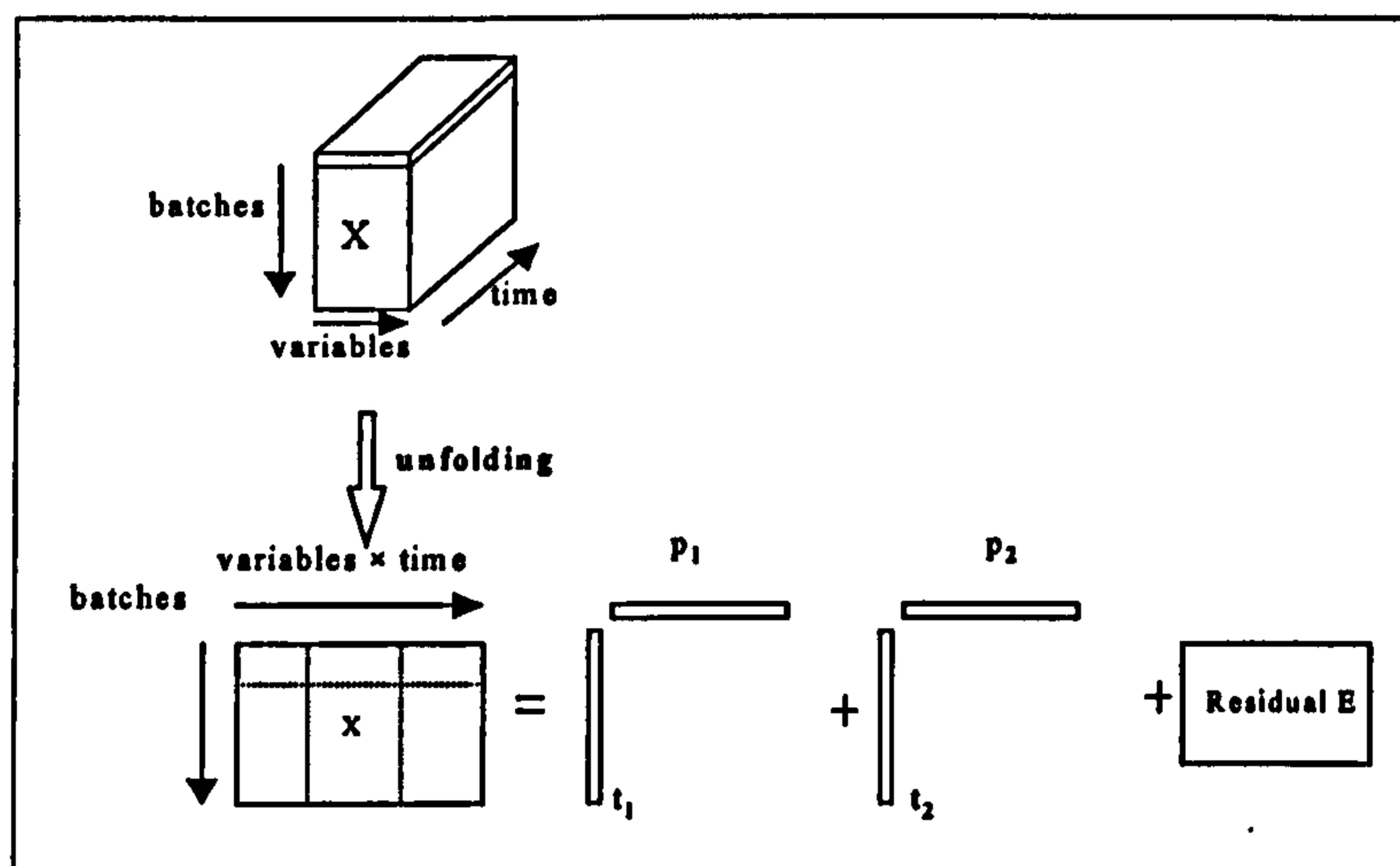


Fig. 2.5. Unfolding of three-dimensional data array and multi-way PCA.

These studies have focused on the following issues:

- (1) A practical problem with on-line monitoring using MSPC to batch processes is that when a batch process is in progress the measurements for the future time periods are unknown, and this means that the new data set is incomplete. To monitor a new batch at the current time, one must replace future observations with appropriate values, such that the predicted scores at each time will be as close as possible to those that would be calculated if the complete trajectories were available. Nomikos and MacGregor (1994)

assumed that the future deviations of the observations from the mean trajectory remain constant at their current values, for the rest of the batch run. Louwerse and Smilde (2000) developed a different method. The method divides the total run time K of a batch process into several time periods according to scheduling points so that each section can be treated separately. Rännar et al. (1998) presented a method, which does not require estimates of the future data. The approach is based on a recursive hierarchical or multi-block PCA or PLS algorithm which processes the data in sequential manner.

- (2) Because the original method and its later extensions were mainly based on simulated case studies, researchers and industrial practitioners have been very interested in applying them to industrial problems. A number of papers have been published which led to interesting findings. For example, in industrial processes, the batch lengths can be different from batch to batch runs.
- (3) The way of unfolding the data has also attracted interests. In the original multi-way PCA, the three way data $X(I \times J \times K)$ was unfolded to a two-way data $X(I \times JK)$. Later various other methods for unfolding the data were proposed, such as the parallel factor (PARAFAC) (Wise et al., 1999) and Tucker3 (Tucker, 1966; Claus and Rasmus, 1998). Louwerse and Smilde (2000) compared the various methods and concluded that their performance depends on the type of fault occurring in the batch process.
- (4) Some researchers have studied the method for variable contribution analysis in multi-way PCA and found that the relative importance of variables varies at different stages of a batch run (Dong and McAvoy, 1996b, Kosanovich, Dahl and Piovoso, 1996).
- (5) Yuan and Wang (2001) emphasised the importance of monitoring batch operations according to stages and developed a wavelet method for automatically identifying stages. A rule-based method was also proposed in the study.

2.4.3 Other Developments in PCA Based Process Monitoring

- (1) Many researchers have pointed out that PCA is a linear operation. This has stimulated study on non-linear principal component analysis. Kramer (1991) proposed to use auto-associative neural networks as a non-linear PCA method. Dong and McAvoy (1996a) developed an alternative non-linear PCA method using the concept of principal curves. Wang (1999) indicated that while both methods are able to reduce the dimension of the original data effectively, the principal components obtained are still correlated or

dependent. This is unlike linear PCA in which the PCs are known to be linearly uncorrelated.

- (2) Multi-scale PCA. Bakshi (1998) proposed the idea of integration of wavelets with PCA to analyse signals in multi-scales.
- (3) Multi-level PCA. Yuan and Wang (2001) have developed a multi-level PCA method, which makes use of rules.

Kosanovich et al. (1996) used multi-way principal component analysis to improve batch process understanding and to identify the major sources of variability of process data. Recently, Tates et al. (1999) presented an application of the method. They use multivariate statistical process control charts to monitor a PVC batch process on-line. Louwerse and Smilde (2000) focus on the decomposition of batch process data with three dimension to propose three different models: Unfold-PCA, PARAFAC and Tucher3 and compare these models.

2.5 Supervised and Unsupervised Neural Networks

Neural networks (NNs) have also been widely studied in process fault diagnosis. NNs can be broadly divided into two types, i.e., supervised and unsupervised. A supervised NN requires training data from which a non-linear mapping model is learned to map the symptoms of faults to sources of faults. Unsupervised neural networks do not need training data. They group process operational data into classes corresponding to normal and abnormal operational zones only based on symptoms.

2.5.1 Supervised Neural Networks

The most widely studied supervised NN is the error back-propagation neural network (BPNN). Simply speaking, BPNN is an algorithm or software system, which can learn from data the non-linear relationships between multiple inputs and outputs, without requiring specific information on the fundamental mechanisms relating them. The learning mimics the human learning process through continuously correcting the errors. A BPNN is made up of interconnected computational processing elements called neurons which process input information and give outputs. The neurons are divided into layers. A typical three-layer BPNN consists of an input layer representing the input variables, an output layer corresponding to the output variables and a hidden layer (Fig. 2.6). Neurons between two

adjacent layers are fully connected by branches. Attached to each branch there is a weight reflecting the strength of the connections. The training (or learning) of the network involves finding the connection weights, which minimise the sum of squares of difference between the network outputs and the target values:

$$E = \sum_{m=1}^M \sum_{i=1}^N (t_i^{(m)} - y_i^{(m)})^2 \quad (2.3)$$

Where M - Number of training data patterns

N - Number of neurons in the output layer

$t_i^{(m)}$ - The target value of the i th output neuron for the given m th data pattern

$y_i^{(m)}$ - The prediction for the i th output neuron given the m th data pattern

The BPNN learning process involves a forward propagation pass calculating the outputs using the inputs, weights and neuron transfer functions, as well as a back-propagation pass correcting the weights using the error between predictions and target values. The major advantage of a BPNN model is its ability to learn from data without requiring principle knowledge of domain problems. In addition it is very effective in dealing with a large amount of data. The structure of a BPNN model can be easily constructed according the domain problem and availability of data attributes.

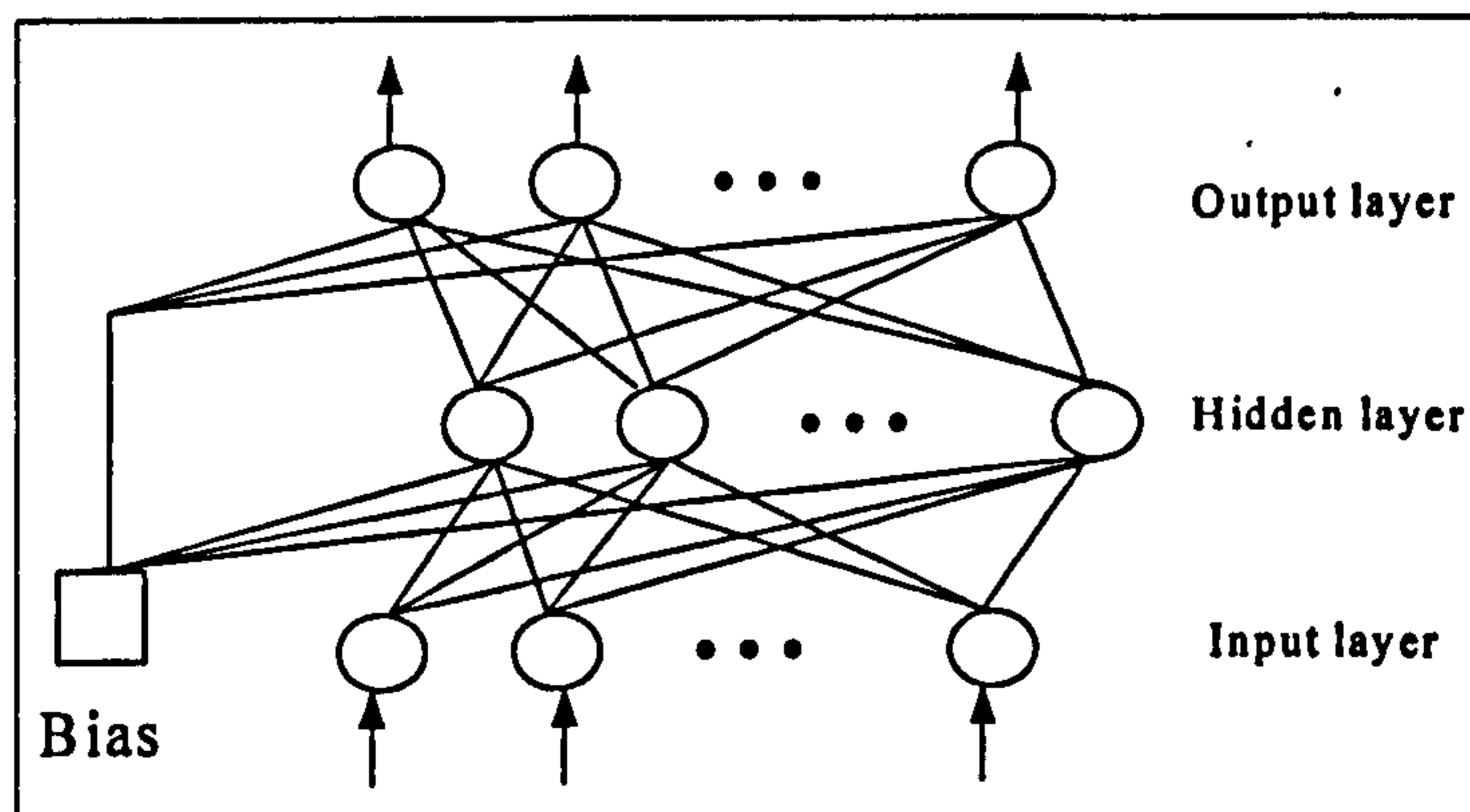


Fig. 2.6. A three layered back propagation neural network.

As one of the earliest applications of BPNN in process fault diagnosis, Hoskins and Himmelblau (1988) studied six types of faults using a process consisting of three CSTRs in series. Venkatasubramanian et al. (1990) investigated some fundamental issues using a more

complex process. Hoskins et al. (1991) studied 19 types of faults using a process having 418 measurements. Kramer and Leonard (1990) made a useful analysis on use of BPNN in process fault diagnosis and introduced radial basis function network. Ungar et al. (1990) looked at the application of adaptive networks to fault detection and adaptive control. They used two neural networks, one for fault diagnosis and one for the controller. The connection strengths for the models represented by the correlation between inputs such as alarms and sensor measurements and the outputs such as faults and action, which are learned using rules and the back-propagation algorithm. The outcome of the system is a pattern recogniser, which learns non-linearly for controlling simple process, and to learn the logical relationships between the alarm and measurements with faults as well as their linear correlations. Farrell and Roat (1994) proposed a framework for enhancing neural network performance in fault diagnosis, which could also be described as an elementary classification (clustering) technique. The network is trained using not the actual values of variables, but normalised distances from normal operation values. Improved performance was observed. An unsolved problem is how to determine the threshold value, which specifies the size of each cluster. Sridhar and Seagrave (1996) came up with a methodology of combining different neural models by using stacked generalisation. It attempts to solve the problem of model selection and model combination simultaneously, to improve model predictions. The drawback of this approach is the increased computational time. Zhang et al. (1997) used the same principle but the purpose was to build a neural soft sensor for quality prediction in a polymerisation reactor. Lennox et al. (1998) employed the artificial neural networks in two practical applications. The first application was modelling verification process using real process data (Verification is a process that encapsulates highly active liquid waste in glass to provide a safe and convenient method of storage). The second application employed the neural network to capture non-linear system characteristics and then recalled to provide a means of detecting imminent failure of a vessel in the same verification process. Because real data is employed, the method is limited to a number of known failures therefore needs further training for new conditions. Simani and Fantuzzi (2000) developed a fault diagnosis methodology consisting of two stages. In the first stage the fault is detected on the basis of the residuals generated from a bank of Kalman filters, while in the second stage, fault identification is obtained from pattern recognition techniques implemented by a neural network. Comparative study was carried out using a three-layered radial basis function network and a back-propagation neural network. It was found that the radial basis function did not perform satisfactorily.

Wang (1999) indicated that supervised neural networks have two major limitations in fault diagnosis. The first problem is that it is not an effective method for identification of abnormal operations. Some researchers used neural networks trained with normal operational data to identify faults: if the output is not in the normal region then abnormal operation is expected. The second and most important limitation of supervised neural networks is that training data is not readily available. It is unthinkable to initiate faults in a real plant in order to get training data. Many researchers have proposed to use dynamic simulators to generate the necessary training data. These limitations make supervised neural networks less attractive in fault identification and diagnosis compared with unsupervised neural networks.

2.5.2 Unsupervised Neural Networks

To distinguish supervised and various unsupervised NNs, it is useful to make a detailed classification of the data that is used. Table 2.3 listed four types of data and the types of neural networks that can be used to solve the classification problem. The most important advantage of unsupervised NNs compared with supervised NNs is that they do not need training data. They classify the operation of a process into normal and abnormal operations only based on the assessment of the measurements.

Table 2.3. Types of data and neural networks.

Types of data	Types of neural networks
Part of the database is known, i.e., the number and descriptions of classes as well as the assignments of individual data patterns are known. The task is to assign unknown data patterns to the established classes.	Supervised NNs, e.g. back-propagation NN (BPNN)
Both the number and descriptions of classes are known, but the assignment of individual data patterns is not known. The task is then to assign all data patterns to the known classes.	Unsupervised NNs, e.g., Kohonen (1982)
The number of classes is known but the descriptions and the assignment of individual data patterns are not known. The problem is to develop a description for each class and assign all data patterns to them.	Unsupervised NNs, e.g., Kohonen (1982)
Both the number and descriptions of classes are not known and it is necessary to determine the number and descriptions of classes as well as the assignments of the data patterns.	Unsupervised NNs, e.g., adaptive resonance theory (ART2)

Whiteley and Davis (1994) and Whiteley et al. (1996) studied the adaptive resonance theory (ART2) developed by Grossberg (1976a,b) and Carpenter and Grossberg (1987, 1988) for the purpose of process fault diagnosis. In addition to being an unsupervised technique, ART2 is also recursive, or in the terms used in ART2, it is plastic, that is able to acquire new knowledge and retain stable in the sense that existing knowledge is not

corrupted. This property is apparently very useful for on-line monitoring where information is received continuously and the model can be continuously improved.

Chen et al. (1999) and Wang et al. (1999) found that ART2 is very sensitive to noises and to the threshold value; therefore they developed a new method called ARTnet, which uses wavelets to replace the signal pre-processing element of ART2. ARTnet proves to be robust to noise and the threshold values, and faster than ART2.

Kohonen network (1982) has also been studied for fault detection and diagnosis (Chowdhury and Wang, 1996). The difference of Kohonen network from ART2 and ARTnet is that it needs the number of classes to be determined before learning starts.

2.6 Other Methods

2.6.1 Data Pre-Processing

Data pre-processing has the following purposes,

- (1) Filtering out the noise components otherwise this may result in wrong conclusions being reached from the data. On-line measurements are characterised by noises and uncertainties. At high noise to signal ratio, the real trend of variables and the process cannot be clearly identified.
- (2) Extracting features, reducing the dimensionality of the original signal and retain as much relevant information as possible. The main reasons for feature extraction are, first of all to minimise the dependencies between attributes and secondly to reduce dimensionality.
- (3) Dealing with the problem of variable sampling periods for data, such as on-line real time signals and laboratory analytical data.
- (4) Qualitative interpretation of measurements, for the purpose of expert systems and qualitative reasoning.

Although techniques for noise removal and data reconciliation exist, some new techniques have been developed in recent years, which are more effective than the traditional methods in handling noise and uncertainty in data. More importantly these techniques can be

used for qualitative interpretation, feature extraction and dimension reduction of dynamic trend signals.

2.6.1.1 Qualitative Interpretation

The most notable method for qualitative interpretation of dynamic trend signals is the episode method, which was originally developed by William (1986). Janusz and Venkatasubramanian (1991) adapted the method and produce nine primitives to represent any plots of a function, as shown in Fig. 2.7. Each primitive consists of the signs and the first and second derivatives of the function. This means, each primitive possesses information about whether the function is positive or negative, increasing, decreasing, or not changing, and the concavity. An episode is an interval described by only one primitive and the time interval the episode spans. A trend is a series of episodes that when grouped together can completely describe the qualitative states of the system. C and D in Fig. 2.7 are actually not primitives because they can be regarded as the combination of A, F and B, E. Therefore they can be reduced to seven primitives as shown in Fig. 2.8.

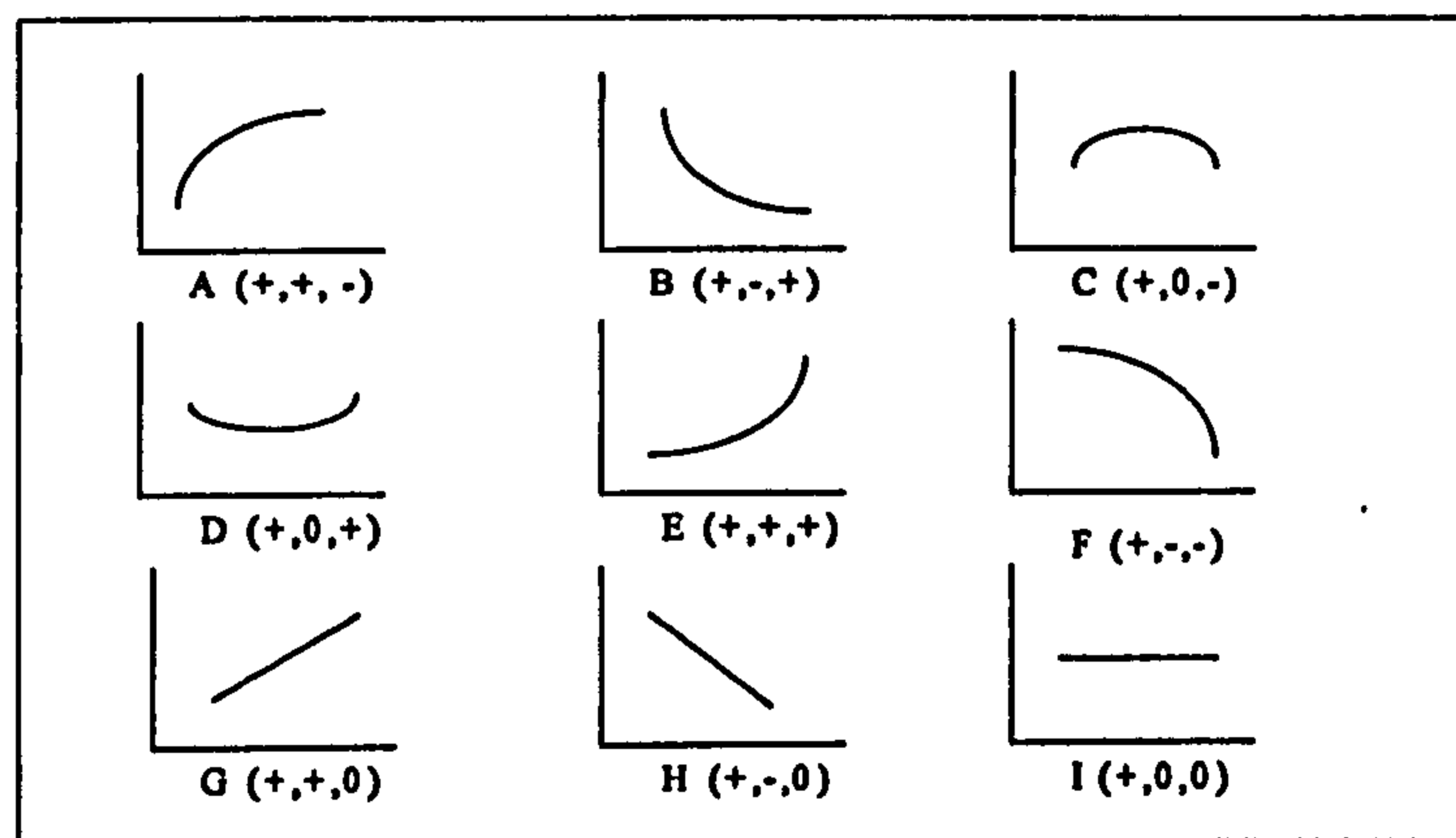


Fig. 2.7. Nine primitives used in episode approach.

A combination of episodes will form a trend over an interval and is described by a primitive and the associated time. Primitives are different for first and/or second order derivatives, so the distinguishing points between episode segments are the extrema and inflexions where

$$\frac{\partial x}{\partial t} = 0 \quad \text{or} \quad \frac{\partial^2 x}{\partial t^2} = 0$$

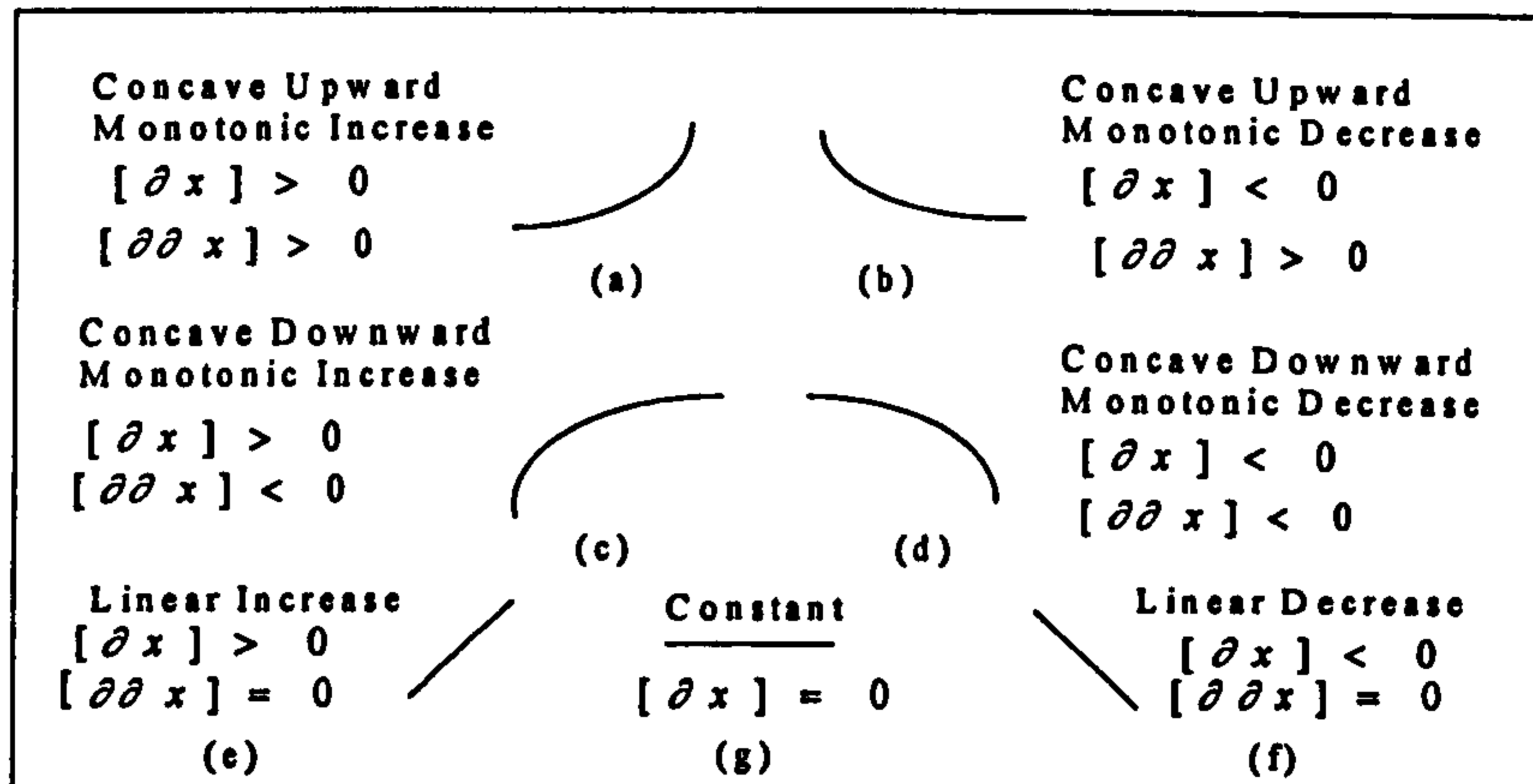


Fig. 2.8. The seven primitives episodes.

The task of identifying the episodes from a signal is simply to identify the inflexions and/or extrema, i.e., singularities in the signal since they correspond to distinct points of the episode segments. This means that the singularities of a signal contain the most important information about the trend. Using singularities for feature representation therefore completely defines the episodes characteristics of a signal.

However, the singularities are strongly influenced by noise and this is the major weakness of this approach. Noise components must be identified and filtered from the features; otherwise the representation will be misleading. Bakshi and Stephanopoulos (1994 a&b) used the wavelet approach to simultaneously remove the noise components and automatically identify the inflection points.

Wang and Li (1999) developed a different approach for qualitative representation of dynamic trends using principal component analysis. The main advantage of the method is that it can qualitatively describe a dynamic trend using only a single qualitative value, without the need to break the trend into segments.

2.6.1.2 Feature Extraction and Dimension Reduction

There are two aspects in dimension reduction of process dynamic trends: feature extraction from a trend of an individual variable and removal of dependencies among a number of correlated and sometimes redundant variables. The former is concerned with using minimum number of values, called features to represent a trend. Wavelets (Bakshi and Stephanopoulos, 1994 (a&b); Chen et al., 1999; Chen, 1998) have been studied for this

purpose. The methods of episodes (Janusz and Venkatasubramanian, 1991; Cheung and Stephanopoulos, 1990) and principal component analysis (Wang and Li, 1999) can also be considered as belonging to this category. The later is aimed at removing the dependencies among variables so that the process can be monitored in a reduced dimensional space. The most notable method for this purpose is principal component analysis (PCA) (MacGregor and Kourti, 1995).

2.6.2 Hybrid Methods

There are also research interests in integration of different techniques. Examples include integration of expert systems and neural networks (e.g., Ozyurt and Kandel, 1996), fuzzy logic with neural networks (e.g., Zhao et al., 1997; Wang et al., 1997), and fuzzy logic with graphical methods (Shih and Lee, 1995; Han et al., 1994; Wang et al., 1995).

2.6.3 Graphical Methods

The most well studied graphical method for process fault diagnosis is signed digraphs (SDG). SDG is attractive because of its ability to translate the complex inter-relationships between process variables into an easily understood form and make a complex problem traceable. In relation to development of a new graphical method for fault diagnosis in a joint process – operator system, a detailed literature review will be made in chapter 6.

2.7 Human Factors in Process Operational Safety

As has been addressed earlier that operators are an integral part of modern computer control systems who are responsible for assessing process operational status and take corrective actions when he/or she perceives that things may go wrong. Human factors in process operational safety (Mill, 1992; Redmill and Rajan 1997) are concerned with what happens when the operator receives information, reviews it against his/her experience and feeds back to the operation. Many things may go wrong at the interface between the operator and the process. For example the operator's observation may be faulty, assessment on the situation may be wrong and the feedback or action may commit failure and cause more faults in the process.

According to a survey conducted by a consortium led by Honeywell around the world including UK, USA, Canada, Europe and Japan, about 40% of abnormal operation were caused by the human errors (Nimmo, 1995). However as indicated by Health and

Safety Executive (UK), there is only limited information on how human factors can be assessed and even less that is specific to chemical engineering. There are two main methods which, have been used to address human factors in process safety, i.e., training and human-machine interactions.

2.7.1 Operator Training using Computer Based Systems

Traditionally operator training has been based on on-site learning and practising. More recently, computer based training systems have been widely used. The most widely used technique is using training simulators. On a dynamic training simulator, operators learn to identify abnormal operations and observe systems responses to faults and corrective actions, as well as learn start-up and shutdown procedures. Since various faults can be easily initiated and the dynamic response time is much shorter than in a real plant, operators can experience more operational scenarios in weeks on a training simulator than in the real plant in months to years.

Knowledge based expert systems can also be used for training operators (Su and Lin, 1997). Emergency management of chemical spills was employed to exemplify the rule based decision task. Expert systems were used as the training tool for 40 students who were asked to resolve spill scenarios under the manipulation of training and deadline conditions.

The function of operator training systems can be greatly enhanced with the use of multimedia technologies including 3D motion pictures, sound effects and interactive communications (Goh et al., 1998).

Research on human factors often considers one human user interacting with the machine. In practice, it often involves several operators working together and communicating between each other. Goal setting and goal sharing are important prerequisites for co-operative work. Elliot and Entin (1999) developed a team training procedure designed to train teams to adapt by shifting from explicit to implicit modes coordination and choosing strategies that are appropriate during period of high stress and workload condition. The result of their study indicated that several underlying team process measures exhibited pattern indicating that adaptive training improved various team processes, including efficient use of mental models, which in turn improve performance.

2.7.2 Addressing Human Factor Issues at the Design Stage

Human errors can also be introduced to safety check procedures during the process design stage, such as the symbolic model verification procedure, hazard and operability studies (Kletz, 1999; Lees, 1996), and process simulation (Moon et al., 1997; Probst et al., 1997; and Dimitriadis et al., 1995). In these procedures, modes of operator activities are needed.

2.7.3 Reliability Modelling and Risk Simulation of Operators

With the increasing awareness of the importance of human factors in operational system safety, human reliability assessment (HRA) is gaining increasing attention (Broadbent et al., 1990). Early work attempted to evaluate the probability of human erroneous actions such as the method developed by Swain and Guttman (1983), which was known as the Technique for Human Error Rate Prediction (THERP) and regarded as the first generation of HRA methods. THERP is a schematic representation of human actions and related system events, the so-called HRA Event Tree. The drawback of THERP method is that it does not include a consideration of the dynamic cognitive factors that effect operator's behaviour. The development of a second generation of HRA methods (Dougherty, 1990, 1991) failed to overcome the drawback of THERP due to failure to provide a proper treatment of human cognition. Consequently the natural evolution of the human reliability assessment approaches led to attempts to solve the problem of HRA in terms of the Reliability of Cognition (Hollnagel, 1991). These solutions account for dynamic effects of endogenous and exogenous factors on the inappropriate decision-making and actions (Cacciabue et al., 1993; Cacciabue, 1998; Roth et al., 1991). In parallel to the evolution of the HRA methods, the taxonomies dedicated to human erroneous behaviour have also gradually modified their focus from the simple omission/commission alternative to more structured taxonomies of work environment based on cognitive analysis (Norman, 1981; Rasmussen et al., 1981; Reason, 1990). These approaches for the study of the reliability of cognition need to be coupled to appropriate taxonomies accounting for the socio-technical factors of the working environment (Bagnara et al., 1991) and for well-structured definitions of causes, or genotypes and manifestations, or phenotypes and consequences of human erroneous actions (Hollnagel, 1993, 1996). Yoshikawa and Wu (1999) developed a framework for estimating Human Error Probability, which is used for HRA. The approach relies on the comparison between the experimental data and human model simulation, an estimated human cognitive reliability curves are used to confirm the applicability of human

model for estimating these human error probability parameters. Vanderhaegen (2001) developed a method called ACIH, a French acronym for analysis consequences of human unreliability. The method aimed at identifying both tolerable and intolerable sets of human behavioural degradation, which may affect the system safety.

The limitations of human reliability approaches are no greater than the equivalent limitations of the system reliability approaches, which is that the lack of cognitive or human modelling accuracy is no more of a drawback than the lack of deterministic physical analysis, typical of a fault-tree approach, in performing the reliability analysis of the system. However the drawback of HRA methods mainly falls within modelling and simulation of the human behaviour such as human planning and decision and human-machine interaction such as dynamic and time dependent nature of interaction. Johnson (1999) discussed the barriers to the practical application of human error analysis and explained why the human error modelling failed to help in systems development. Human behaviour modelling is also employed in other applications such as design of interface (Johannsen, 1995, 1997; Yoon and Kim, 1996; Nishitani et al., 2000) and operational procedures (Grant and Mayes, 1991; Moray et al., 1992).

2.8 Conclusions and Final Remarks

Over the last fifteen years significant progress has been made in research in applying artificial intelligence techniques to process monitoring and fault diagnosis. This chapter has reviewed some of these including real-time expert systems, univariate and multivariate statistical process control, supervised and unsupervised neural networks as well as data pre-processing techniques and graphical methods. In the review, the focus has been put on examining the advantages and limitations of various methods rather than exhausting the literature. To make a clearer and more concise comparison of some of these methods, Table 2.4 gives a summary.

Apart from the comments made on individual methods in the above review, we also have the following observations. Firstly, there is a need to benchmark the techniques in industrial applications. Although there have been comparisons of various methods in literature, they often are qualitative and not comprehensive. Secondly, the methods need to be integrated with modern computer control systems. This has just started, for example, some DCS control systems now provide fault detection and diagnosis programs as standard configuration modules. However, it has not become a routine practice. Furthermore, with

extensive use of these methods, the need to improve existing techniques and seek more effective methods will arise.

Table 2.4. Comparison of various methods for fault identification and diagnosis.

Techniques	Advantages	Disadvantages
Real-time expert systems	Knowledge is transparent and causal Can give explanations to Why and How Rules can be easily added and removed Can be considered as a principle knowledge based method Human experts experience and knowledge can be stored and used	Human experts knowledge is subjective Unable to learn from data therefore not able to automatically improve performance during use Causal relationship can be buried in a large knowledge base Difficult to maintain and inconsistency may occur in a large database Lack of statistical basis because data is not used. Can have difficulty in describing system having strong interaction of variables Qualitative interpretation of measurements cause loss of information
Multivariate Statistical Process Control (MSPC)	MSPC is a data driven method Principle model is not needed Has a statistical basis Well developed	Human expert's knowledge can not be used Principle knowledge can not be incorporated into the system Need a large amount of historical data Knowledge is opaque
Supervised Neural Networks (NNs)	Supervised NNs are data driven approaches Principle model is not needed Well developed and easy to be trained	Require training data of fault – symptom pairs, which is often not available Human expert's knowledge can not be used Principle knowledge is often not used Knowledge is opaque
Unsupervised Neural Networks	Unsupervised NNs are data driven approaches Principle model is not needed Do not need training data	Not as well developed as supervised NNs Knowledge is opaque Human expert's knowledge can not be used Principle knowledge is not used
Signed digraphs (SDG)	a useful tool for qualitative, causal and first principle analysis represent a complex problem in a causal and traceable way System's overall causal relationship can be visualised	Being a qualitative method drawing a SDG for a process involving strong interactions of variables and control loops can be difficult. Not a data driven approach Qualitative interpretation of measurements cause loss of information

In almost all the above-reviewed methods, it has assumed that after a fault occurring, the process will evolve without intervention of operators. For example, dynamic simulation systems have been widely used in developing and testing fault detection and diagnosis systems. The simulators only emulate the process's behavior under disturbances or faults, without considering operators possible interventions during the dynamic transition of the process. The dynamic behaviour of the process clearly will be different and more complex if operators intervene during the process of system evolution. Most of the studies on operator's factors in systems operational safety have been in other industries such as the

nuclear and air space, rather than chemical industries. These studies have been focused on stress and behaviour models of operators and the purpose has been on improving management culture, working environment such as light and operational procedures. They have not been linked to development of computer aided fault detection and diagnosis systems.

A further observation is that all the studies on automatic fault detection and diagnosis have focused on only part of the integrated dynamic system, i.e., the process part. No effort has yet been made on automatic monitoring and assessing the other part, i.e., the operators. This may be partly due to the difficulty associated with automatically detecting the fault committed by operators, but is certainly inconsistent with the statistics. According to Nimmo (1995), 40% of fault happened in process history was due to human factor. Lardner and Fleming (1999) indicated 80% of accidents involved human errors. The difference in the figures may have been caused by the definition on what can be called human errors (direct human error or process error with inappropriate reaction of operators), they all stressed the importance of human factors in operational process safety. However, as reviewed above, work so far has been restricted to training and prediction of human reliability. There has been no effort to develop techniques and systems that can automatically characterise, monitor and assess operators behaviour and actions in operation.

Chapter 3

The Joint Process-Operator Simulation System

This chapter describes the role and implementation issues of the joint process-operator simulation system.

3.1 Introduction

Data, information and communication are very important to the analysis of the human-machine interactions. In the chemical and allied industries, it will take years to collect sufficient data and then catalogue them for the human-machine behaviour study. The collected data, from which, the accidents/incidents have been experienced by human operators, only covers events that have happened and reported. There are still plenty of unexpected errors in plant design, operations, human or equipment. Hence, other scenarios, which have not happened, may happen. To overcome this deficiency, it is advantageous to develop a computer-based system, which can generate data and information in a very short time to cover most of the possible events lurking in the process plants waiting to materialise. In fact, this computer-based system should also be able to catalogue, analyse, communicate and predict the human-machine interactions readily.

For this proposes, a joint process-operator simulation system to carry out all analyses, interaction and model development is developed in this chapter. The system is used as the main tool to generate the training data to be used in Chapter 6, validation data in Chapter 7, human behaviour data in Chapter 4; and to develop the process and human behaviour qualitative models in Chapters 4 and 6. It is also used to monitor the process and human behaviour (Chapters 4 and 5), undertake data analysis (Chapters 4 and 7), and evaluate the developed models (Chapter 7). The system development and testing are based on a joint simulation framework for human-process interactions. The operator's performance is modelled as a knowledge-based system, which is a collection of rules representing the skills of operators in perception and interpretation of on-line signals, and the subsequent planning and sequence of actions. Moreover, a CSTR dynamic training simulator generates data of the process behaviour. One of the objectives of the joint system is to develop a framework for

analysing the operational records in detail and to study the proposed human factor studies. In the case of human factor studies, special attention will focus on the human errors in operational process safety in an attempt to identify the good and bad behaviour and performance of both process and personal operation. The generic knowledge can be used to improve the operator's skills, design process of equipment and control systems, develop decision support system and carry out hazard and operability and reliability studies.

In order to develop a framework that can provide guidelines and support the above analyses, it is important to start by illustrating some basic concepts and definitions that generically characterise the human-machine interaction system. Therefore, in Section 3.2, the outline of a classical architecture for process-operator interaction and simulation of cognition is given. To define the structure and the functions of the developed system, several types of process-operator interaction systems used for simulation, analysis and application are investigated in Section 3.3. In Section 3.4, the architecture of the proposed process-operator interaction system is detailed. Finally, the conclusive remarks are made in Section 3.5.

3.2 The Joint Human-Machine Interaction System

Human-machine interactions always occur in a realistic context, which is characterised by the machine under control, the socio-technical working environment and by the operator in-direct contact with the process. The plant interacts with the operator through its interface, i.e. display panels, indicators, and decision support tools. The socio-technical working conditions, such as the context and environment, influence the human behaviour. These conditions comprise:

- (1) The actual environment such as noise, space, light, temperature, etc. in the operation place.
- (2) Other operators cooperating directly or collaborating at distance with the decision maker.
- (3) The whole social context represented by the management, the company, the society, and the cultural climate.

The process interface and socio-technical working conditions are the main source of incentive for the operator. They affect the allocation of the resources (i.e. data and information) and knowledge base. They may modify the unfolding of the reasoning and

cognitive processes, as well as the performances of manual or control actions, for examples, causing error or inappropriate behaviour, or altering the amount of knowledge accessible to the human in a given circumstance. Therefore, the human-machine interaction system must include an interaction model, so that the system will be able to account for other aspects of the interaction, such as dynamic features, human errors, component failures, control panel and display units, and working environment. Therefore the joint system requires an interaction model to carry out the above functions and data architecture model for managing the data that supports the simulation and permits the interaction model to manage the data exchange between all human-machine interaction systems. A typical architecture of a human-machine interaction system is shown in Fig. 3.1. The system is comprised of a number of models linked to dynamic memory to allow a fast and bi-directional data flow between the system models.

An efficient interaction (i.e. easy but fast data, information and knowledge exchange) between the data architecture and the interaction models must be established since all knowledge and information. The types of disturbances influence the operator behaviour regarding the overall joint system required by the interaction model is stored in the data architecture model. For example, in order to let the operator model to take an action or decision in an accident situation, the data architecture model will provide all knowledge and information, such as the type and mode of error, the type of component failure, level of operator stress and expertise, amount of information available for the operator by the support system, etc., required by the interaction model to carry out the accident scenarios. The operator model will produce a number of actions or procedures during the accident to represent his/her own behaviour, which will be recorded by the joint system. The operator behaviour will be analysed and assessed also by the interaction model. As a result, new knowledge and information will be created and used to update and modify the existed knowledge and information, which are located in the data architecture model. The new information is used to create new scenarios under accident situation, rules and facts related to operator and process, and models to represent the behaviours of both operator and process.

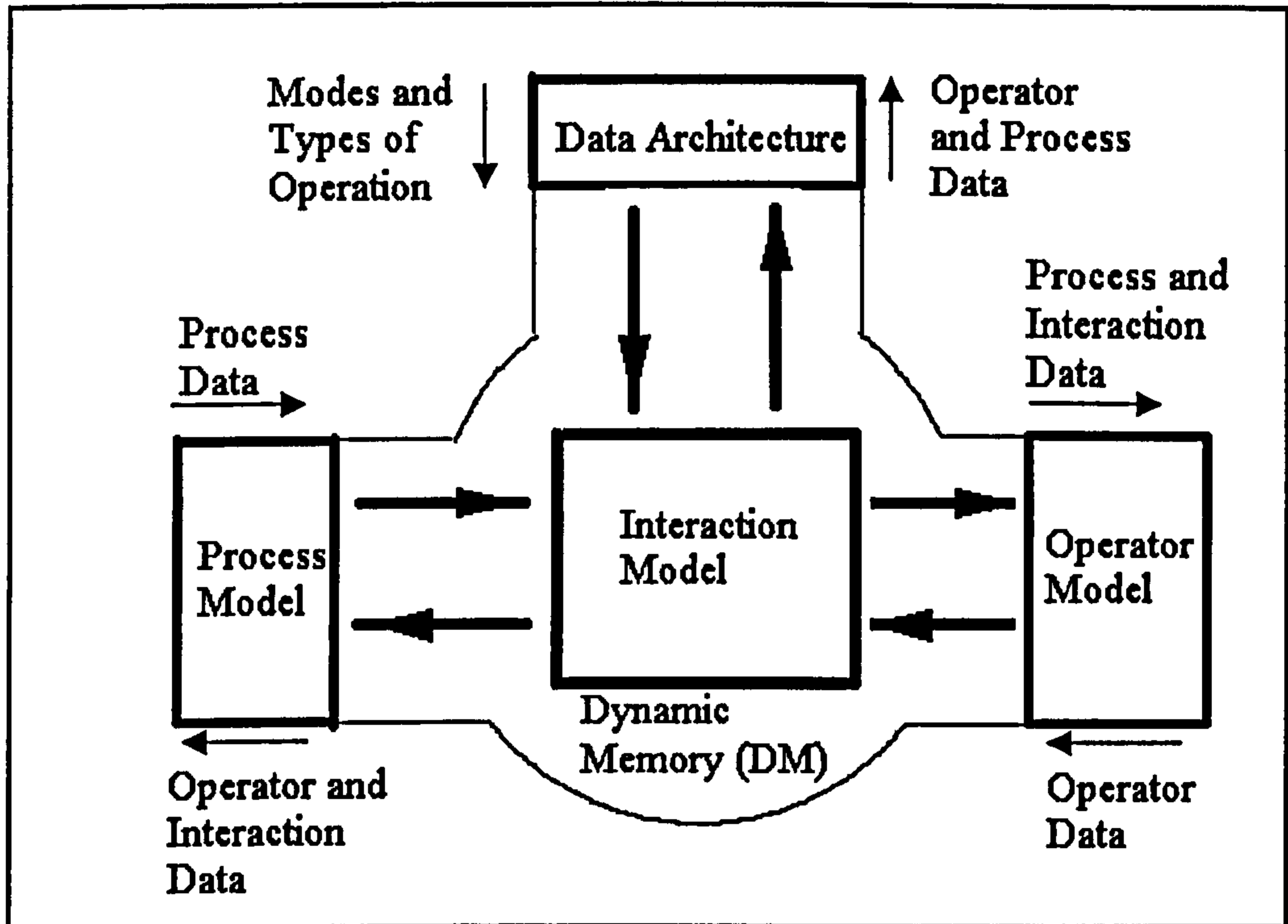


Fig. 3.1. Architecture of a process-operator interaction system.

Figure 3.2 shows a general architecture proposed by Cacciabue (1998). It was developed for all prospective analysis, which is mainly concerned with analytical description of the plant behaviour. A human model is linked directly to the machine model, i.e., a human action is executed directly by the machine model without any filtering from the interaction model. The information of the entire content of an incident without filtering is vital to safety analyses. There are no bi-directional links between the interaction and human models (i.e. Fig. 3.2 shows one way arrows therefore data flow in one direction only) because the human behaviour is determined by the human model and not by the interaction model. The joint system (Fig. 3.2) must be initialised at time zero ($t=0$) with an accident or event, i.e., either a human erroneous action or a system failure, or both. Then the process model produces responses to represent the plant behaviour and control mechanisms over a certain time period (Δt). These will combine the internal/external conditions to produce human error modes and new system failures. The operator model calculates the human behaviour and ends the loop of the interaction. A new configuration of the control setting, system failures and human action is defined and new time integration ($t=t+\Delta t$) can be calculated. The main drawback of this system is that limited to safety assessment application only and not for improving the

system design such as operation procedures, computer interface, and fault diagnosis, and for accident analysis. The system also needs to be initiated in every new safety analysis case with appropriate initial conditions. Further more the accuracy of dynamic and time dependent nature of the interaction is not known.

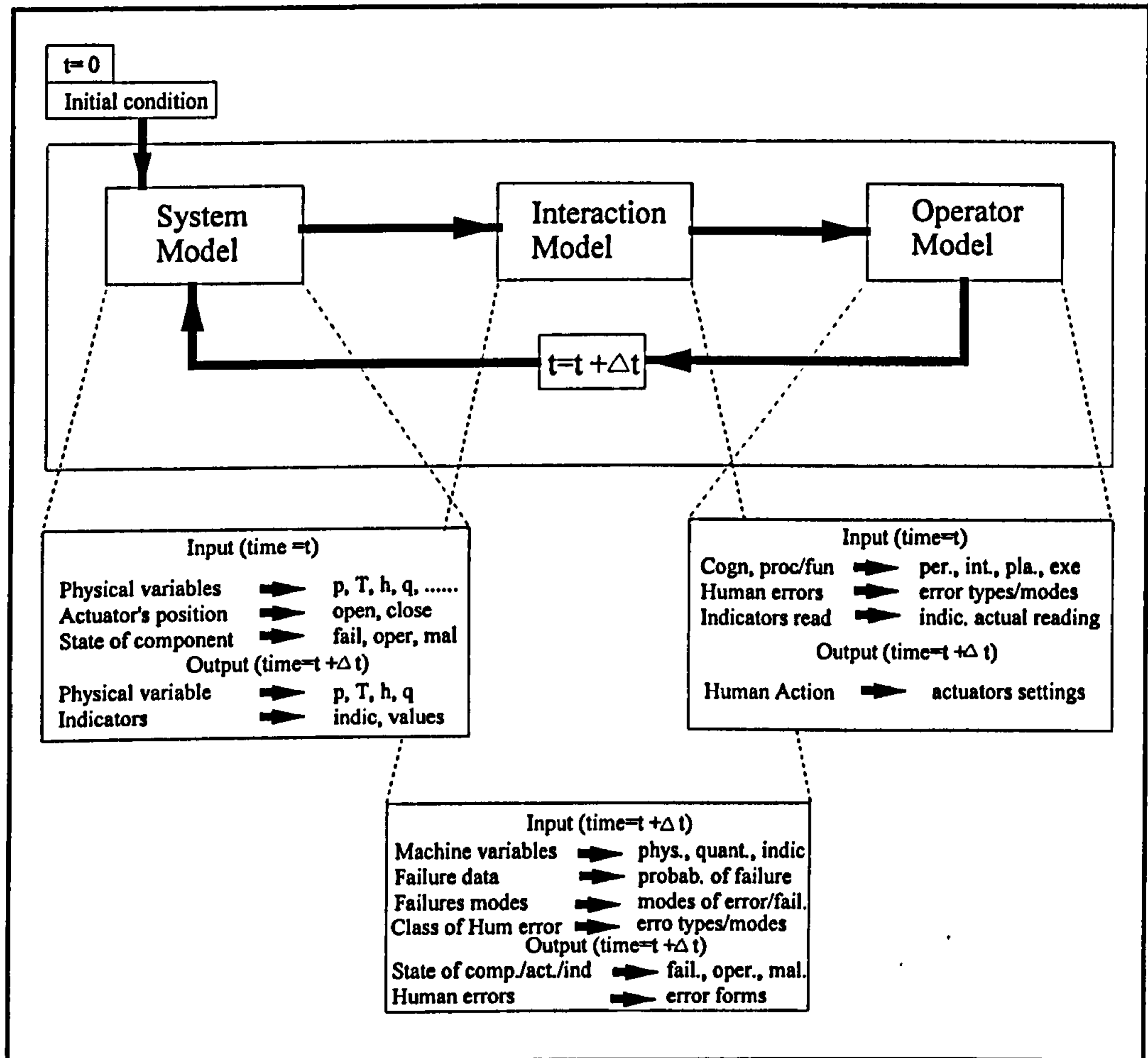


Fig. 3.2. Architecture of human-machine interaction simulation (Cacciabue, 1998).

Kazuo et al. (1999) developed a simulation system known as operator crew cognitive simulation (OCCS) (Fig. 3.3), where interactions exist between the operators and environment, and among the operators. The operator information is obtained from the environment and other operator, or agent, in addition to its own knowledge. The simulation system is used to see to what extent these interactions are relevant for operator crew performance, and whether the simulation of operator crew performance is useful in human-machine system design. Fig. 3.3 also shows the message transfer sub module, which controls

the flow of bi-directional messages exchanged between the interface simulation, plant simulation and operator simulation sub modules.

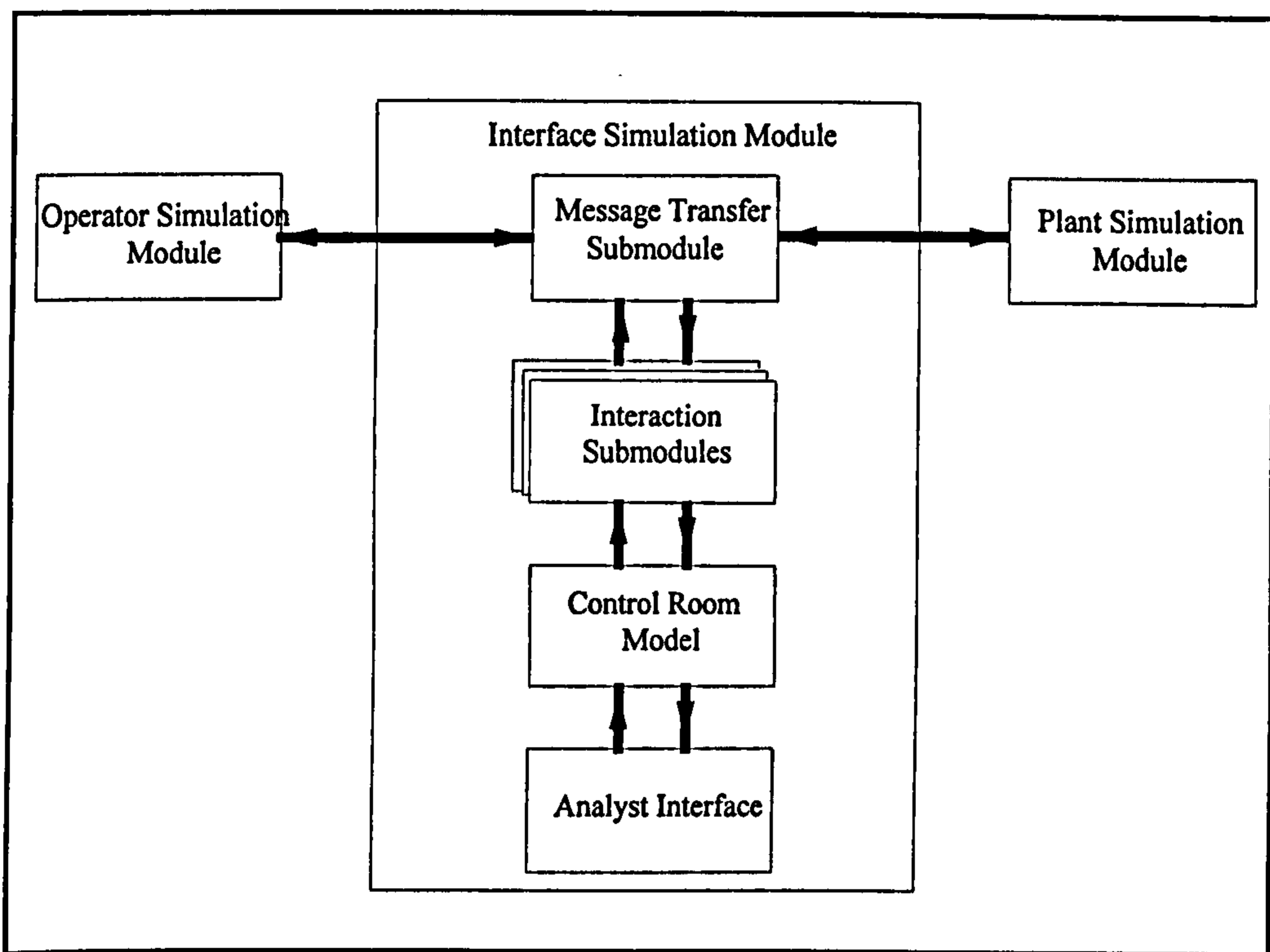


Fig. 3.3 Operator crew cognitive simulation architecture (OCCS) (Kazuo et al., 1999).

The OCCS system mainly deals with the factors affecting the human behaviour, such as the performance of a group of operators during the operation. Although this type of joint interaction system will be useful for theoretical study in improving the operator crew communication, designing control panels and designing a large control room where the operation depend on a number of operators, the result of any of these studies is not reliable because an accurate model for human cooperation behaviour cannot be developed since the mentality and the background of each operator are different. For example, the team cooperation is a function of stress level, operator confidence, operator training, etc. (Entin et al., 1999). The limitation of the system is mainly derived from its limited application to operator crew performance and design of human machine system cooperation. Therefore, the system is not capable to improve the operation procedures, the fault diagnosis, the decision support system and the safety analysis.

Nevertheless, a compromise between the Cacciabue (1998) system and that of Kazuo et al. (1999) could produce a more reliable system, which can be used for prospective analysis, such as the evaluation of data, parameter and probabilistic related to human actions and decisions, and retrospective analysis, such as events and fundamental reasons and facts that promote certain human behaviour during operation. To develop the process-operator system as illustrated in Fig. 3.1 for both retrospective and prospective analyses, the requirement and the specification of each element in the system must be set as follows:

- (1) Human behaviour model and simulation can be represented by the basic cognitive function such as perception, interpretation, planning and execution. These cognitive functions can be implemented using engineering methods of detection, diagnosis and action, such as the mathematical theory of communication (Shannon and Weaver, 1949), the theory of signal detection (Peterson et al., 1954) and linear control theory (McRuer and Krendel, 1957), and engineering methods of planning and decision making such as fuzzy set theory and mathematics (Zadeh, 1965), qualitative physics theory (De Kleer and Brown, 1984), artificial intelligence (Cohen and Feigenbaum, 1986), and expert systems (Alty and Guida, 1985). The human model also requires rule and knowledge base to describe procedure and to support the cognitive function.
- (2) Machine behaviour can be modelled using sets of analytical and differential equations translated to a computer programme as a dynamic simulator. The dynamic simulator should emulate the dynamic behaviour of the process under various operational modes and continuously send information of alarm status and variable values to the system. Example of human-machine systems includes the simulation of context and working environment in the machine model (Cacciabue, 1999) and the context and working environment in the interaction model (Kazuo et al., 1999).
- (3) Interaction model and simulation can be implemented using logic algorithms, analytical expression, statistical techniques and rule and knowledge bases, which can deal with the requirement of the system such as time management, reliability and systematic safety analysis, forming sequences and exchange of data and messages. The logical and numerical algorithms or analytical expressions manage the correlation of failure and error modes and types. The statistical methods or rule-based approaches are useful in probabilities and frequencies of occurrences and uncertainty bounds.
- (4) Data architecture elements can be implemented through data classification according to their physical, structural and mathematical features and by a specific body of data, such

as the database and knowledge base, which support the simulation of human, plant and environment.

3.3 Simulation, Analysis and Application Types of Joint Human-Machine Systems

Simulation of system behaviour can be broadly divided into two types, i.e., qualitative and quantitative simulations. Qualitative simulation explains qualitatively how process-operator interaction occurs by describing the structure, the links and the logical and dynamic evolution of cognitive process. Quantitative simulation is the computational part of the system simulation as well as the numerical estimation of the human behaviour. It is necessary that all quantitative simulation performed in parallel. There are a number of reasons using simulation study instead of real practice study, such as, the access to simulation is much easier and much faster; simulation can be controlled, i.e., can be stopped at any point and restarted from the same point; simulation covers wide range of situation in very short period; and simulation provides a structured way to the analysis of events. Two types of analysis can be considered in the process-operator interaction simulation. First, retrospective analysis is the assessment of events, such as incident and accident to identify the root causes that have triggered a certain human behaviour using qualitative model and simulation, i.e., analysis of past accident data and knowledge for root cause studies (evaluation of decision in accident analysis) using expert system. Second prospective analysis is prediction and evaluating the outcome of human action or malfunction, i.e., human and process behaviour evaluation studies, such as the operation reliability (Human Reliability and Process Reliability Assessment in Probabilistic Safety Assessment), and interface and procedures design. Prospective analysis is based on quantitative simulation and requires probability and expectation of human and machine behaviour, i.e., statistical mathematics. The applications of analysis and simulation of cognition are:

- (1) Design purpose aims at developing and evaluation of procedures and interface (Degani and Wiener, 1994; Nishitani et al., 2000; Beka Be Nguema, 2000) and improving communication and control design (Johannsen, 1997). Different procedures, interfaces, control and decision support systems can be designed, compared and tested using different initial and boundary conditions derived from the normal and abnormal plant conditions made by the operators. Design is a typical application of prospective analysis using quantitative numerical simulations since various operator behaviours are used to determine a number of designs.

- (2) The safety assessment purpose aims at evaluating the probabilities associated with certain accidents, their consequences and frequencies of occurrence, in relation to predefined selection of initiating events. These events are represented by a combination of structure of classes or levels of erroneous, reliability data and error/failure probabilities and reliability methods for human and hardware/software system (Hollnagel, 1993). A process model is required in this application to describe the machine response, which will be used in process reliability assessment; and the human actions, which will be used in human reliability analysis (Cacciabue, 1998; Yoshikawa and Wu, 1999), which is to predict human error rates; and to evaluate the degradation to human machine system likely to be caused by human errors in association with equipment function, operational procedures and practice which affect the system behaviour. Therefore, the safety assessment is a combination of human reliability analysis with process reliability assessment according to the rule of probability. The design basis for the accident analysis is also classified as the safety study of specific accidents. The designer sets the boundary and initial conditions, which represent a set of worse possible accident scenarios. The design of safety measure and protection devices of the system such as alarms, safety valves, position of fire extinguisher and instruction, etc., are based on the quantitative results of design basis accident analysis. The quantitative effect of the safety assessment can also employed in modifying the design of the process and the associate controller so that it deals with the considered events or disturbances (Dimitriadis et al., 1996).
- (3) Training human factors insight has nowadays become practice for highly specialised operators, such as the nuclear power plant operators, pilots and air traffic controllers. There are two types of human factor training: classroom and simulation training. Classroom human factor training covers an introduction of concepts in human behaviour, human-human and human-machine interactions in very specialised discussion and lectures, as part of the standard and recurrent training (Wiener et al., 1993). Simulation training is carried out during practical sessions on a full-scale simulator. Operators are trained in these sessions with the objective not only to develop their technical skill in controlling and supervising the machine during abnormal conditions, but also to manage and exploit human competence and potentialities at their best, especially when working as a team (Kazuo et al., 1999). The instructor in both human factor training must master the simulation of the human behaviour in order to describe, review and characterise different human performance. Therefore the model must be well constructed and descriptive in nature, as to offer a solid paradigm of

reference to the instructor. The most frequent application of such a model in training occurs when instructor has to explain punctual performances and patterns of behaviour.

- (4) Accident analysis and investigation are oriented to the identification of the root-cause of an accident. They are related to human errors and system failure and malfunctions, and to prevent the same types of accidents in future by taking preventative measures. Accident analysis aims at establishing the correlation between causes, effects, and consequences that may be recurrent within the system at all levels, and have contributed to the sequence of events. From the human analysis viewpoint a method for accident analysis require a models of cognitive process, which leads to classification schemes that categorise the observed behaviour. A framework representation of the dynamics of events and human-machine interactions is required where dependences, contextual occurrences and logical links are accounted for.

3.4 The Proposed Architecture of the Process and Operator Joint Simulation System

Figure 3.4 shows the overall architecture of the proposed process and operator joint simulation system. The system is developed for the following purposes: monitoring the process and operator's behaviour during operation particularly when the process is under the affect of disturbances, developing qualitative models representing both process and operator behaviour, and as a tool for extracting information and knowledge from data, which will be used for designing decision support systems, procedures, interfaces and safety measures.

The interaction model is one of the main elements in the joint simulation system. It is implemented using a number of quantitative and qualitative simulation functions linked to data architecture and the graphical user interface. The types of simulation functions used in the interaction system are fuzzy logic and fuzzy *c*-means clustering, combinational logic, mathematical statistics, and rule and knowledge based techniques. These simulation functions are supported by the physical, structural and mathematical data of the data architecture embedded in the interaction model. There are other functions performed by the interaction model, such as handling the graphical user interface and data exchange within the interaction model. The input data to the interaction model is the operator and process variables, parameters and the mode and types of errors and failures exist in the data architecture of the interaction model. Unlike other systems, errors and failure modes and types exist outside the interaction model or are initiated by the user (Cacciabue, 1998). There are two reasons to integrate the data architecture in the interaction model, firstly, it allows

the model to access the data much faster and secondly to reduce the complexity of the time management of the interaction model (i.e. reduction of time dependent of data structure). This is very beneficial since the interaction model has to deal with the data exchange between the process and operator models, which can be evolving continuously and independently. The outputs of the interaction model are the disturbances, operator's errors, and indicators and controller states. The interaction model receives and transmits data from and to the operator and process models as shown in Fig. 3.4.

A qualitative simulator is implemented by combining rules and facts used as operator model. The model can represent a number of operators; each has different responses and behaviour to the same event or process malfunction. The operator model input is the indicator reading, controller status or the mode and the type of operator, such as his/her stress level, operator response and operator output constant. The output of the operator model is the action to be carried out.

The process model imitates the dynamic behaviour of the process under various operational modes and continuously receives operator's action and transmits its status to the interaction model for carrying out the required analysis and assessment.

The process, operator and interaction models communicate with each other using dynamic data exchange (DDE). Fig. 3.5 shows a screen shot of the CSTR process model implemented using MS Visual C++, the operator model implemented by Visual Prolog and the interaction model implemented using the Matlab. A communication link is established in a way that the three models can send and receive a command and data from one model to another. The DDE is based on the dynamic data exchange management library (DDEML) of the MS Windows platform.

Each model can be a client or server, or both. The client's role is to initiate and control the communication, while that of the server is to respond to a request from clients by obtaining information and then format the information to be usable by the clients. For example, the interaction model acting as a client-program requests data and information from the server-program (operator and process models) and sends command to server-program to be executed. The operator model consists of both the client and server programs because it serves the interaction model and is served by the process model.

All the models shown in Fig. 3.5 are supported by a graphical user interface (GUI), which is used to override the process and operator joint simulation system, to stop and carry

out from the same point, and to display the behaviour of each model during the operation. This gives the process and operator joint simulation system a number of advantages, such as monitoring the behaviour of all models, initializing any event during the operation by direct access through the GUI, and stopping the simulation at any point to perform a visual inspection of a certain process or operator behaviour.

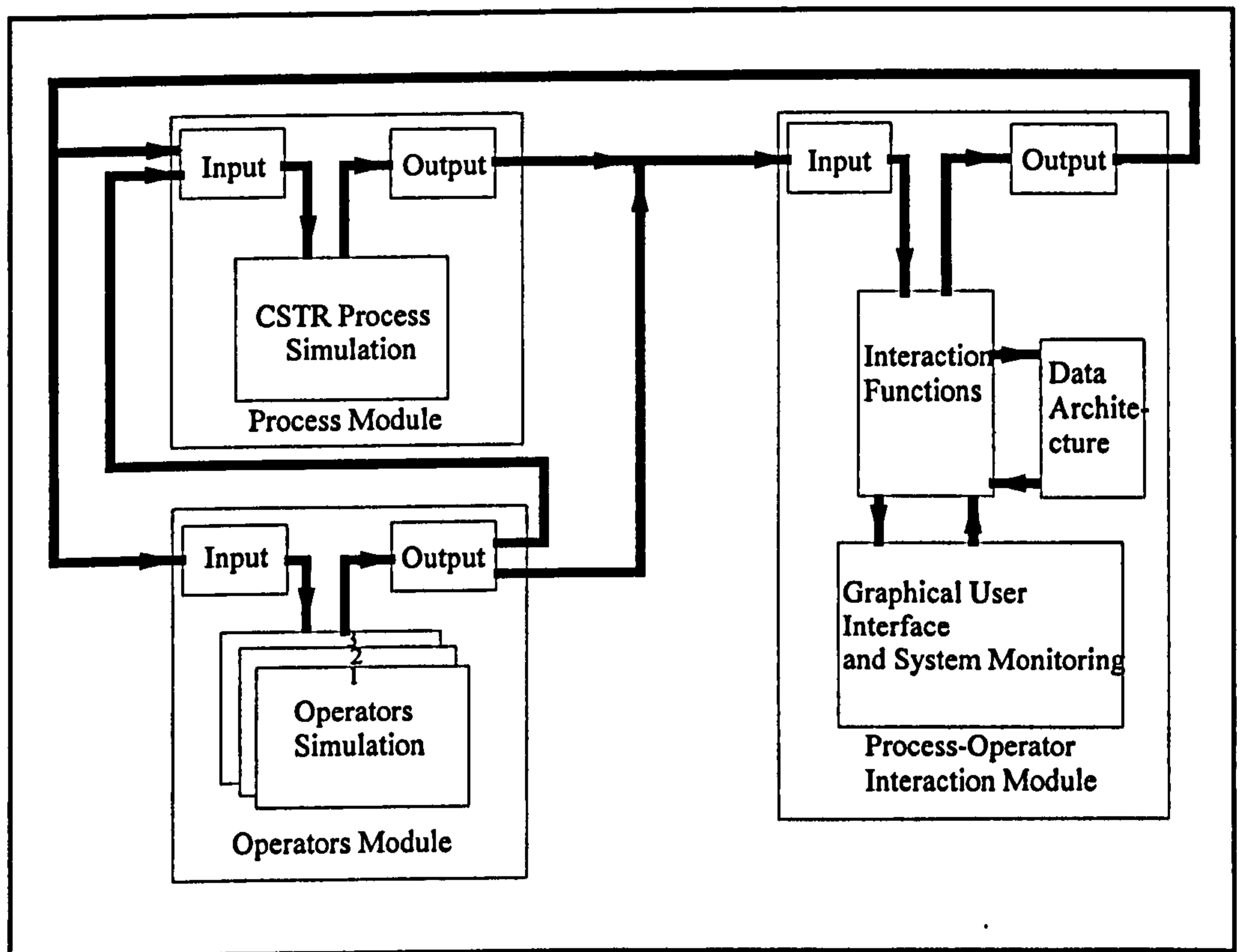


Fig. 3.4. Architecture of process-operators joint simulation system.

The proposed system can contribute in both the retrospective and prospective analyses. Prospective such as design decision support system, operator procedures for start up and shut down operations, computer interface and safety measure. Retrospective analysis is an investigation of past accident and human/process behaviours. The propose system can also perform operator and process data classifications during identification of the good and the bad operation and operators. For example, the joint system is capable to develop a qualitative representation of operator and process operations and classify these operations according to the status of the operation region such as abnormal, normal, emergency, good operator, bad operator etc.

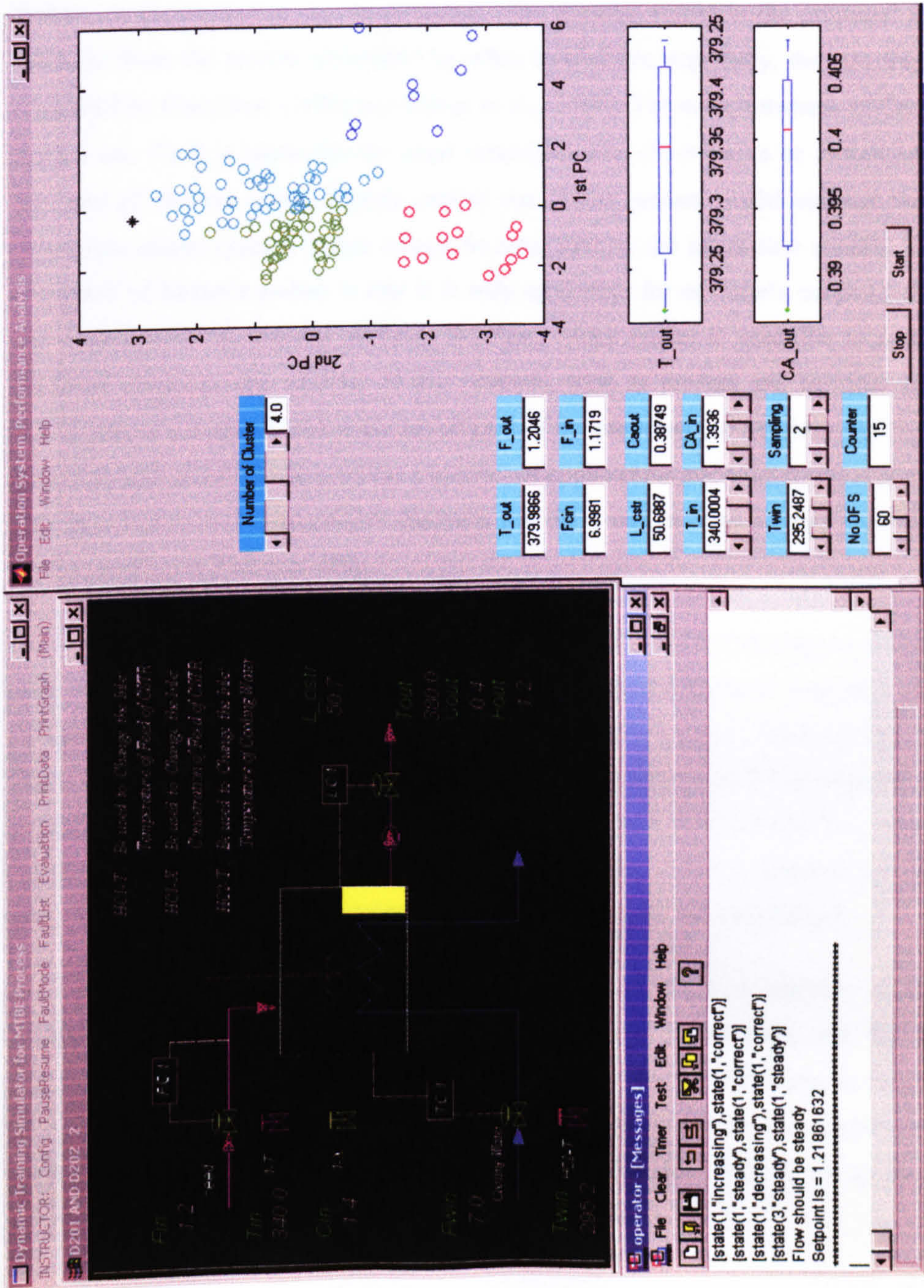


Fig 3.5 Screen shot of process, operator and interaction models during dynamic joint interaction simulation.

3.5 Summary

The general framework of the proposed joint process-operator interaction simulation system, as shown in Fig. 3.4, is presented. The operator model in the proposed system is different from the models developed by other researchers, especially, the two frameworks suggested by Cacciabue (1998) and Kazuo et al., (1999). The main drawback of Cacciabue's system are: (1) It is applicable for plant behaviour only, (2) It has to be initialised in each run, and (3) human action directly carried out by the process model and not through the interaction model (human action cannot be perceived by the interaction model). The main drawback of Kazuo's system is that it is only applicable for operator's cooperation studies and investigation of operator machine interface, which makes it incapable to perform the proposed functions and analysis of this research, such as process and operator behaviour monitoring and analysis. The main advantages of the proposed joint system are: (1) it has a powerful GUI, (2) it can be used for a number of applications and studies, (3) it can perform both prospective and retrospective analysis, and (4) it can be used to carry out analysis of both dynamic and historical data.

The advantages of employing the simulation study over the real practice study and the type of analysis, simulation and application of joint process-operator simulation system is emphasised. In the present development, the proposed framework is shown in Fig. 3.4. The interpretation and the planning of the human model is composed of one element, and the human stress model is developed using fuzzy logic and is located outside the human model and calculated dynamically during the operation. Moreover, the elements and the data exchange methods of the joint process-operator simulation system are detailed.

The process-operator interaction simulation can have a number of different architectures or frameworks depending on the analysis requirement and the type of application. In reality, there are no limitations in any of these architectures as long as they can perform the required functions. However, with minor and simple modification, the human-machine joint operation system can perform other classes of analyses and assessments so that it can cover a wide range of applications.

Chapter 4

Operator Behaviour Modelling and Simulation

This chapter describes the system of operator behaviour modelling and simulation, including the functions, elements, models and implementation issues.

4.1 Introduction

Mathematical modelling of human behaviour is not a completely new subject. Sheridan (1985) described a number of examples of human models going back to the 1950s, and the field has been growing ever since. It is well worth pointing out, however, that the general acceptance of operator modelling was declined in the 1960s and 1970s, and the concept of an operator model was very different from the present time. The present view of the human model was formed in 1980's with the development of cognitive science and artificial intelligent (AI) and of human-computer interactions (HCI). The issue of human model in machine control has been dealt with in several books by Rasmussen (1986), Hoc et al. (1995) and Cacciabue (1999), and in numerous papers and conference proceedings, such as Wan and Young (1996), Johannsen (1997), Yoshikawa et al. (1997), Kazuo et al. (1999) and Hirokazu et al. (2000). Improvements in human modelling often aim to increase automation, hence change the balance between the roles of operators and machines. The research on human modelling has also been aimed at improving operational safety although there are still limitations to what can be modelled, the success in improving automation and safety cannot be ignored. Chemical engineers interest in process safety has focused on the plant and its monitoring and control systems, mainly because they regard human behaviour as a management and cultural issue.

This chapter will describe the system developed in this study, which is a constituent component of the operator-process interaction system. In the following discussion, we will deliberately use the word operator instead of human to refer more specifically the personnel, who is directly responsible for monitoring and controlling the process. The purpose is not to develop a new theoretical model for operator's behaviour

modelling. Instead, it is aimed at developing a system that can be used to carry out the studies outlined at the beginning of the thesis. In the next section, theoretical models on operator modelling and system architectures, most of them developed in domains other than chemical industries will be reviewed, and the method used in this study will be described. In section 4.3 the implementation of the model will be discussed. In section 4.4 simulation runs will be presented to demonstrate the joint operator-process interaction system under the proposed operator model and operator's stress models. In section 4.5 an industrial case study of operator's performance analysis will be presented and discussed. Finally a summary of the chapter will be in section 4.6.

4.2 Theoretical Models on Operator's Behaviour and System Architecture

4.2.1 The Human Model of Yoshikawa

Yoshikawa et al. (1997) developed a human model using Petri-net (Fig. 4.1) to analyse and evaluate the effectiveness of man-machine system design through computer simulation from various viewpoints of human factors. There are six elements in the model, three cognitive functions and three cognitive processes. The first function is perception. After getting data from the man-machine interface, the perception function interprets and filters the data and then transmits the information to peripheral working memory (PWM). The second cognitive function is the focal working memory (FWM). This function fetches information from PWM and stores and indexes them in FWM conscious world according to their priority, modes and types. The final cognitive function is the knowledge base retrieval. It retrieves the information from the KB using keywords exactly agree with the higher priority information in the FWM conscious world index. The cognitive processes PWM unconscious world and FWM conscious world are simply temporary memories and the difference between these two is PWM hold unorganized information and FWM hold organized and indexed information. The KB database process is a long-term memory, which holds the information, representing the human behaviour modelled via Petri-net. However, this system has a number of limitations. The model is totally dependent on the KB database represented by Petri-net, which is not sufficient and does not describe all the operations because of the limited knowledge of the users and operators to enable them to learn or dynamically improve its performances. The model also cannot predict new events and does not give clear and detailed description about how the results were obtained.

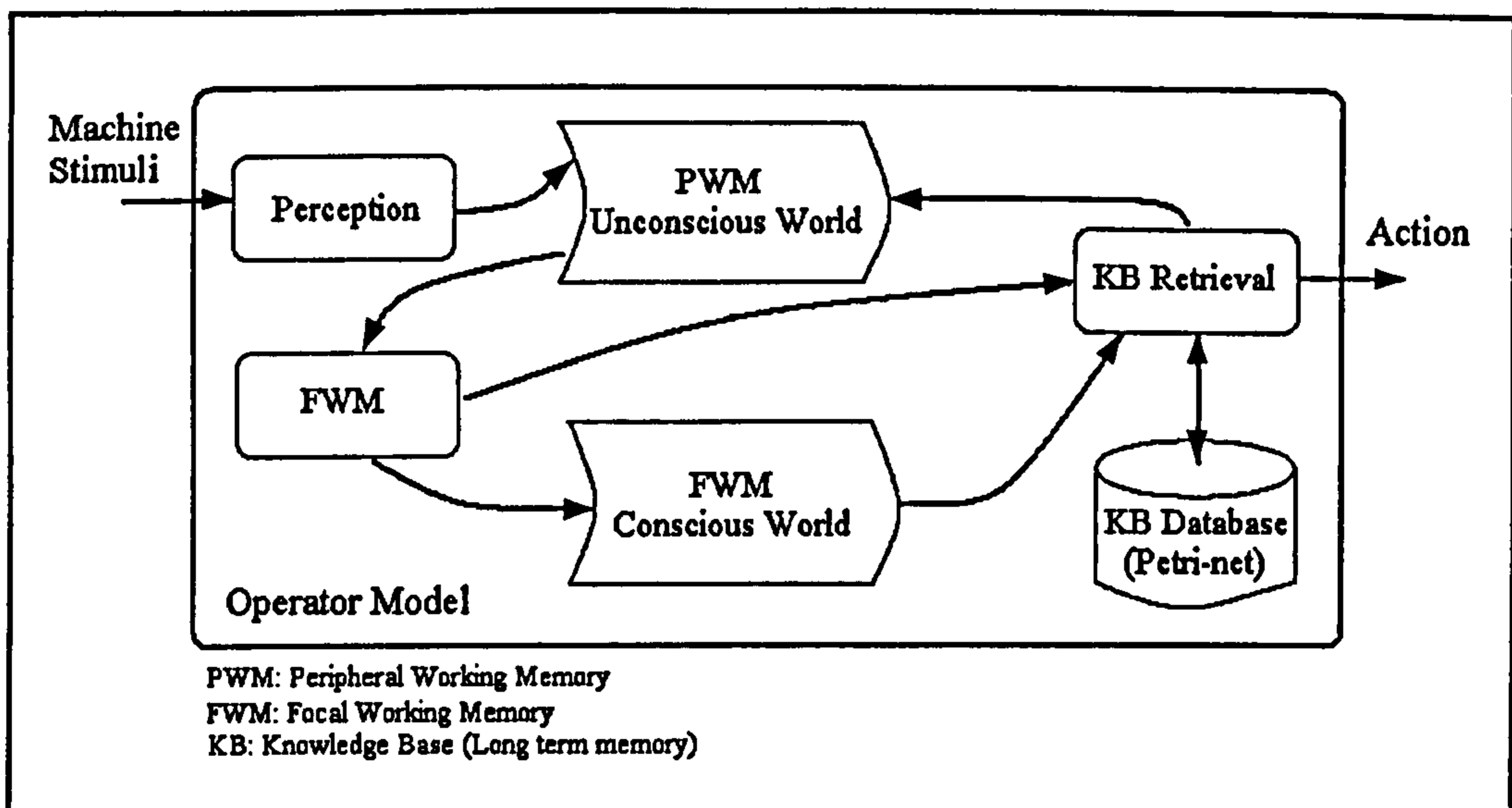


Fig. 4.1. Human model structure in simulation architecture (Yoshikawa et al., 1997).

4.2.2 The Human Simulator of Nishitani et al.

Nishitani et al. (2000) developed a human simulator, (Fig. 4.2) for the design and evaluation of the computational models of the human information processing of plant operators and psychological approaches to measure the mental state of human operators. This operator model composes of three processors and two memories. The perceptual processor simulates the operator's awareness of the operational panel information, i.e., whether operator notices panel information. The cognitive processor simulates the operator's recognition of the current plant state. When the alarm sounds, the cognitive processor using the information provided by the knowledge base long-term memory would develop an urgent procedure. This procedure will be stored in the short-term memory as temporal sequential control program, which can deal with the occurred alarm. The motor processor actuates the intended action given by the program created by the cognitive processor. The cognitive processor has two modes, a state monitoring mode and emergency mode. At monitoring mode, the operator model uses a number of rules stored in the knowledge base long-term memory to deal with the normal operation. Once an abnormal state is recognised, the cognitive processor switches to the emergency mode where an urgent procedure is generated instantaneously. This operator model is much better than the previous one because it has the ability to create its own plan from the knowledge provided by the long-term memory, while the previous model is not capable to do so. However, this model is not capable of updating its own knowledge and information dynamically. Therefore, the planning capability depends heavily on the

amount and the type of knowledge and information of long-term memory. This limitation shows very clearly in Fig. 4.2. The one-way arrow links between long-term memory and the cognitive processor, indicating that the data flows only from the long-term memory to the cognitive processor.

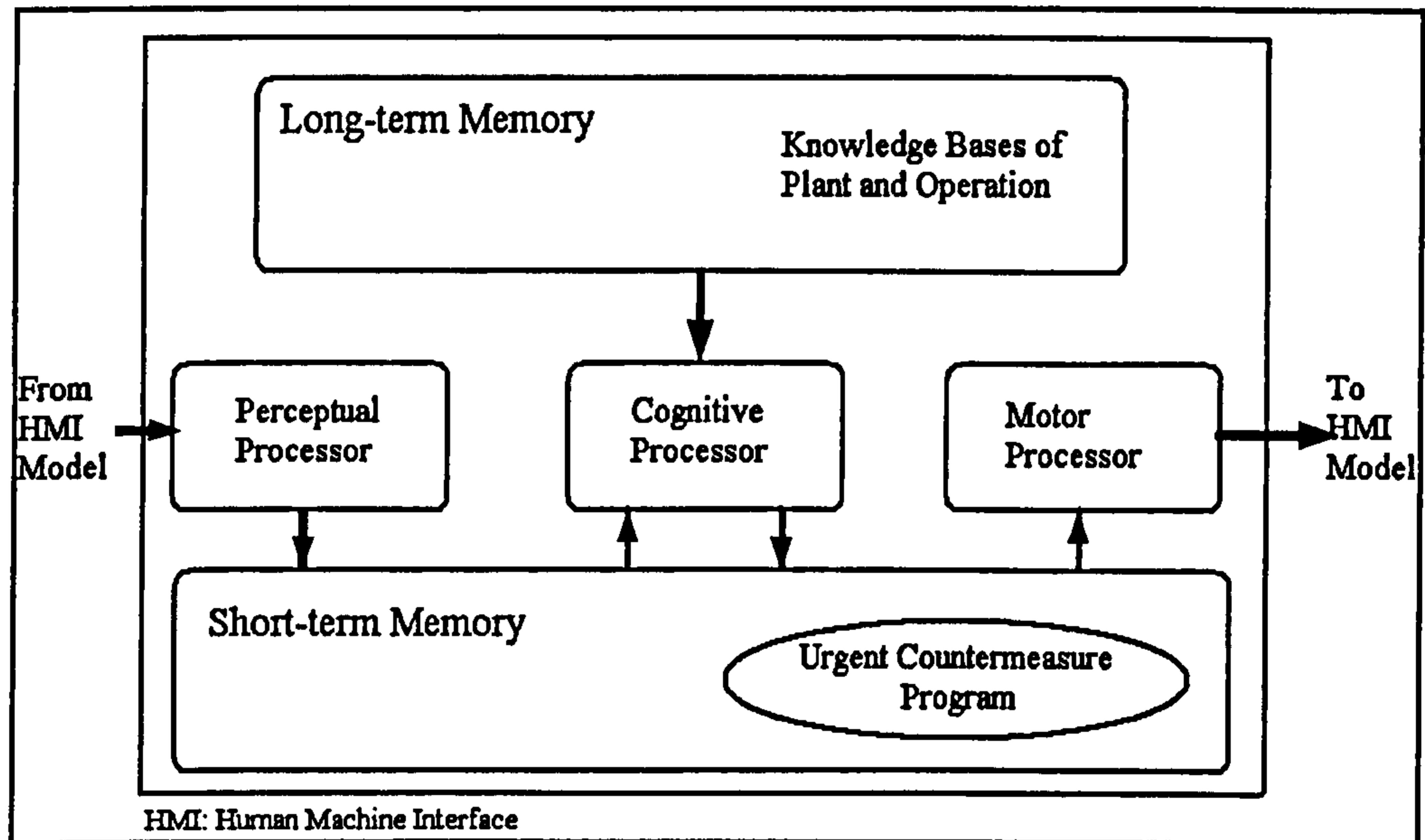


Fig. 4.2. Human model structure in simulation architecture (Nishitani et al., 2000).

4.2.3 The Model of Cacciabue

The above work shows that the first activity of human model is perception. However, they mainly focused on system implementation, fall short in giving a comprehensive and theoretical analysis of operators' activities. The most comprehensive theoretical treatment of operator's model was given by Cacciabue (1999) and therefore is adapted in this study. Cacciabue (1999) has reviewed various activity models and classified operator's cognitive functions into four, i.e., perception, interpretation, planning and execution PIPE (Fig. 4.3). *Perception* implies that some, or all of the information produced by the models of the process is actually perceived by the human sensors. The second cognitive function of *interpretation* or recognition is related to the elaboration of perceived information, such as identification of cues, pattern recognition, trend analysis, and fault detection. *Planning* implies development of a plan for control or manual action carried out as a result of the previous steps of cognitive processes. Finally, the fourth

cognitive function of *execution* entails the implementation of the decision, which may take the form of manual responses or control actions, but may also be the beginning of a new cognitive process.

The above four activities rely on another two resources, i.e., cognitive process memory/knowledge base (KB) and allocation of resources (AoR). The memory/knowledge base cognitive process embodies previous experience, qualitative and quantitative knowledge and rules, which support the four cognitive functions. The allocation of resources describes how the resources available to the human are distributed throughout the model and how they affect the cognitive functions.

A conceptual framework depicting the relationships is given in Fig. 4.3, the connection between the PIPEs shown in Fig. 4.3 represents the human model mechanisms, which generates human behaviour such as human actions and procedures. These actions and procedures developed by the human model are considered as the human model response to a number of events initiated by the interaction model. Cognitive functions and processes of the interaction model create these events with the knowledge base support.

The simulation of cognitive functions can be implemented using computational means such as fuzzy functions, logic, qualitative rules, and analytical expressions. The connection amongst the cognitive functions of perception, interpretation, planning and execution is established to maintain the cyclical nature of cognition, by which information is perceived from external stimuli, combined with reasoning over past events, and with anticipation about planning future response to produce further perception, reasoning, and planning. This process is simulated by the repetition of looping the four PIPE cognitive functions until the execution of an action is generated.

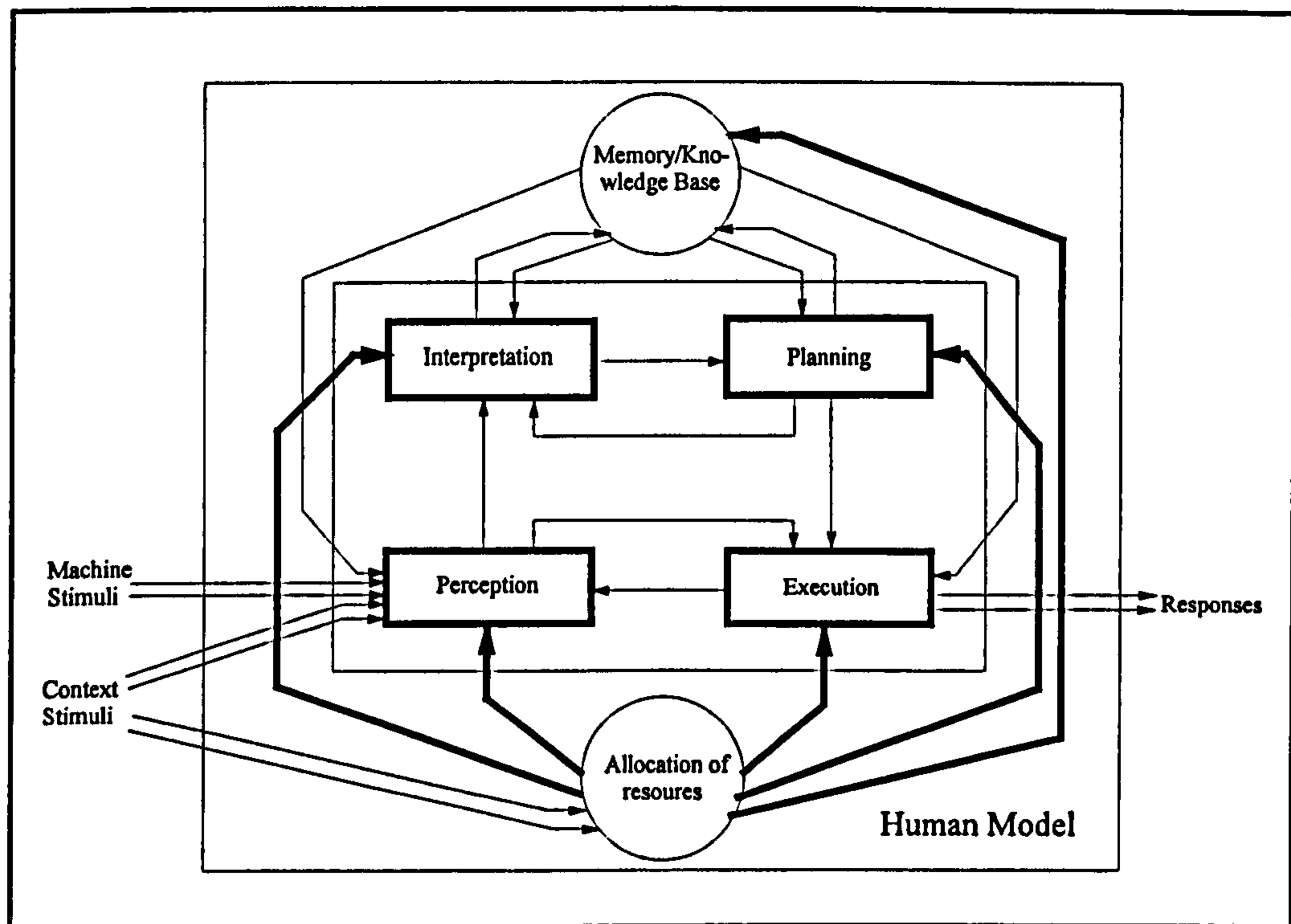


Fig. 4.3. Structure of human model (Cacciabue 1999).

4.3 The Operator's Model Proposed in This Study

Figure 4.4 shows system's architecture. The system for operator's behaviour is developed based on the theoretical framework of operator's activities, i.e., perception, interpretation, planning and execution, with the exception that perception and interpretation is implemented in a single module. The core part of the system is implemented as a real-time expert system emulating operator's activities of perception of information, interpretation of received signals, planning of activities and their execution. The main consideration of using an expert system is that the rules can be easily revised to reflect various cognitive scenarios, e.g., operator behaviour. Numerical models are integrated into the expert system only when it is necessary, e.g., the stress model of operators.

The rules have been compiled specifically for a case study of a continuous stirred tank reactor (CSTR), though some rules apply in principle to any systems, e.g., those regarding operation of PID controllers. The system is implemented using visual Prolog, which was originally designed to be an artificial intelligent language and is very well suited for developing expert systems. Frame and rules, forward and backward chaining,

pattern-matching, and constraint-resolution are all natural and elegant expressions of Prolog's underlying semantics. Instead of a series of steps specifying how the computer must work to solve a problem, a Prolog statement consists of a description of the problem. Conceptually, this description is made up of two components. The first component is the description of the objects involved in the problem. The second component is the facts and rules describing the relations between these objects. The rules in Prolog's program specify relations between the given input data and the output, which should be generated from the input.

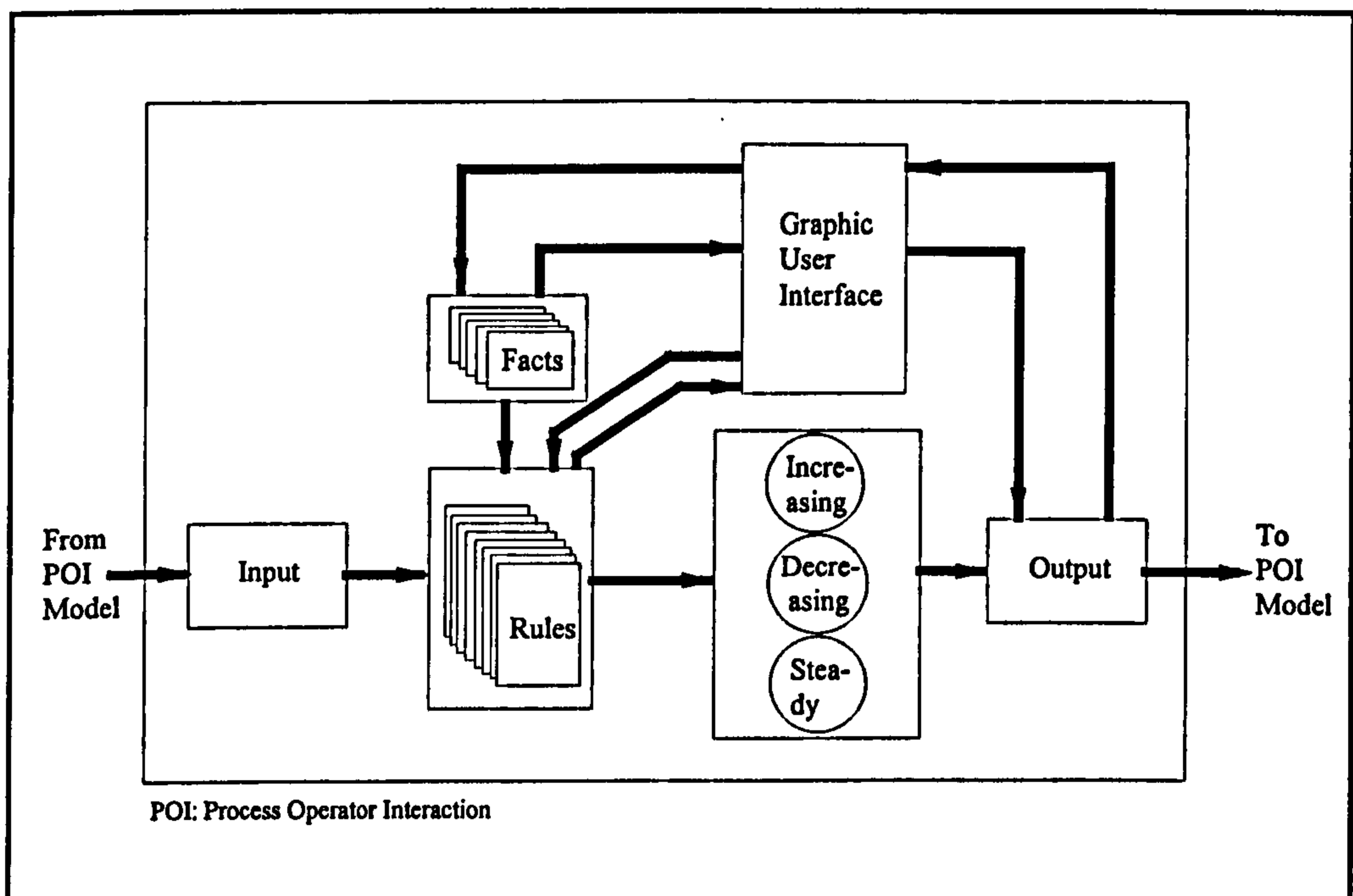


Fig. 4.4. The proposed human model structure.

Here are some important considerations in implementing the system:

- (1) The problem boundaries and aim of simulation must be clearly defined. The first step is crucial and may be the most important one as it can affect the whole model. The main goal or objective of the operator model is to monitor CSTR process continuously and to intervene in the process when it is perceived to be necessary. The operator model is allowed to change the set point of the controllers (in this case the reactant inlet feed flow controller F_{in} has been chosen). The operator model should also keep the product outlet temperature constant during the process operation, and has the capability of representing a number of operators during the dynamic simulation. Finally, the knowledge of controlling the F_{in} controller can

also be used to control other controllers, such as fresh water inlet feed flow controller in auto or manual modes.

- (2) Qualitative technique has been selected for developing the operator model and the cognitive tasks are described by a number of facts and rules. Visual Prolog (Version 5) is used for the implementation, which is Window-based and capable of interacting with any other Windows applications dynamically.
- (3) The operator model is represented by a number of facts, rules and the correlation between them. Facts, such as the normal state and conditions of the CSTR process, in terms of normal temperature, flow and concentration of the product, set points of all controllers, and a number of empirically determined coefficients. Rules are created from a number of conditions to present the operator mentality process during cognition. For example, if the temperature is low but increasing, the operator might increase the temperature because it is still low; decrease the temperature because it is increasing very fast and the offset from the set point reducing; or not intervene because the offset from the set point is very small and it is increasing slowly. Therefore, the rules created depend on the value of current temperature differing from the set point and the value of the rate of change of temperature. The statements, which all rules are based on are, for example,
- Low temperature and increasing.
 - Low temperature and decreasing.
 - Low temperature and steady.
 - High temperature and increasing.
 - High temperature and decreasing.
 - High temperature and steady.
 - Correct temperature and steady.
 - Correct temperature and increasing.
 - Correct temperature and decreasing.

For each statement above, the operator model takes only one of the three actions, to increase, decrease or not intervene in the reactant inlet flow controller set point. An example of the rules in Prolog format is shown in Fig. 4.5. The statement in Fig. 4.5(a) means that if the temperature is not very low and increasing slowly, do not intervene in the process.

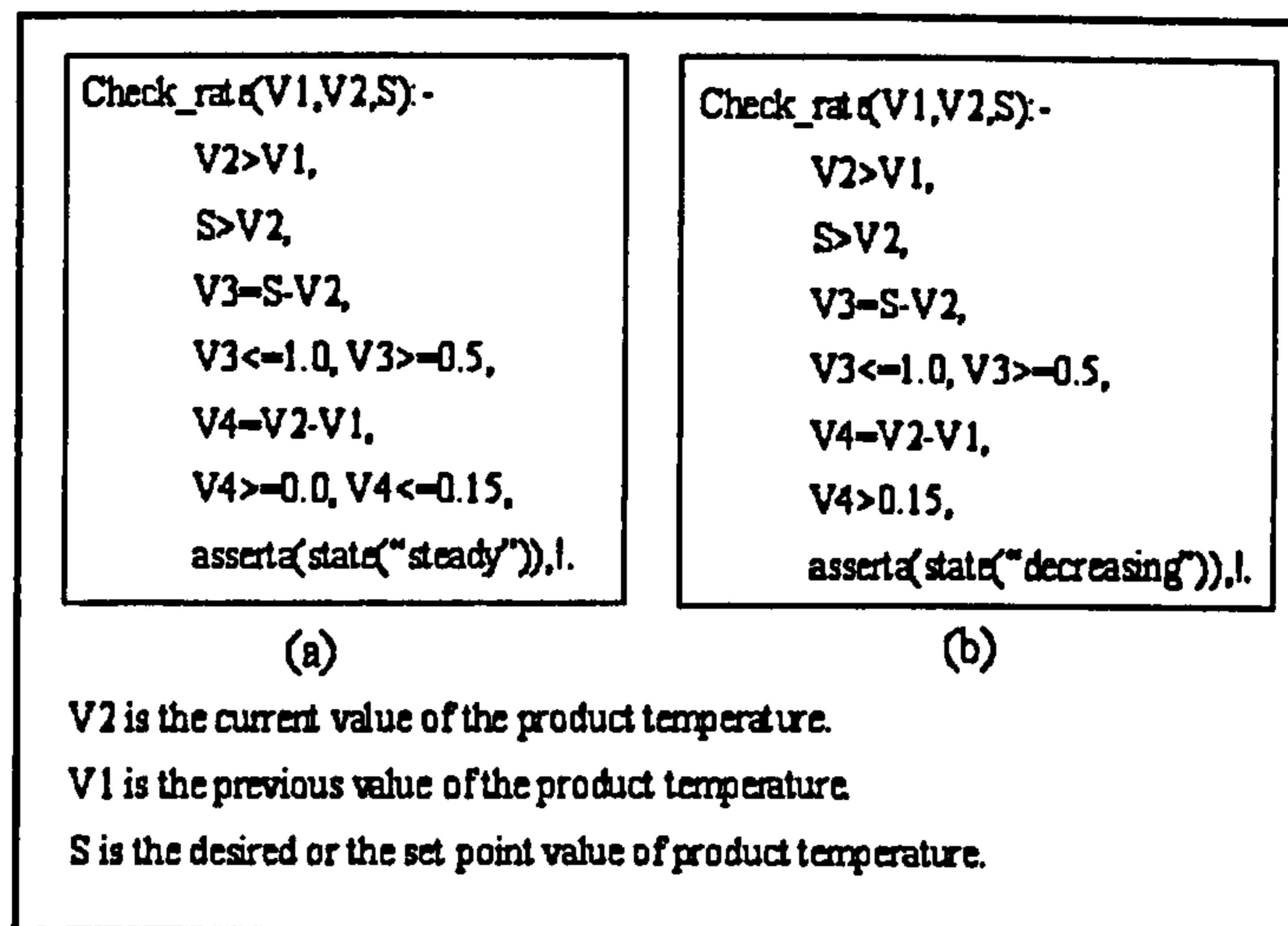


Fig. 4.5. Samples of operator model rules in Prolog format.

The result of the statement is stored in the internal database using Prolog command `asserta`. Obviously the operator model in this case observes the process and decides not to take any action, but in Fig. 4.5(b), the operator decides to decrease the temperature because the temperature is not very low and increasing rapidly. In this case, the operator model must convert its action from qualitative to quantitative values and then transmit the value to the process model. This is simply done by the following steps:

- (a) Error (E) = current temperature value (V) – temperature desired value (S).
- (b) Set gain coefficient multiplier (K), based in the error value E.
- (c) Present gain (K2) = gain constant (K1) * K.
- (d) Controller set point = K2 * E + previous controller set point (U).

Note that K and K1 are determined empirically and different value of K1 can be used with the sampling time to represent a number of operators behaviour.

- (4) The initial operator simulator must be tested continuously to tune all the coefficients, so that all types of process disturbances can be dealt with and the process operation can be brought to steady state condition with minimal time and maximum accuracy. The next step is to improve the simulator to fulfill the objective of the first step. Fig. 4.6 shows the screen shot of the operator model simulator during the process and operator joint interaction simulation. The figure also shows a dialog box for the integral gain constant K1 and a message box showing the some rules, the decision and the final output.

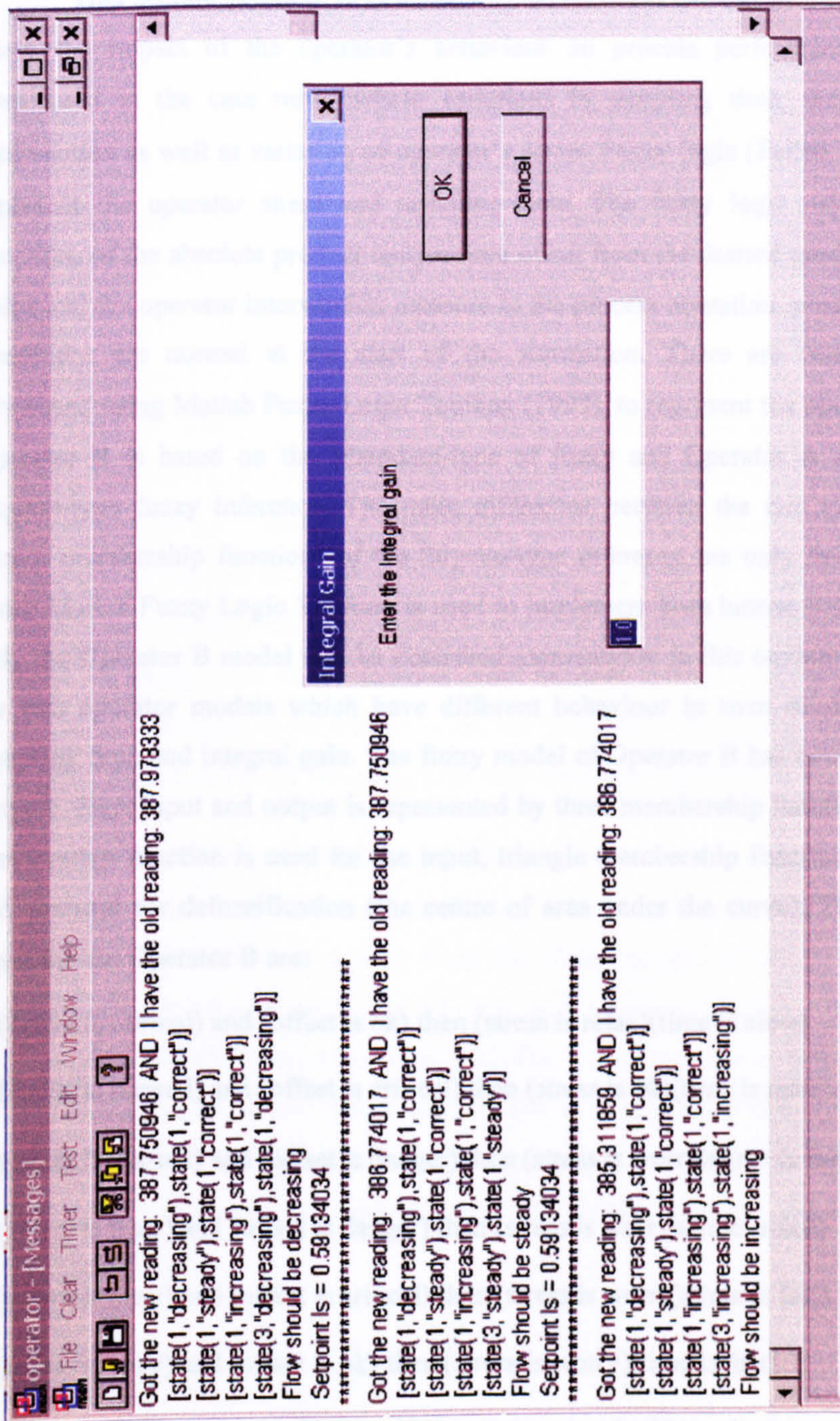


Fig 4.6 Operator model simulator during process and operator interaction in joint simulation .

4.4 Behaviours of Operators During Joint Process-Operator Simulation

This section presents case studies to demonstrate the use of the system, and to study the impact of the operator's behaviour on process performance. The factors considered in the case runs include variations in sampling time, ways of operators intervention as well as variation of operator's stress. Fuzzy logic (Zadeh 1965) is used to represent the operator stress and sampling time. The fuzzy logic model outputs are functions of the absolute product temperature offset from the desired product temperature value and the operator intervention measure in the process operation, providing the initial conditions are normal at the start of the simulation. There are two fuzzy models developed using Matlab Fuzzy Logic Toolbox (1998), to represent the operators A and B. Operator B is based on the Mamdani-type of fuzzy and Operator A is based on the Sugeno-type fuzzy inference. The main difference between the two types is that the output membership functions of the Sugeno-type inference are only linear or constant. Since Matlab Fuzzy Logic Toolbox is used to implement both human behaviour models, only the Operator B model will be described momentarily in this section. However there are two operator models which have different behaviour in term of stress, intervene, sampling time and integral gain. The fuzzy model of Operator B has two inputs and two outputs. Each input and output is represented by three membership functions. Trapezium membership function is used for the input, triangle membership function for the output and centroid for defuzzification (the centre of area under the curve). The rules, which represent the Operator B are:

If (active is normal) and (offset is ok) then (stress is relax)(time is slow)

If (active is normal) and (offset is critical) then (stress is ok)(time is medium)

If (active is normal) and (offset is danger) then (stress is worry)(time is fast)

If (active is busy) and (offset is danger) then (stress is worry)(time is fast)

If (active is busy) and (offset is critical) then (stress is worry)(time is fast)

If (active is busy) and (offset is ok) then (stress is worry)(time is fast)

If (active is cautious) and (offset is ok) then (stress is relax)(time is slow)

If (active is cautious) and (offset is ok) then (stress is ok)(time is medium)

If (active is cautious) and (offset is danger) then (stress is worry)(time is fast)

The first input of If statement (active) is represented by cautious, busy and normal membership function. The input parameter is a measure of the operator intervention in the process operation. Initially this measure is set to zero and every time the operator intervenes in the process operation, the measurement will be increased by one. If the operator does not intervene in the process operation but only observes, intervene measurement will be decreased by one. The maximum measurement of the operator intervene is 10 and the minimum is -10. A value of 10 means that the operator is very active due to abnormal process operation and the value -10 means that the operator does not intervene in the process operation for a long period of time. If statement second input (offset) is represented by ok, critical or dangerous membership function. The input parameter is the absolute value of the difference between the desired and the actual value of the product output temperature. The fuzzy model outputs are the stress and the sampling time of the operator. Stress is represented by relaxes, ok or worry membership functions and timing is represented by slow, medium or fast membership function. The Maximum and the minimum value of stress is 0.1 and -0.1. A value of 0.1 means the operator under considerable load and a value of -0.1 means the operator is relaxed. The operator sampling time varies from 2 to 7 seconds. Operator observes the process operation or intervenes in the process operation more frequently during abnormal process operation. Therefore his/her sampling time must be shorter, down to 2 or 3 seconds.

As soon as the interaction model detects the operator's low stress measurement, it will initiate disturbance and start monitoring and recording the operator's activities. When the process starts to recover from the disturbance's influence after operator's intervention, the operator will start to relax and whose stress measurement starts to decrease and eventually becomes very low. The interaction model will detect the low stress measure and initiates a new disturbance to monitor and record the subsequent operator activities and behaviour. New knowledge, rules and information will be extracted from these records and used to identify the operators' features for future operations and design.

4.4.1 Behaviour of Operator B

Figure 4.7 shows the projection of the CSTR operation in the reduced low dimensional space (the low dimensional 1st PC and 2nd PC space is obtained using principal component analysis). The red, blue and green colours represent three operational zones. The black asterisk point shows the trajectory of the operational point

when the process is under the influence of disturbances. In this case, three disturbances are the reactant feed temperature, the reactant concentration and the cooling water feed temperature. Fig. 4.7 shows 250 samples of the operational path of Operator B during an abnormal operation caused by three disturbance events. Fig. 4.8 is the decomposed operational path of Fig. 4.7, showing the starting and the ending position of the operational path for the first disturbance event in 4.8a, the second disturbance event in 4.8b, and the final disturbance event in 4.8c. Both figures indicate that Operator B is able to maintain the operation within the normal operation and avoid other operational zones. Referring to Figures 4.9 to 4.11, the behaviour of Operator B to each disturbance can be summarised in the following three steps:

- (1) The absolute offset of the reactor temperature from the set point (Fig. 4.9b) is suddenly increased by 2°K due to an external disturbance event at the sample point 9. Operator B detects the change and develops a sudden stress measure, (Fig. 4.10a) of 0.1 (maximum stress). Operator B then decides to intervene (Fig. 4.9a) in the process operation every 3 seconds, (Fig. 4.10b) at sampling point 13 and stops intervention at the sample point 57, while his/her stress is still at a high level. When the temperature offset drops dramatically, the operator stress decreases and his/her intervention time becomes 4 seconds instead of 3. This occurs only once at sampling point 31. After sample point 57, the operator's stress starts to decrease and the intervention in the process stops completely. The operator at this point considers that the process is recovering and is under his/her control, so it needs only to observe the process every 7 seconds without any intervention in the process operation. Figs. 4.11a & 4.11b show the reactor temperature shoots up to 390K while the operator decreases the reactant feed flow set point to bring the product temperature back to 380K. The operator starts to increase the reactant feed flow set point at the sample point 31 before the product temperature reaches 380K because he/she realises that the temperature decreases so fast and it will drop below the set point value.
- (2) At the sample point 85, the temperature offset suddenly jumps up by 3.6°K , (Fig. 4.9b), and the operator stress instantly reaches to maximum, (Fig. 4.10a) from a low stress state indicating that the operator is at a state of great stress. And at once, the operator starts to intervene in the process operation every 3 seconds. The operator stops to intervene in the process at the sample point 106 and starts again after 7 seconds, then stops completely at the sample point 116, where the offset temperature becomes very low. The operator continues to observe the process at every 6 seconds

with no more intervention in the process operation until the sample point 189. From sample point 83 to 163 (Figs. 4.11a and 4.11b), show how the operator manages to control the product temperature without any overshoot, just by reducing the set point at an earlier time than the first process operation recovery.

- (3) At the sample point 164, the temperature offset increases only by 0.6 °K (Fig. 4.9b). The operator detects the temperature changes after 2 sample points and does not react instantly as in the previous event. This is due to the long duration of the operator relaxation time, which is indicated by the duration of the negative stress measure before the sample point 166 (Fig. 4.10a). The operator starts to intervene in the process at that point with a sampling time of 6 seconds and then gradually reduces his/her intervention time to 3 seconds. At the sampling point 178 the operator stress drops to -0.05 , which makes the operator to change his/her attitude from intervention to observation every 6 seconds.

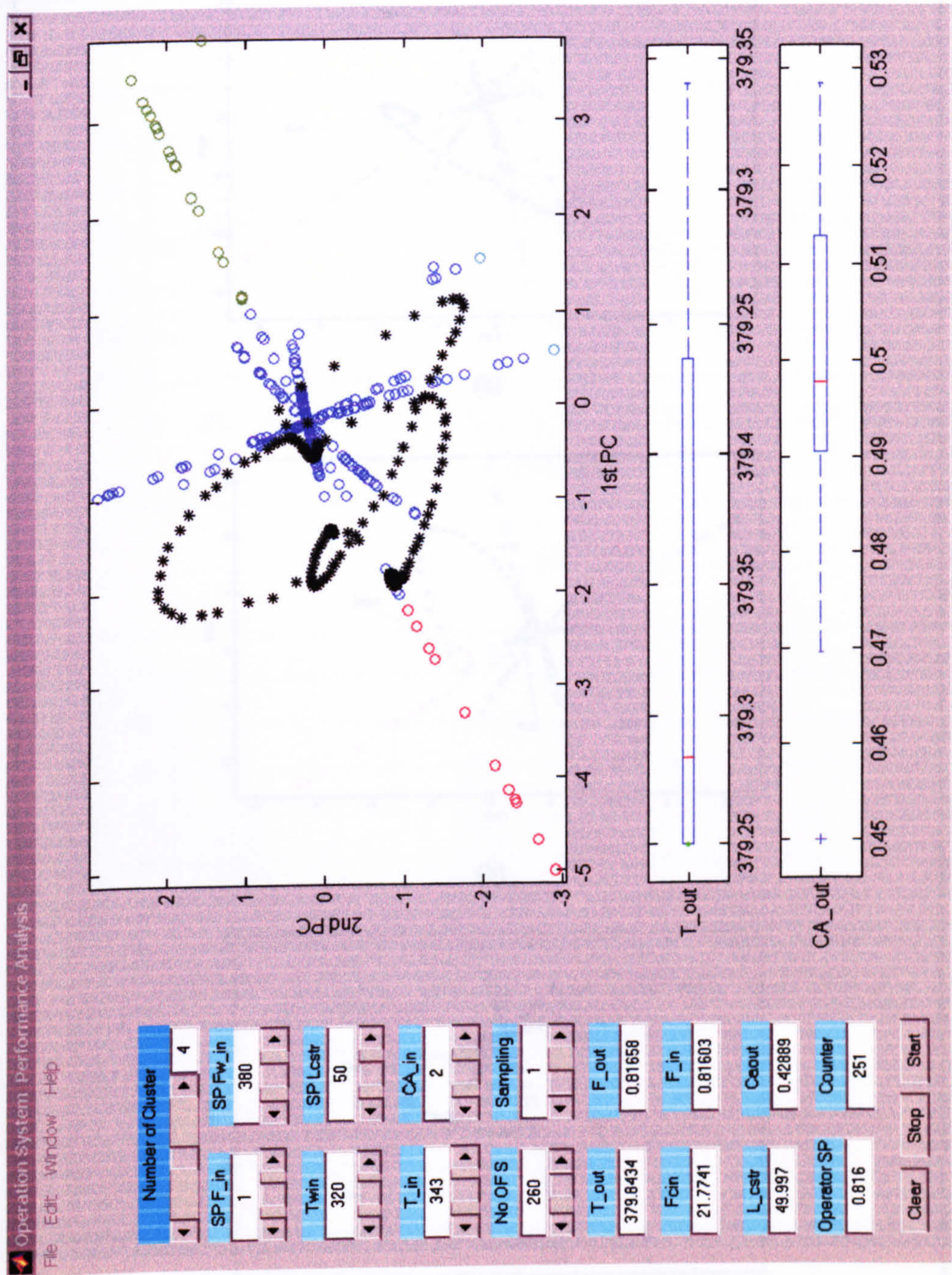


Fig 4.7. Operation path of operator B, represented by the dark asterisk .

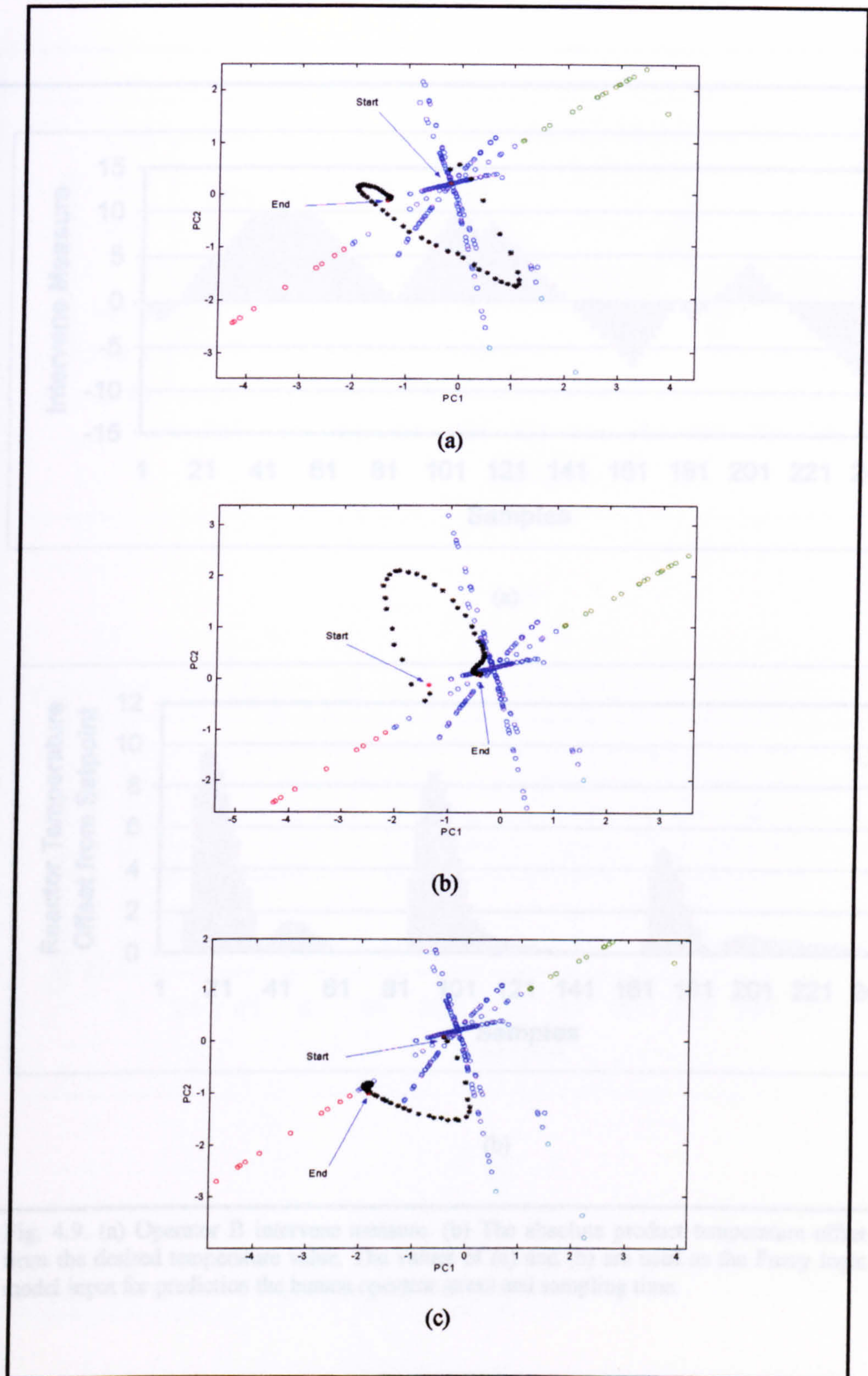


Fig. 4.8. Operation path decomposition of Operator B, showing three-captured activities of the operator during disturbed operation.

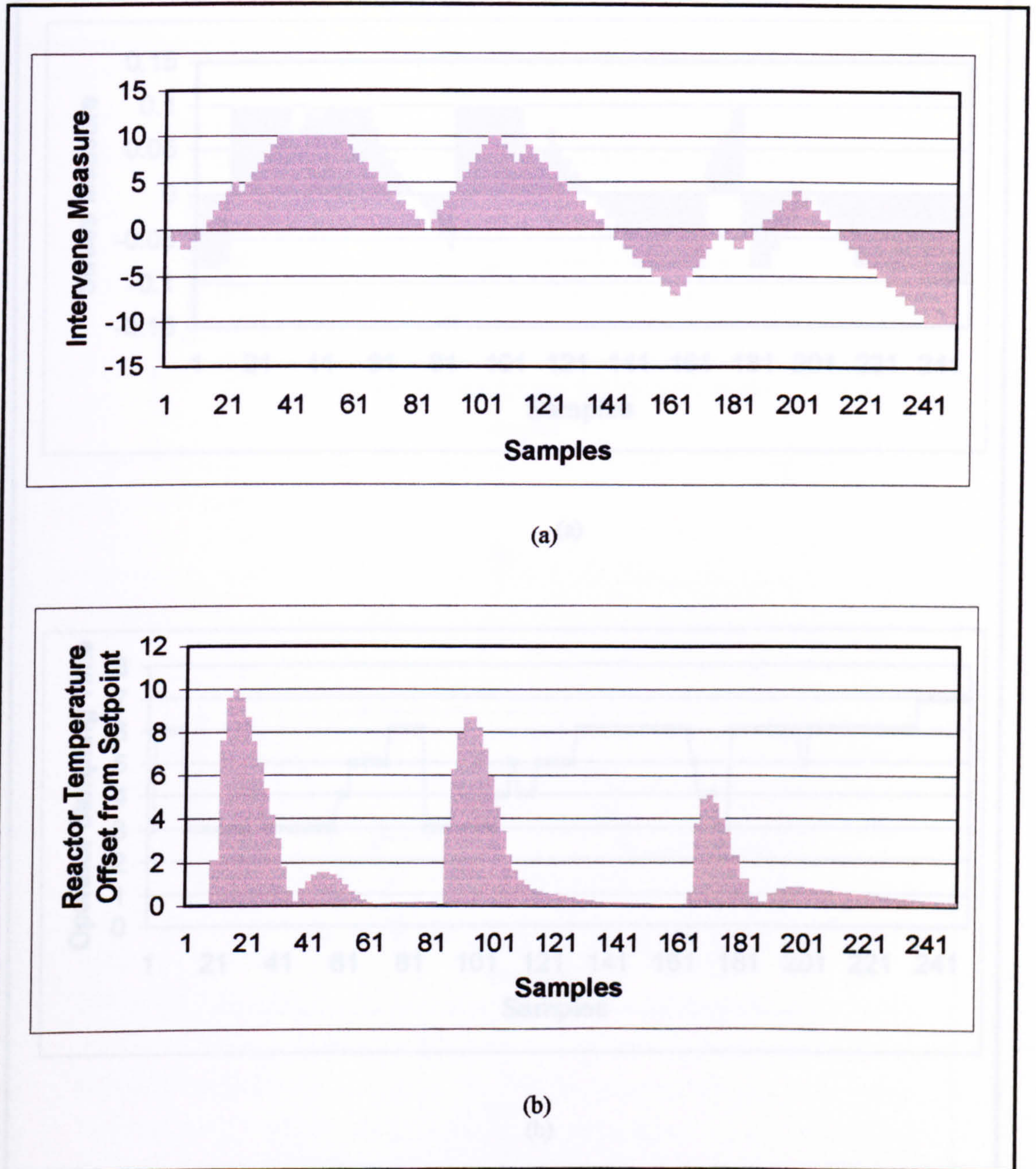
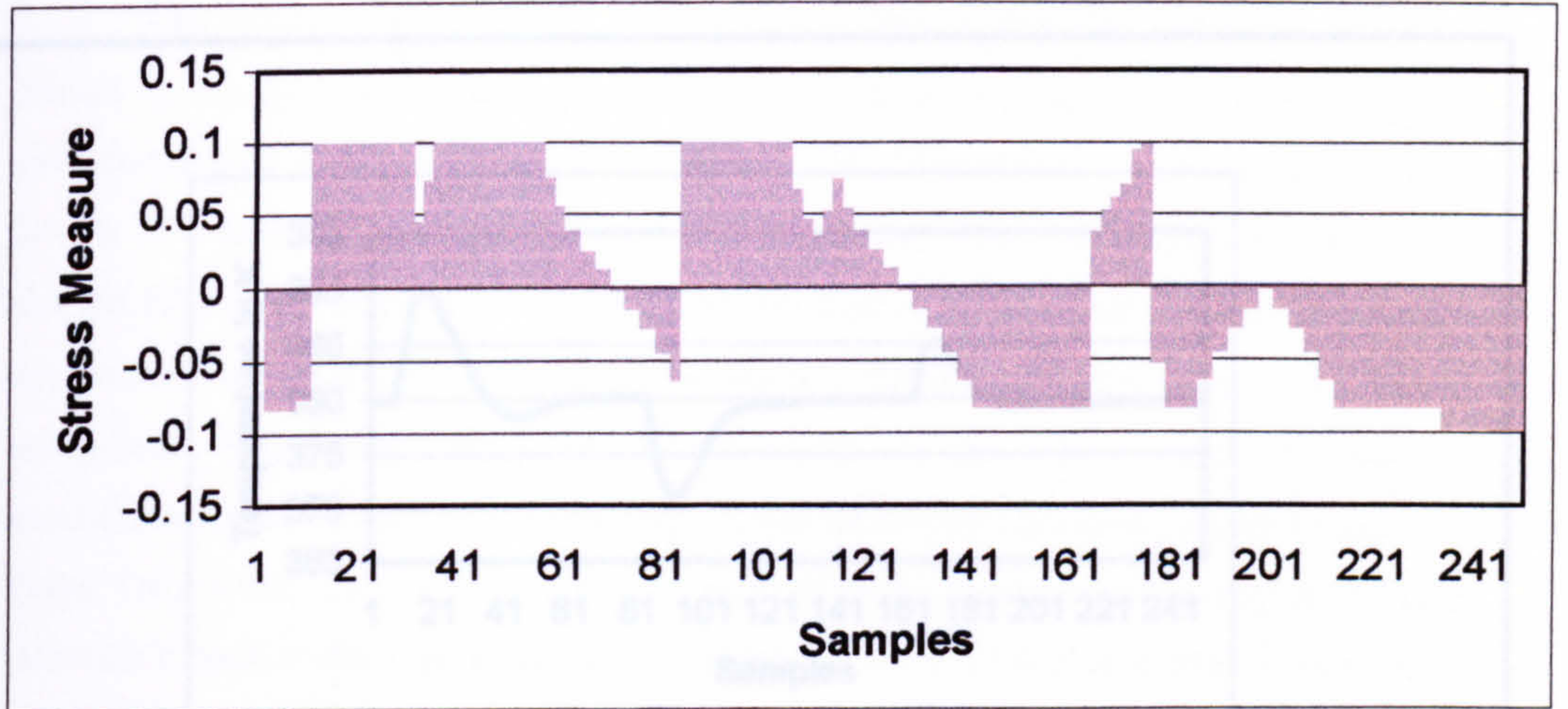
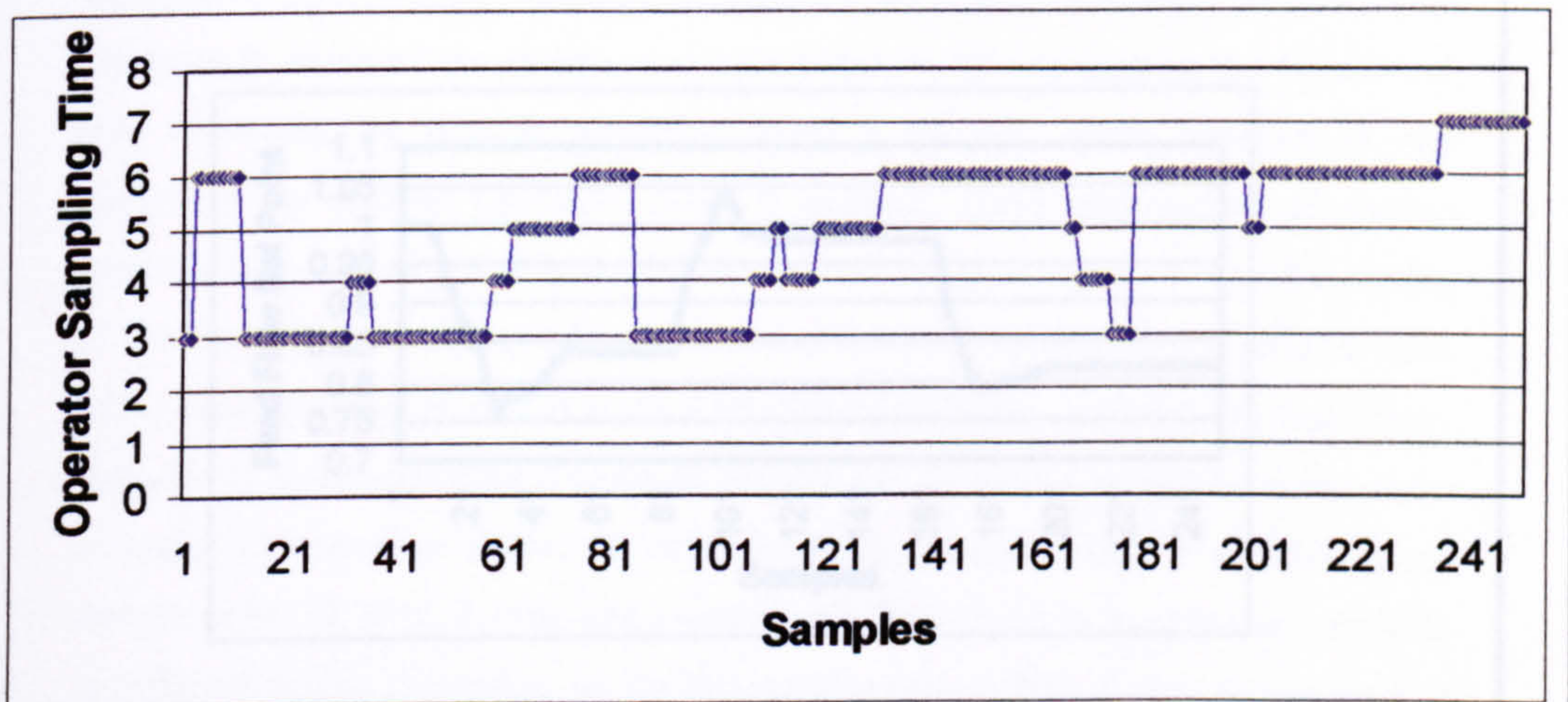


Fig. 4.9. (a) Operator B intervene measure. (b) The absolute product temperature offset from the desired temperature value. The values of (a) and (b) are used as the Fuzzy logic model input for prediction the human operator stress and sampling time.



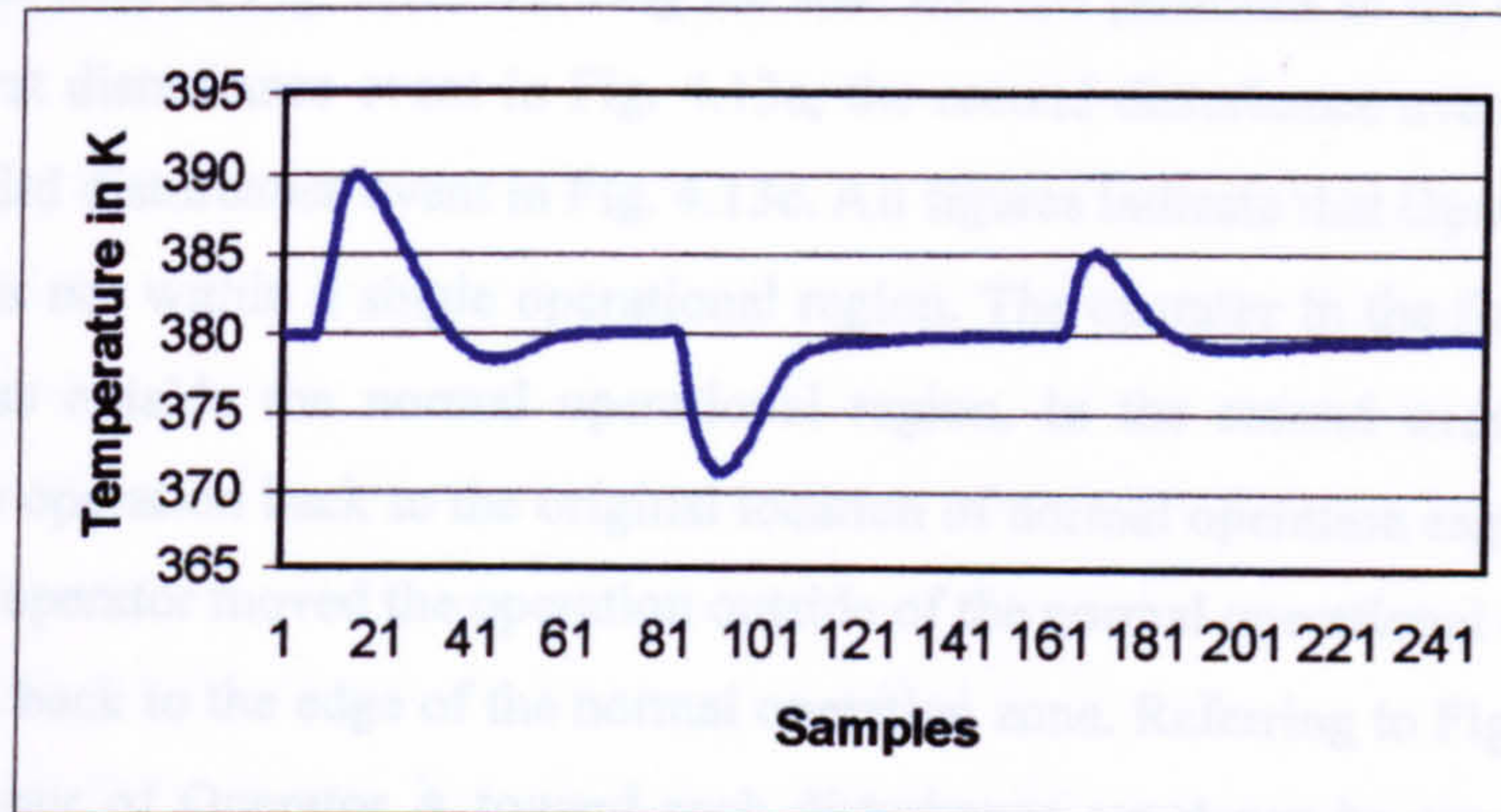
(a)



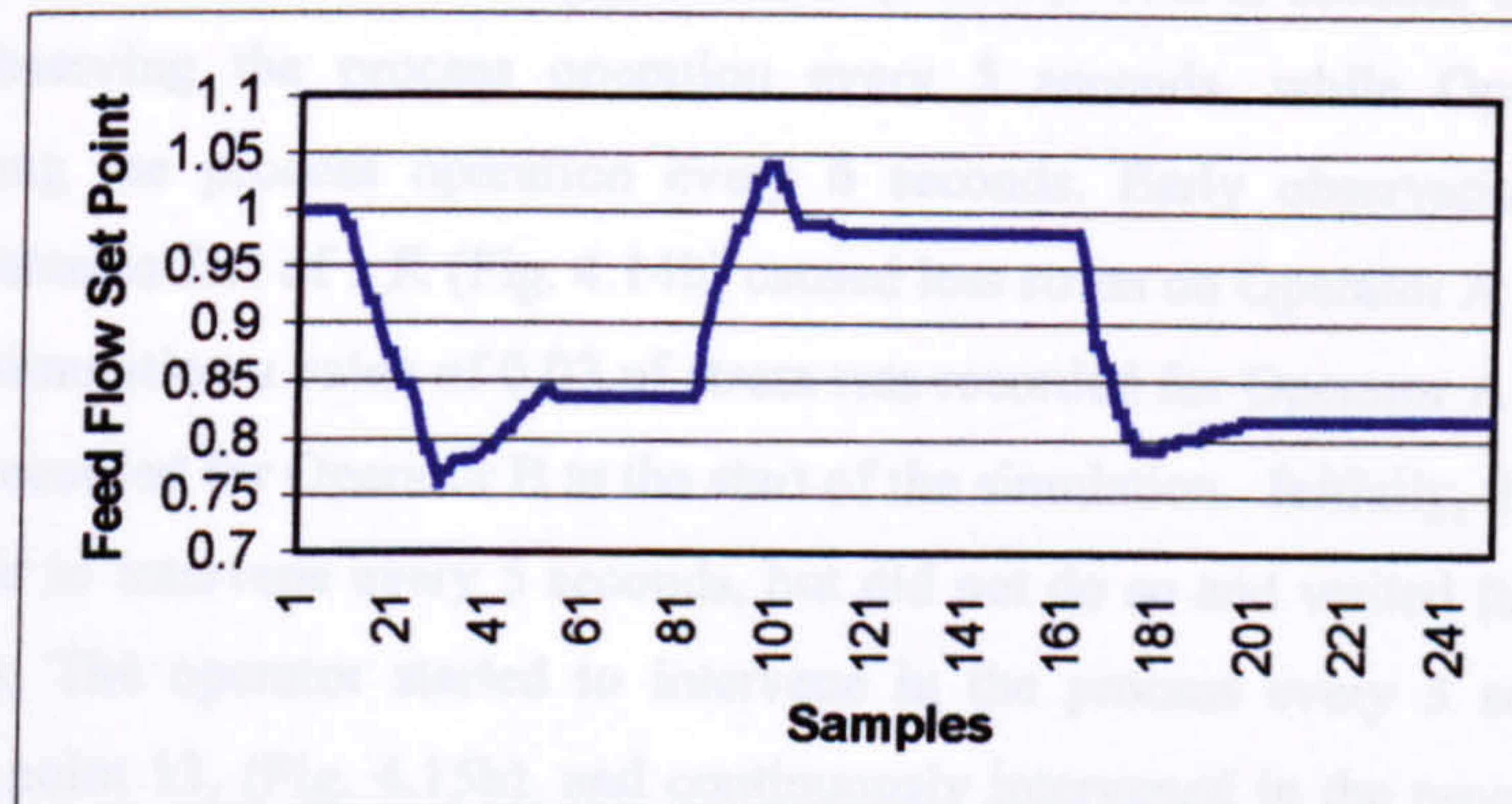
(b)

Fig. 4.10. (a) Operator B stress measure. (b) Operator B sampling time during the operation. The values of (a) and (b) are the Fuzzy logic model output.

4.4.3 Behaviour of Operator A



(a)



(b)

Fig. 4.11. (a) the dynamic trend of the product temperature and (b) Operator B intervention in the reactant inlet feed flow controller set point.

4.4.2 Behaviour of Operator A

Fig. 4.12 shows Operator A's operation path during the abnormal operation caused by the same three disturbances applied to Operator B. Fig. 4.13 is the decomposed operational path of Fig. 4.12, showing the start and end positions of the operational path for the first disturbance event in Fig. 4.13a, the second disturbance event in Fig. 4.13b, and the third disturbance event in Fig. 4.13c. All figures indicate that Operator A operates the process not within a single operational region. The operator in the first event moved the process outside the normal operational region. In the second event, the operator moved the operation back to the original location of normal operation region. In the final event, the operator moved the operation outside of the normal operational region and then returned it back to the edge of the normal operation zone. Referring to Figs. 4.14 to 4.16, the behaviour of Operator A toward each disturbance event can be summarised in the following three steps:

- (1) Operator A observed a change in the product temperature output earlier than the Operator B by a sample (Operator A observed the change at sample point 8, while Operator B observed the change at sample point 9). This is because the Operator A was observing the process operation every 5 seconds, while Operator B was observing the process operation every 6 seconds. Early observation of product temperature offset of 1 K (Fig. 4.14b) caused less stress on Operator A at the starting of the simulation a value of 0.03 of stress was recorded for Operator A while a value of 0.1 recorded for Operator B at the start of the simulation. Initially, the Operator A intended to intervene every 5 seconds, but did not do so and waited for a few more seconds. The operator started to intervene in the process every 3 seconds at the sample point 13, (Fig. 4.15b), and continuously intervened in the process operation at different timing depending on the temperature offset, (Fig. 4.14a). It was noticed that if the temperature offset is more than 1°K, the operator intervenes in the process operation every 3 seconds but if the temperature offset is less than 1°K, the operator intervenes every 4 seconds. From the sample points 0 to 80 (Fig. 4.16 a and b), the operator continuously changed the set point of the reactant feed flow, which caused the product temperature to oscillate at first disturbance event.
- (2) At the sample point 84, a new disturbance event was initiated and the operator stress increased. Operator A did not change his/her intervene time (sampling time), which is every 4 seconds (Fig. 4.15b). This causes the product temperature offset to increase dramatically at the sample point 86. At this instant, the operator panicked

and reduced the intervening time to 3 seconds and then to 2 seconds, which caused the temperature offset to decrease. The operator returned his/her intervention time to 3 seconds until the temperature offset becomes less than 1°K at the sample point 108. From sample point 80 to 160 (Fig. 4.16a and b), the operator at this event managed to keep the product temperature closer to the desired value with slight oscillations.

- (3) At the sample point 163, the temperature offset increased and the operator stress started to rise (Figs. 4.14b and 4.15a). Obviously, the operator reduced his/her intervening time to 3 seconds and started to be more active to avoid a surge of temperature offset. During this event, the operator thought that he/she was in control. At the sample point 172, the operator increased his/her intervening time to 4 seconds, which caused the temperature offset to increase. In turn, this caused the operator stress to rise. This situation repeated at the sample point 86, which made the temperature offset to rise and cause the operator to reduce his/her intervening time to 3 seconds. The operator finally stopped to intervene in the process operation at the sample point 230, where the stress dropped to less than 0.4. Samples point from 160 to the final sample (Fig. 4.16) shows that the operator managed to control the product temperature eventually after a few oscillations.

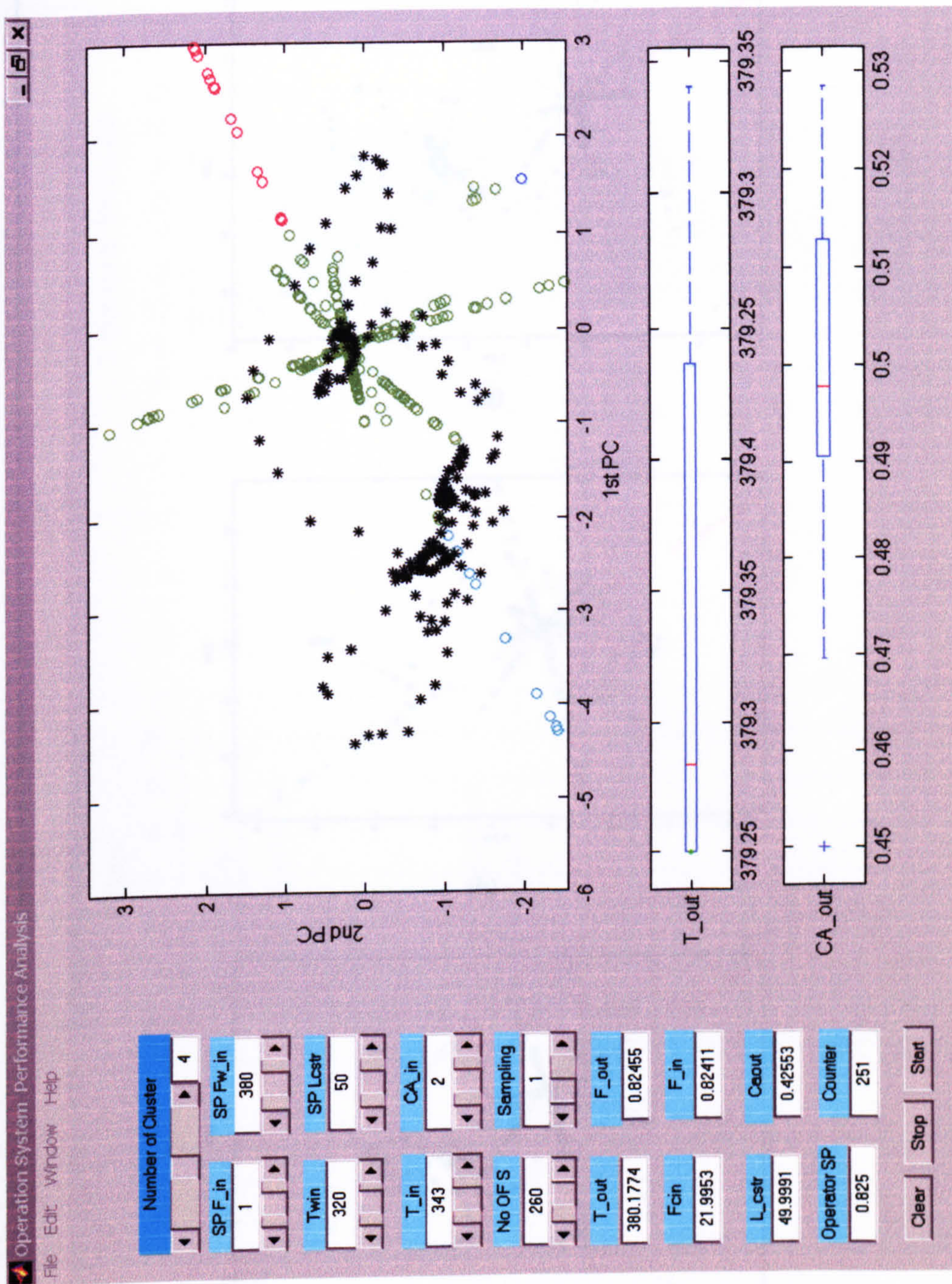


Fig 4.12. Operation path of operator A, represented by the dark asterisk .

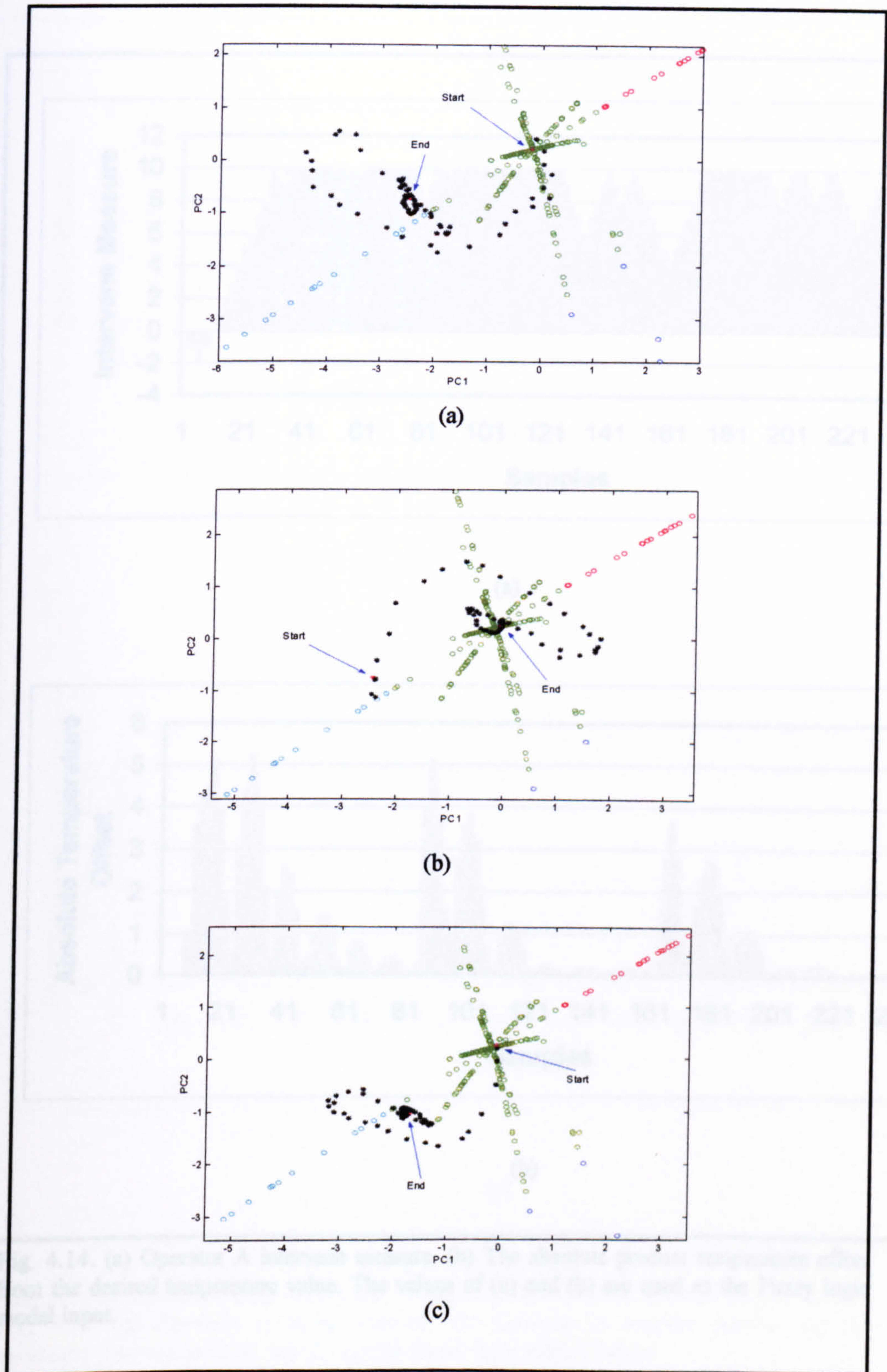
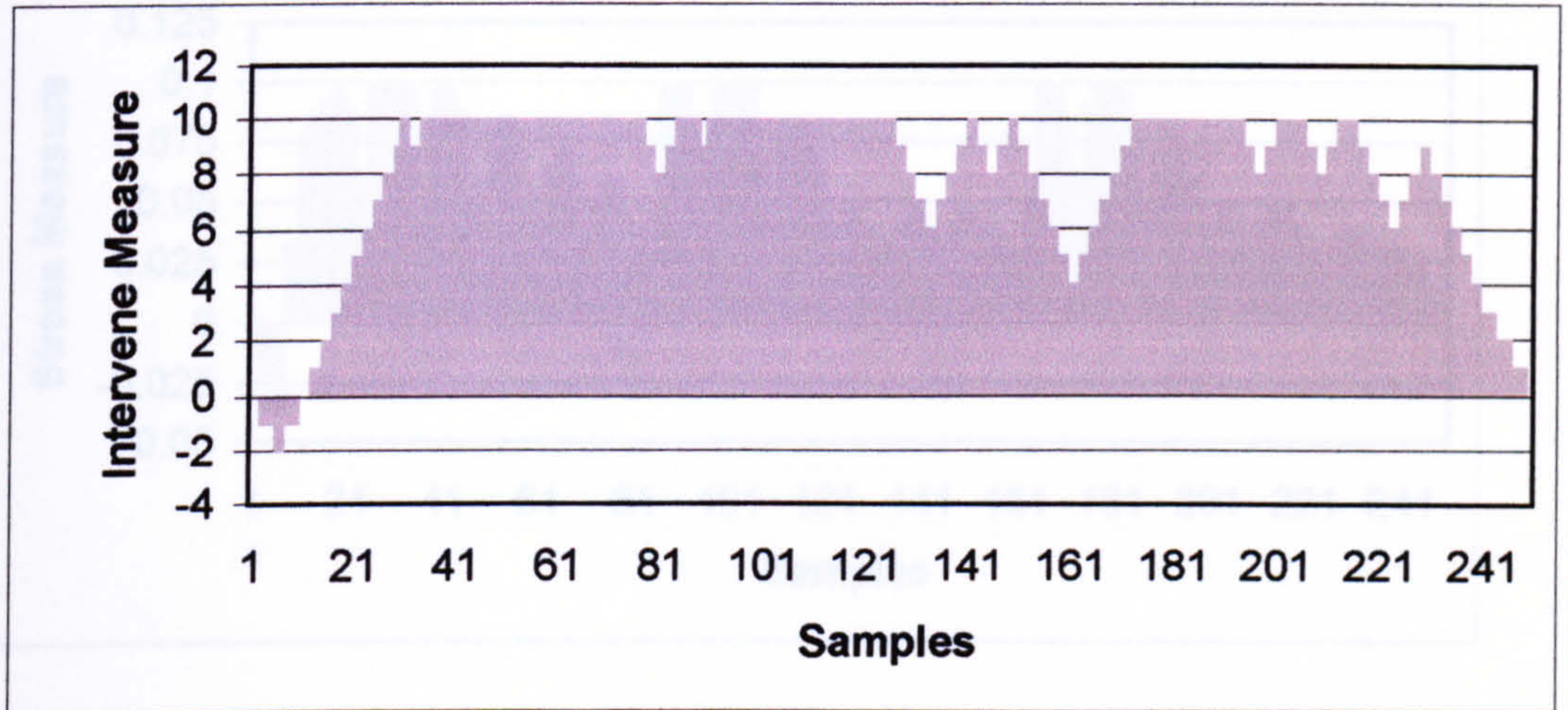
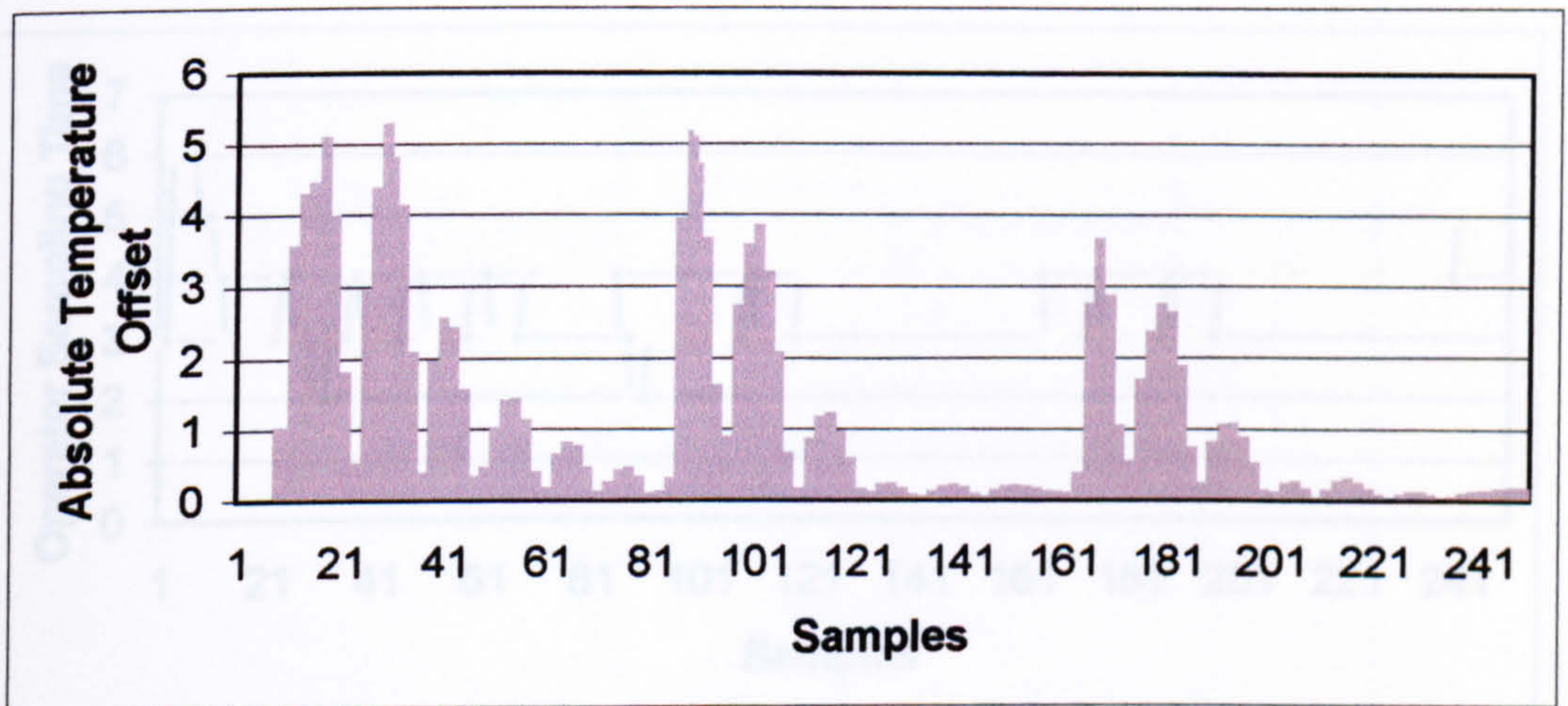


Fig. 4.13. Operation path decomposition of Operator A, showing three-captured activity of the operator during disturbed process operation condition.

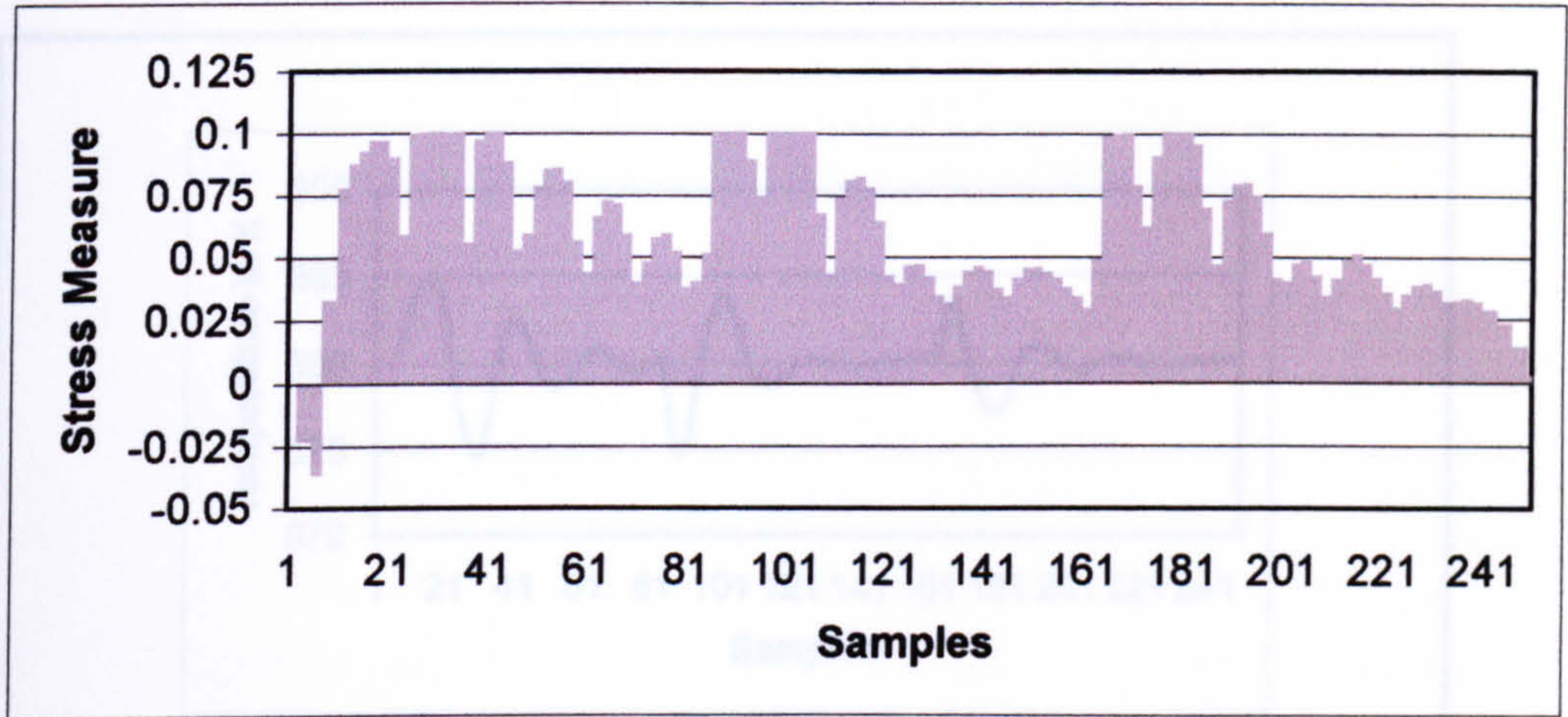


(a)

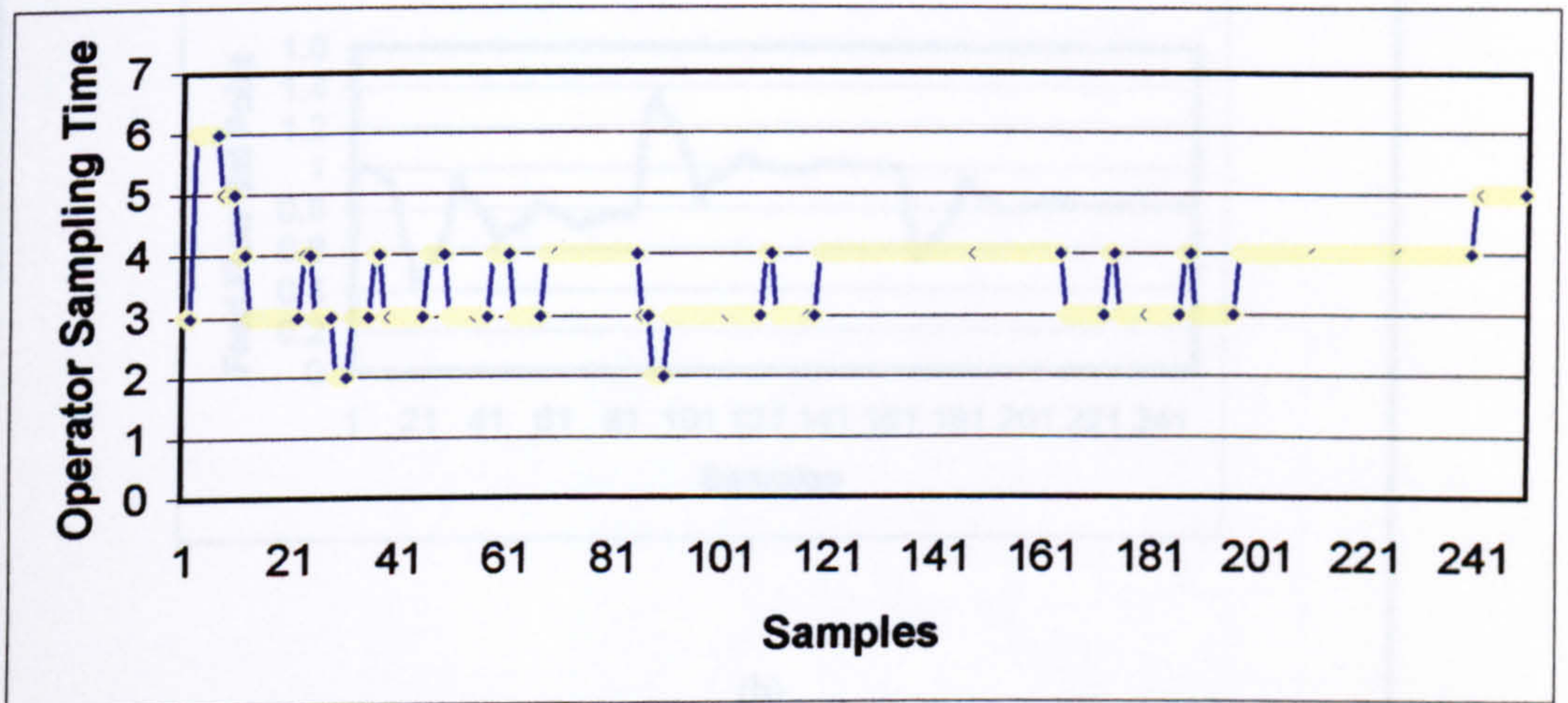


(b)

Fig. 4.14. (a) Operator A intervene measure. (b) The absolute product temperature offset from the desired temperature value. The values of (a) and (b) are used as the Fuzzy logic model input.



(a)

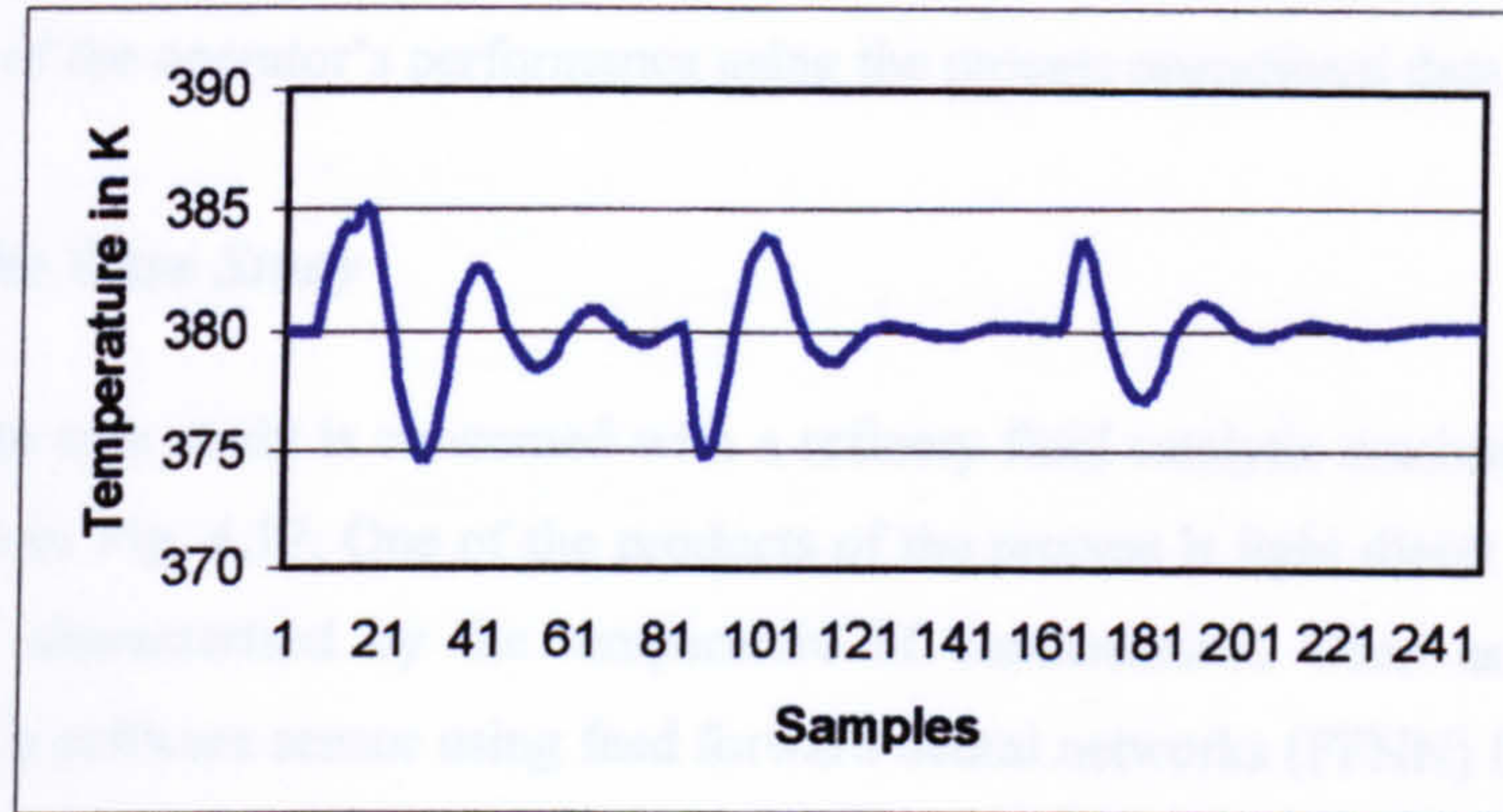


(b)

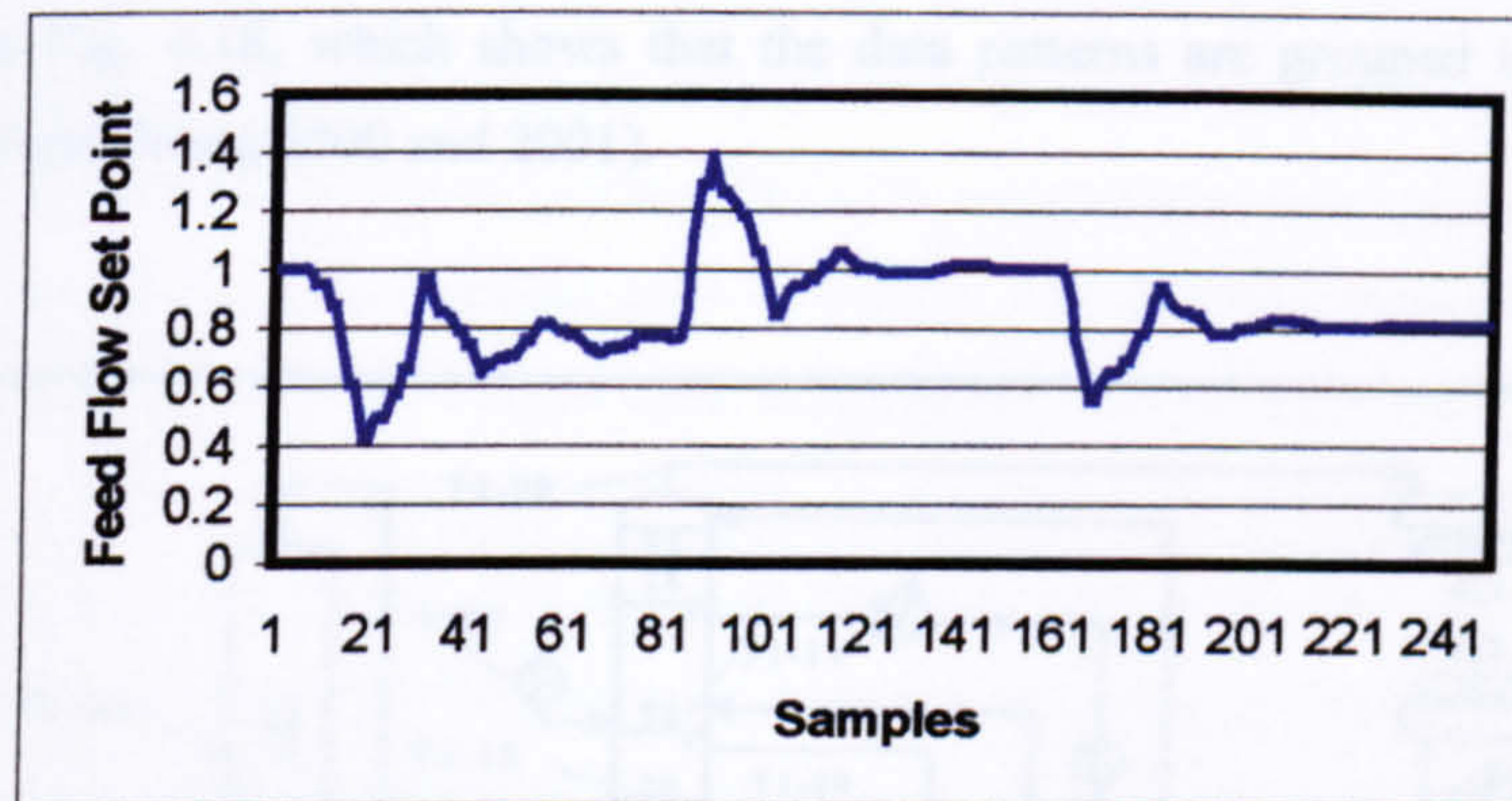
Fig. 4.15. (a) The dynamic trend of the operator stress measure and (b) Operator A interventions in the reactor when feed flow controller set point.

Fig. 4.15. (a) Operator A stress measure. (b) Operator A samples time during the operation. The values of (a) and (b) are the Fuzzy logic model output.

4.16 An Industrial Case Study of Analysing Operator's Performance



(a)



(b)

Fig. 4.16. (a) the dynamic trend of the product temperature and (b) Operator A intervention in the reactant inlet feed flow controller set point.

4.5 An Industrial Case Study of Analysing Operator's Performance

This section describes an industrial case study that further demonstrates the analysis of the operator's performance using the process operational data.

4.5.1 The Case Study

The case study is concerned with a refinery fluid catalytic cracking process (FCC) as shown in Fig. 4.17. One of the products of the process is light diesel whose quality is typically characterised by the temperature of condensation. Chen and Wang (1998) designed a software sensor using feed forward neural networks (FFNN) for predicting the condensation point using fourteen easy-to-measure process variables of Table 4.1. The process is required to produce three product grades according to seasons and market demand, namely -10#, 0# and 5# defined by the ranges of condensation temperature. PCA and fuzzy *c*-means were applied to the data of the size 303×14 (number of data patterns \times number of process variables), and the PC1 and PC2 two-dimensional plot is shown in Fig. 4.18, which shows that the data patterns are grouped into four clusters (Sebzalli and Wang 2000 and 2001).

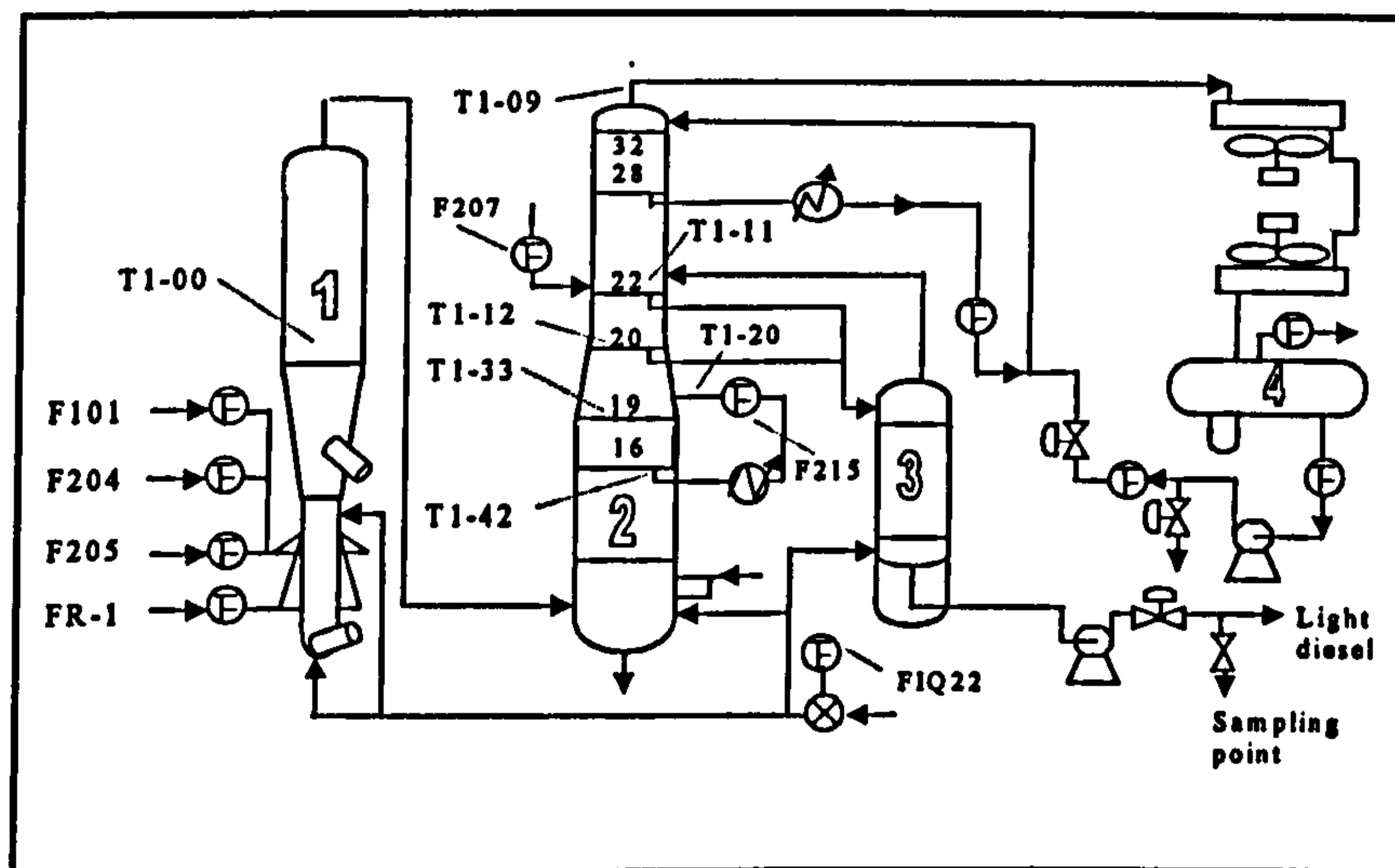


Fig. 4.17. The FCC process.

Table 4.1. Fourteen Process Variables.

T1-11	-T on tray 22 where the light diesel is withdrawn
T1-12	-T on tray 20 where the light diesel is withdrawn
T1-33	-T on tray 19
T1-42	-T on tray 16, i.e., the initialTof the pumparound
T1-20	-the return T of the pumparound
F215	-the flowrate of the pumparound
T1-09	-column top T
T1-00	-reaction T
F205	-fresh feed flowrate to the reactor
F204	-flowrate of the recycle oil
F101	-steam flowrate
FR-1	-steam flowrate
FIQ22	-flowrate of over-heated steam
F207	-flowrate of rich-absorbent oil

4.5.2 Further Analysis

In this study, we have tested two, four and seven PCs to cluster the data into three, four and five clusters. For each cluster, the probability distribution according to the product condensation temperature was plotted. It was found that all clusters follow normal distribution. It was also found that it is more appropriate to cluster the data into four clusters, because in the case of five clusters, two clusters give normal distributions around the same value of condensation temperature. While in the case of three clusters, one has a very poor distribution, which is evidenced by a large standard deviation. Examination of the results also revealed that four and seven PCs though give similar clustering results and the differences is mainly in the assignments of a few data cases, seven PCs are slightly better because they gives smaller standard deviations. Fig. 4.18 shows the distributions according to condensation temperatures of products when four and seven PCs were used. Therefore in the following discussion we will only consider four clusters.

Interestingly, it was found that three clusters correspond to three products -10#, 5# and 0# and the cluster at the bottom-right corner was found to be a cluster that though is close to 0# but has very poor distribution and is an area which has a high probability of product off-specification.

Therefore the strategy for operation should be operating the process in the region of the bottom-left if the desired product is -10#; in the region at the top if the desired product is 5#; in the region at the middle if the desired product is 0#, and try to avoid the

region at the bottom-right corner. Another point is that in order to move from producing -10# to 0#, adjusting PC1 is more important than changing PC2. While to switch from producing 0# to 5#, PC2 is more important than PC1. Both PC1 and PC2 are important in avoiding the region at the bottom-right corner, which produces off-specification product. It is important to notice that the region at the bottom right corner, which should be avoided in operation was not anticipated before the analysis.

Close examination gives a more interesting discovery regarding the region at the bottom-right corner of Fig. 4.17. It is very likely caused by operators during product changeover. For example, 117-124 at the bottom-right corner were due to transition from region of -10# (1-116) to the region of product 0# (125-191). Other data cases in the bottom-right corner can also be explained similarly. Data patterns 211 and 212 were due to transition from the 5# region (192-210) to the -10# region (213-242); 243-244, due to transition from -10# region (213-242) to 0# region (245-271); 278-288 due to transition from 5# (272-277) to 0# (289-303). It shows that some transition took longer time. If the knowledge discovered had been known, the transition time could have been reduced.

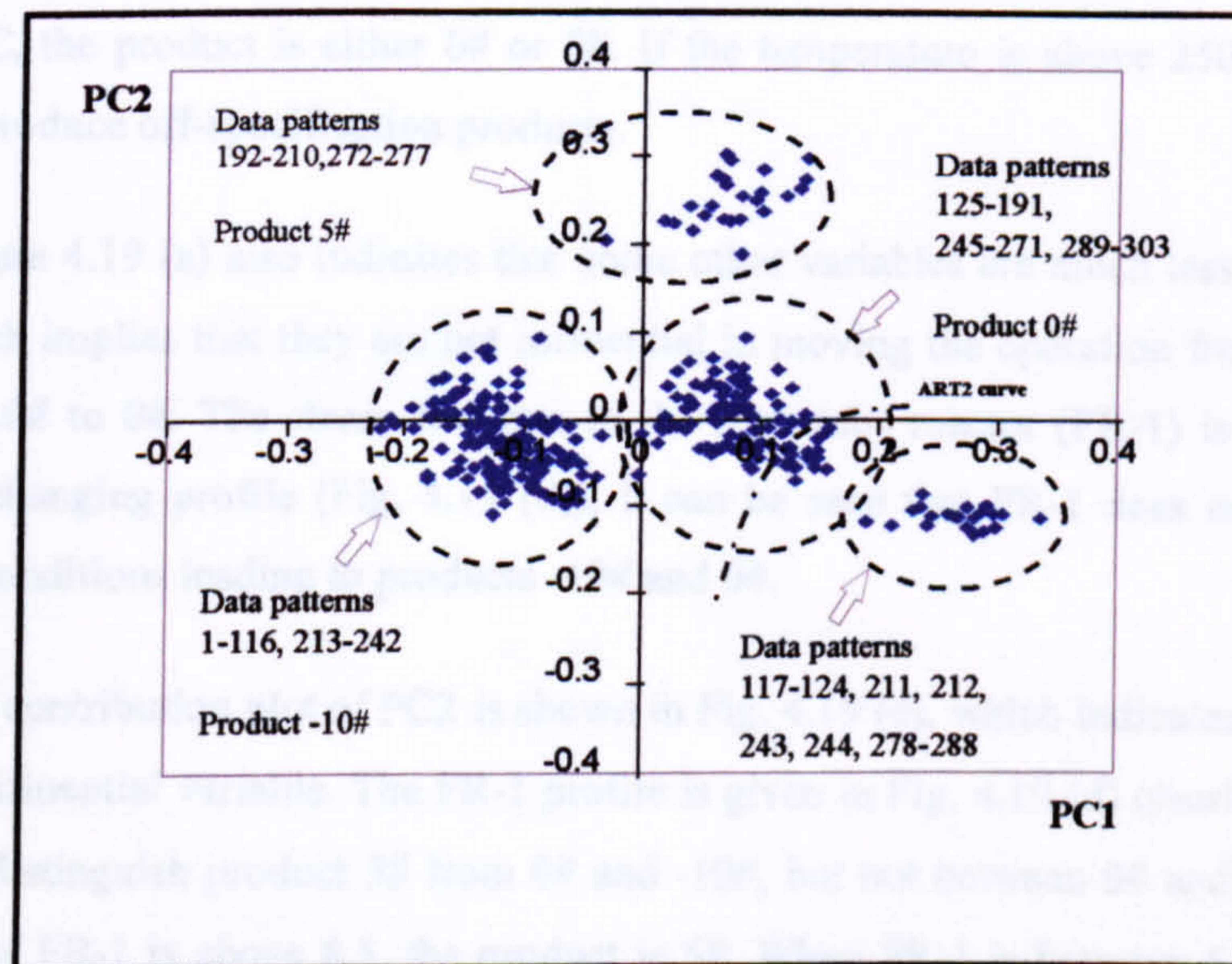


Fig. 4.18. The PC1-PC2 plot.

4.5.3 Discovery of Operational Strategies

Because PC1 and PC2 are latent variables, it is necessary to link PC1 and PC2 to the original variables in order to provide guidance to operators for monitoring and adjustment during product changeover. To this purpose, variable contribution plots were used.

The contribution plot for PC1 is the plot of PC1 against the coefficients for the 14 original variables and is shown in Fig. 4.19 (a), from which it is found that the most important variables are T1-12 (the temperature on tray 20 where the product is withdrawn) and T1-42 (the temperature on tray 16 close to the flashing zone). This result is consistent with the analysis based on principles that the temperature on the tray where the product is withdrawn and the temperature at the flashing zone have most important impact on the sidedraw product. Some other variables are found not important such as FR-1. The above discovery is confirmed by looking at the change of T1-12 over the 303 data patterns (Fig. 4.19 (b)). It clearly shows that from the value of T1-12, it is able to distinguish product -10# from 0# and 5#, but not between 0# and 5#. When the temperature T1-12 is below 230°C, the product is -10#. When T1-12 is between 230°C and 250°C, the product is either 0# or 5#. If the temperature is above 250°C, it is very likely to produce off-specification products.

Figure 4.19 (a) also indicates that some other variables are much less important to PC1, which implies that they are not influential in moving the operation from producing product -10# to 0#. The steam flowrate to the riser tube reactor (FR-1) is an example. From its changing profile (Fig. 4.19 (d)), it can be seen that FR-1 does not reflect the different conditions leading to products -10# and 0#.

The contribution plot of PC2 is shown in Fig. 4.19 (c), which indicates that FR-1 is the most influential variable. The FR-1 profile is given in Fig. 4.19 (d) clearly shows that FR-1 can distinguish product 5# from 0# and -10#, but not between 0# and -10#. When the value of FR-1 is above 8.5, the product is 5#. When FR-1 is between 5 and 8.5, the product is either 0# or -10#. Though not very clear, it can still see that when FR-1 is below 6.5, the operation goes into the region producing off-specification product.

The discovery that FR-1 is the most important variable to PC2 and so in distinguishing product 0# from 5# and -10# was not anticipated. In fact, because of the multivariate and non-linear nature of the problem, some variables, which are important to

product quality in one operational region, may become less important in a different region.

The above analysis on the contributions of individual variables to PC1 and PC2, and so to the operational states is also consistent with the observation on Fig. 4.17 that both PC1 and PC2 are influential to the zone at the bottom-right corner. From Fig. 4.19 (a, b, c & d) we can see that T1-12 and FR-1 all can have significant influence on this zone. Therefore to change the operation from producing -10# to 5#, we should first increase T1-12 and TR-42 and then increase FR-1. In order to avoid off-specification product from being produced we should carefully monitor T1-12, TR-42 and FR-1 to avoid the region at the bottom-right corner. Of course it is important to be aware that fine-tuning of all the variables is necessary but the guidance can help operators to move the process from producing one product quicker to another.

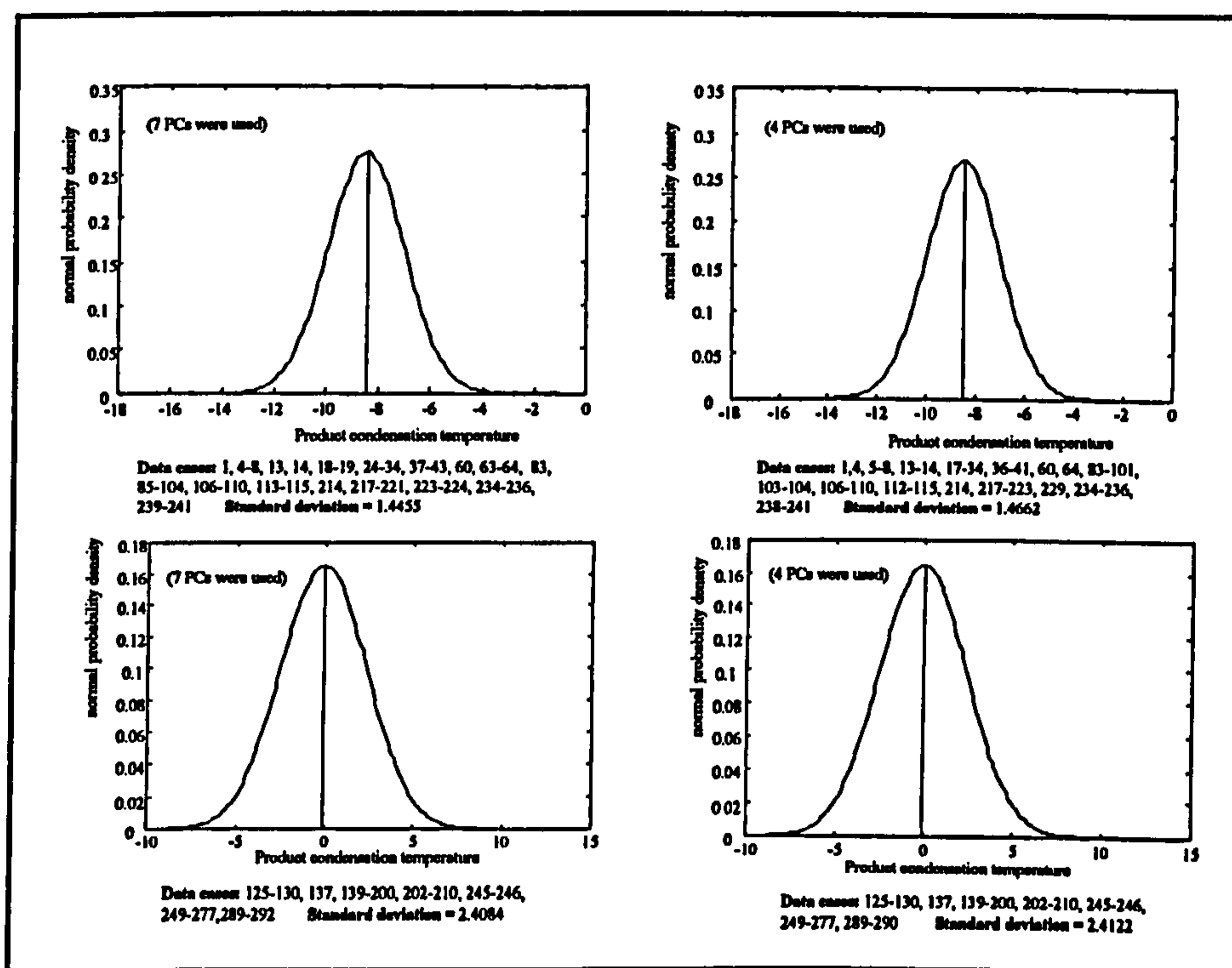


Fig. 4.19. Distributions of product condensation temperatures for the two clusters corresponding to -10# and 0#, when 7 PCs and 4 PCs are used in fuzzy c-means clustering.

4.6 Summary

The structure and functions of the proposed operator module are described. The operator is considered as the most difficult element to model in a joint process-operator interaction system. This is due to the complexity of the human brain and the difference of human mentality measurement, which is influenced by external and internal factors. The major elements of the developed human model are discussed. Although the system is still not very sophisticated, it is sufficient for carrying out the proposed studies in this work. A practical example has been given in a scenario to show, a confident Operator B and a nervous Operator A. Fuzzy membership functions were used to represent the degree of nervousness models of both A and B operators (refer to section 4.4 for a full description). Operator B has low average number of intervention and stress, and higher average intervention time (sampling time). While Operator A has higher average of stress and number of intervention, and lower average of intervention time. Operator B manages to be in control during the process operation while Operator A has some difficulties.

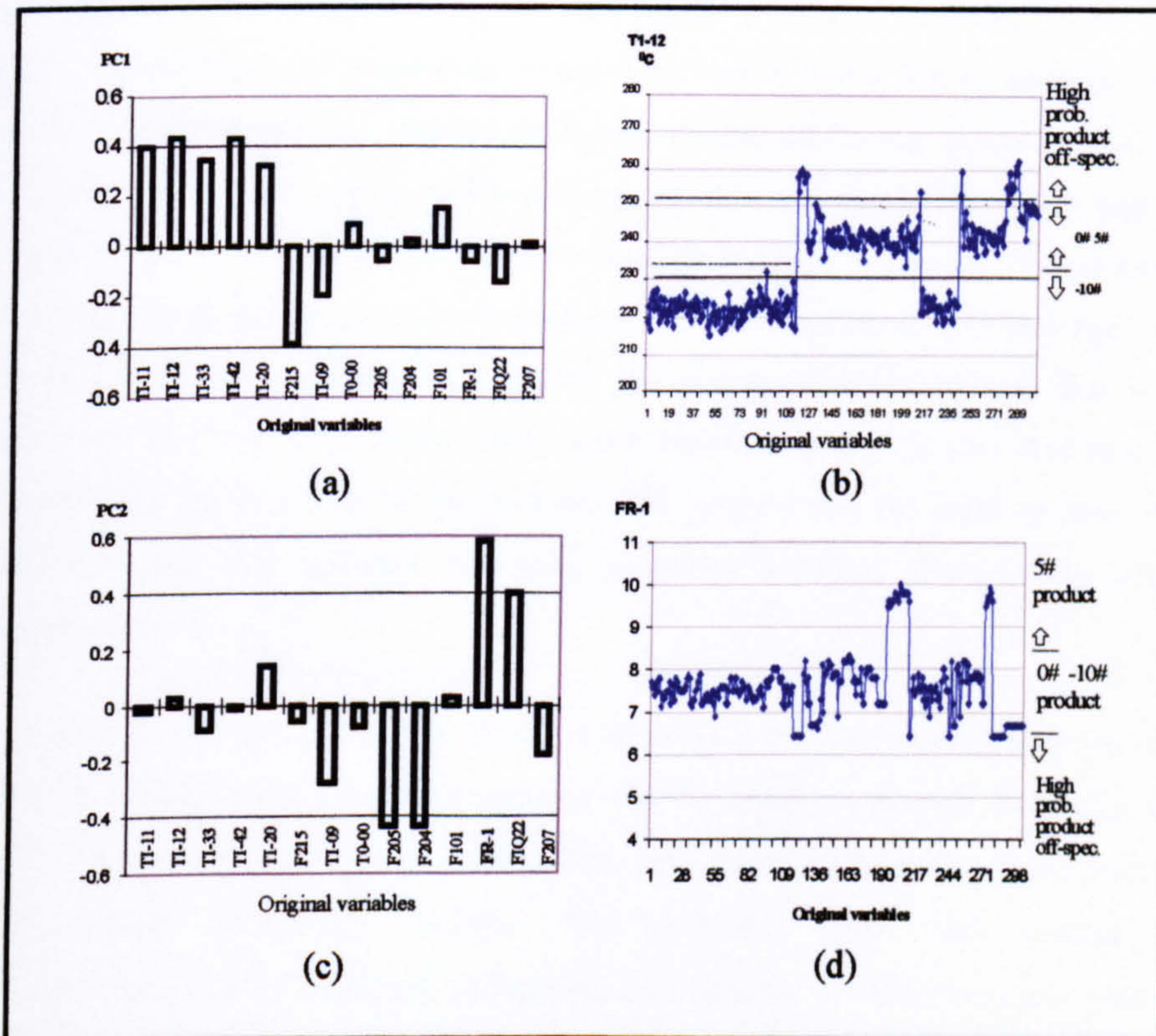


Fig. 4.20. (a) contributing plot of PC1, (b) changing profile of T1-12 (c) contribution plot of PC2 and (d) changing profile of FR-1.

This is clearly shown from the paths of the operation and the results of the graphical analysis. Finally, the results and data can be used to extract the behaviour features of each operator, for example each operator should have different averages, distributions, variances and standard deviations of stress, number of intervention and intervention times. These behaviour features combined with other operator features, such as the operational path, can be used to identify the effectiveness of an operator during the dynamic operation or historical data analysis.

An industrial case study was also presented which further proved that the operator behaviour can be assessed through analysing historical operational data.

Dynamically monitoring the paths or trajectories of operation in the low dimensional operational spaces also presents a useful way for capturing operators near-miss or near-hit. Pervious industrial practices rely on operators to report near-miss situations. However some times operators may not be aware of such situations.

Chapter 5

The Process–Operator Interaction Module

This chapter describes the role and the implementation issues of the process–operator interaction module.

5.1 Introduction

The simplest way of interaction between machine and operator modules in a joint process-operator simulation system is clearly through direct connection, as depicted in Fig. 5.1a. In practice, such a simple and straightforward connection is far from sufficient. There are a number of factors that complicate the interactions. Both the operator and process models generate a variety of complex and highly correlated outputs, which need to be filtered, transformed and sometimes interpreted before being fed to another model. The dynamic behaviour and time dependent feature of interaction also represents an element of complexity, because the effects of the process response and operator's action may not occur in sequence and usually evolve in parallel with different time constants. Thus it requires time management to be embedded in the interaction module. As a result, it is necessary to have an interaction module to manage and control the communication between the process and operator models (Fig. 5.1b). In this study, the interaction module is also used as an interface to monitor the performance of the operator, the process and the joint system. Faults and disturbances are also initiated and data recording managed through the interface of interaction module.

This chapter is organised as follows. In Section 5.2, previous studies on interaction models in man-machine simulation systems will be briefly reviewed. Though none of the models was proposed for process industries, they have inspired the development of our process-operator interaction module. The proposed interaction module and its implementation will be described in Section 5.3. Section 5.4 describes the graphical user interface and the implementation of a proposed fuzzy qualitative methodology for modelling the temporal behaviour of the process–operator joint system. Final remarks will be made in Section 5.5.

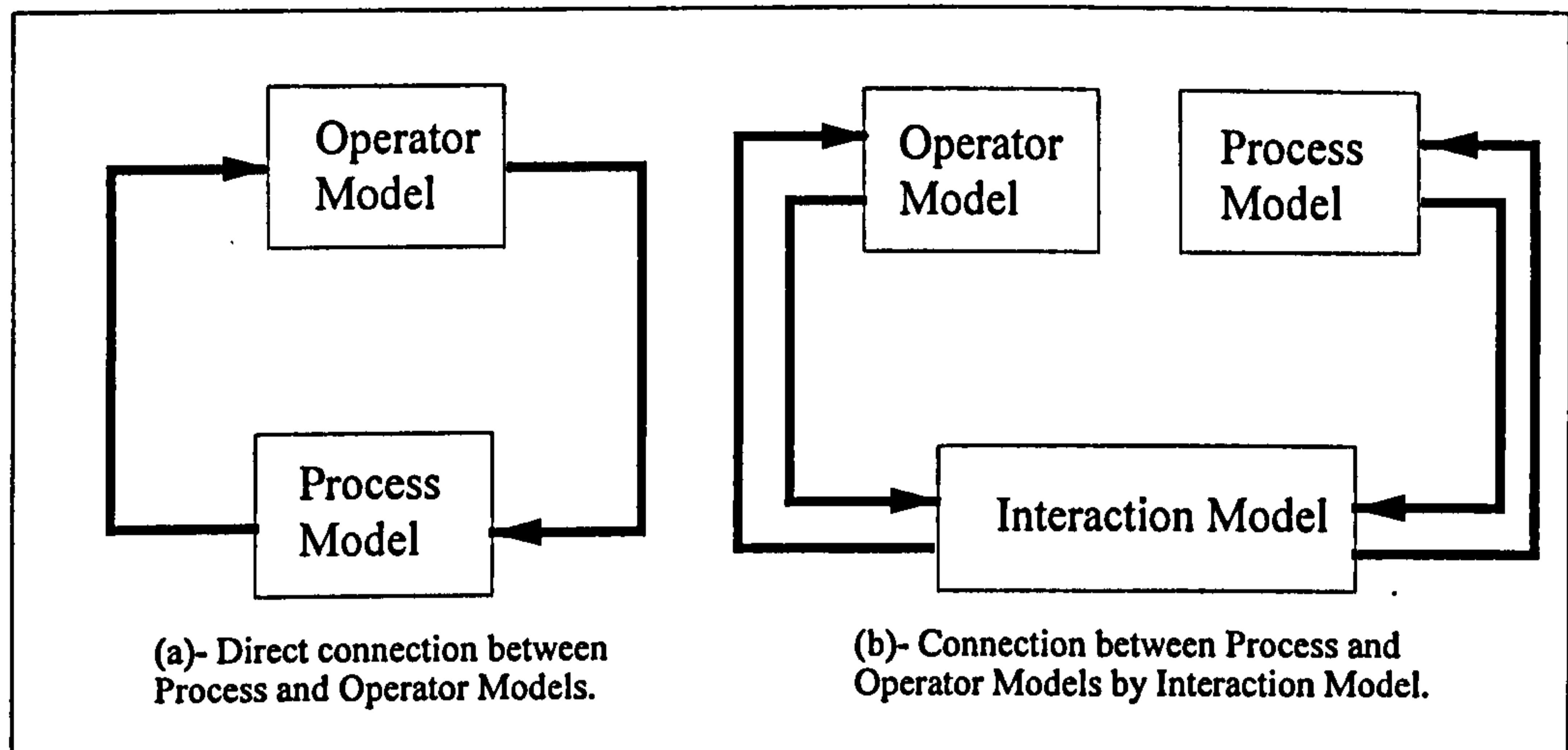


Fig. 5.1. The process-operator interaction module architecture.

5.2 Published Models on Man-Machine Interactions

5.2.1 Reviews of Published Models

Cacciabue (1999) conducted a comprehensive literature review of the man-machine interaction models and identified three major elements in a man-machine interaction system, i.e., time management, logical man-machine interactions and dynamic reliability. Time management deals with the independent time steps for process and operator simulations and the exchange of data to achieve synchronisation between the operator and process simulation. The logical man-machine interaction filters all information that is produced by the process and operator models, using special algorithms, which consider the logical connection that exist between interconnected events. Dynamic reliability handles false and incomplete information or process failures and operator errors, which will provide experiences in the man-machine simulation studies. Fig. 5.2 shows the theories and their computational means employed by the interaction model of Cacciabue (1999). The time management element in the interaction module employs logic models and time management.

The logical man-machine interaction element employs first or higher order logic (Dubois and Prade 1980; Van Orman Quine 1959), which is particular suitable for the representation of qualitative and “quasi-numerical” thinking. Dynamic reliability uses statistical theory such as Markov chains (Bharucha-Reid, 1960), and state transition diagrams such as Petri Nets (Peterson, 1981), which can describe the time dependencies and multiple correlations between the elements of the man-machine system.

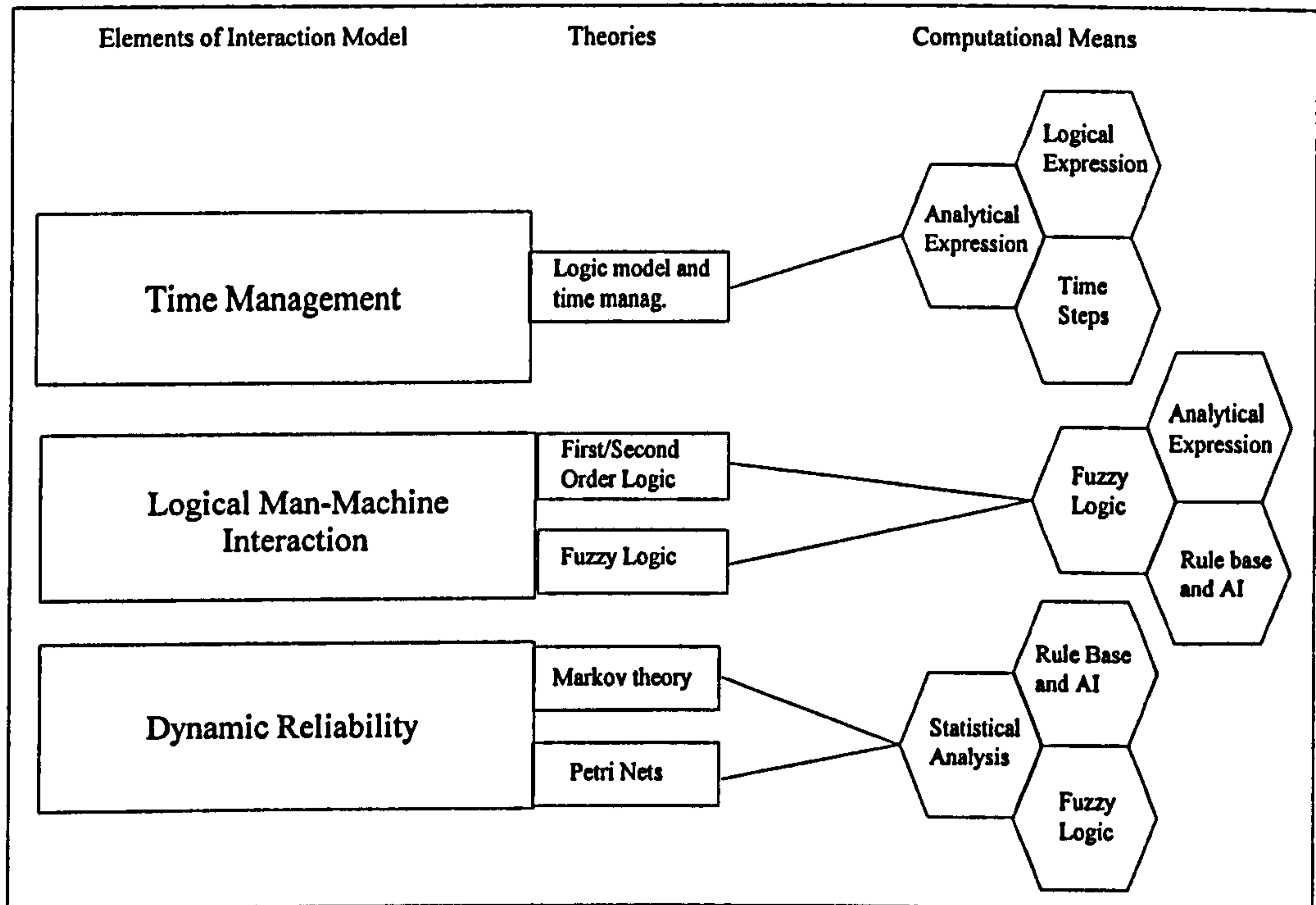


Fig 5.2. Elements of the interaction model and computational means (Cacciabue, 1999).

A major role of the interaction model is to manage the flow of the information and the data in the human-machine interaction system. Therefore, Cacciabue (1999) classified the information and the data into two types. The first type is the dynamic data, which consists of the variables that are dynamically calculated by the human and the machine models and then dynamically changed, such as the set point and auto/manual modes, as well as the various failure and error modes. The second type is static data, which includes the parameters related to the human and the machine models, such as what are normal and abnormal behaviours, and the casual relationships about failures and errors. Static data related to the operator model also includes event sequences, which cause the operator model to perform certain behaviour.

Dynamic data is dynamically generated and exchanged by the human and machine systems, while static data is defined in the design stage and stored in the data or knowledge base. The interaction module manages the specific information to be transferred from one model to another. This needs to be performed continuously during the time step of dynamic evolvment. For example, during the fault diagnosis, the interaction module combines the dynamic data, such as physical quantities and indicator values calculated by the machine model, with static data, such as failure casual relationships defined at the beginning of the analysis, to find the location and the mode of failure.

In order to manage the data exchange between the human and the machine models, the interaction module requires a large amount of input data and information. These large input quantities are classified according to the types, modes and probabilities of operator error and component failures, which are related to process disturbances, and operator actions and decisions. Therefore, all data, information and knowledge have to be organised in data architecture in order to support the operator-process interaction system.

The interaction module can retrieve data from the global database or from its own database, depending on the architecture of the overall process-operator interaction system. Data retrieved from the database by the interaction module mainly concerns the reliability and logical behaviour of process, and operator constituents, which are usually in the form of failure modes, error modes, failure rates, or failure types. The data and information are necessary to predict the temporal operational state. The time management element of the interaction module manages the data flow from the database to the dynamic memory of the interaction module, and vice versa. The data holds the logical behaviour of process and operator constituents, which are usually in the form of failure modes, error modes and failure rate, and are used to determine the present dynamic state of the process and operator behaviours.

The dynamic reliability element of the interaction module is complex. The typical problem of the reliability analysis goes beyond the classical approaches, such as fault trees and event tree methods (Feller, 1968; Hoyland and Rausand, 1994). A number of approaches have been developed to permit the evolution of the probabilistic behaviour of system unavailability versus time and dynamic reliability, when the process is decomposed into a reasonable number of super-components. These dynamic approaches are based on the state transition diagrams theory (e.g. Petri Nets) and Markov chains (Vesely and Goldberg, 1977; Jeong et al. 1987; Aldemir et al. 1994). Although these methods can handle the stochastic behaviour of components very well, they are limited in dealing with the actual interaction between the process of the dynamic behaviour of physical variables and dynamic change of components operating state (Siu, 1994). Hassan and Aldemir (1990) tried to solve logical/reliability problem by developing a methodology that separates the physical and probabilistic analysis, and assesses event sensitivity due to the uncertainty on the component failure data. Another approach by Aldemir (1987) is based on the continuous event tree method, which links the system module to probabilistic treatment using Markovian or semi-Markovian chains in a complete theoretical analysis. Both the dynamic event tree method (Siu and Acosta, 1991) and the dynamic logical analysis methodology (Cojazzi and

Cacciabue, 1994) combine a quantitative dynamic process model and probabilistic analysis in dynamic conditions to evaluate both reliability and physical behaviour in an integrated architecture. The objective of the above methods is to combine the physical simulation and probabilistic evaluation in manageable computer architecture, without requiring too complex analysis. These methodologies generate sequences showing how faults occur (systematic analysis), assign an initial configuration to the process, and study a limited number of critical process conditions.

5.2.2 Observations

One of the problems associated with the above reviewed models is that all possible states of a component need to be pre-defined and stored in the knowledge base before any simulation or analysis of a process-operator interaction. This is not always possible since some states might have never been experienced in practice. Therefore, if a new state of a component occurs, the interaction module will generate incorrect sequence and initiate wrong configuration. This is the nature of the knowledge base, since the knowledge is dependent on past experience of the developed knowledge. The inability of learning or dynamically improve in performance is also a factor. Ideally, the interaction module should be able to learn to create its own knowledge and rules, and to improve its performance continuously during dynamic operation. In addition, the interaction system should be able to deal with both quantitative and qualitative data, and the causal relationships of variables as well as causal relationships of the whole process. The reviewed systems do not have modules that can handle dynamic causal relationships among process variables, operator actions and fault modes. Furthermore, the reviewed human-machine interaction systems focus on studying of the dynamic behaviour of the joint simulation system. One of the fundamental differences of the current effort from the previous work is that we intend to develop a system that can automatically characterise and assess the skills and behaviour of operational personnel. This function has never been considered in the review studies.

5.3 Architecture and Functions of the Proposed Interaction Module

Fig. 5.3 depicts the conceptual architecture of the process-operator interaction module, the constituent elements, data flows, and the control links. The characteristics and the functions of each element will be described below.

The first two elements of the interaction module are the input/output blocks. All data and information from the process and operator simulation, including operator's actions and instant values of process variables are acknowledged of their existence in the input buffer and ready to be processed by other elements of the interaction module. The output buffer contains all the data and information to be transferred to the process or operator modules, such as set points of controllers and manual/auto modes, new and updated knowledge and rule base for the operator model and start-up/shutdown procedures of the process. Disturbance creator is designed to generate various disturbances in the joint system, representing operator errors and external disturbances influencing the process and operator behaviour. This element contains statistical methods, such as normal distributions, which generates disturbances systematically.

The data structure element is responsible for transforming and representing the data and information in the appropriate formats and structures, to allow easy data access and to be processed by all elements within the module. For example, the rules can be represented, stored and processed in three different formats, such as verbose (words), symbolic and indexed (or references). This element is also responsible for adding noise to data and calculating a number of data properties, such as the mean and standard deviation.

The validation and evaluation element is responsible for testing the graphical qualitative model for simulating the temporal behaviour of the joint operator-process system, which will be detailed in Chapters 6 and 7. The mathematical methods used in this element are based on statistical techniques, such as analysis of variance and standard deviation.

The interaction model elements controller of the interaction module (Fig. 5.3) control all data flow between the elements within the interaction module as well as the data flow between the process and operator modules. The element employs both combinational and sequential logic methods to carry out a number of different tasks. The bi-directional links between the interaction module elements, such as the controller and other elements of the interaction module (Fig. 5.3) make it possible to transfer codes and signals all around the joint process-operator interaction system dynamically. Codes representing information about the location of the elements are defined for the data exchange between the system elements, data types and formats identification, and function types to be carried out by each element. This element employs a signal-addressing system to address all elements of the joint process-operator interaction system and to enable/disable each element during any operation.

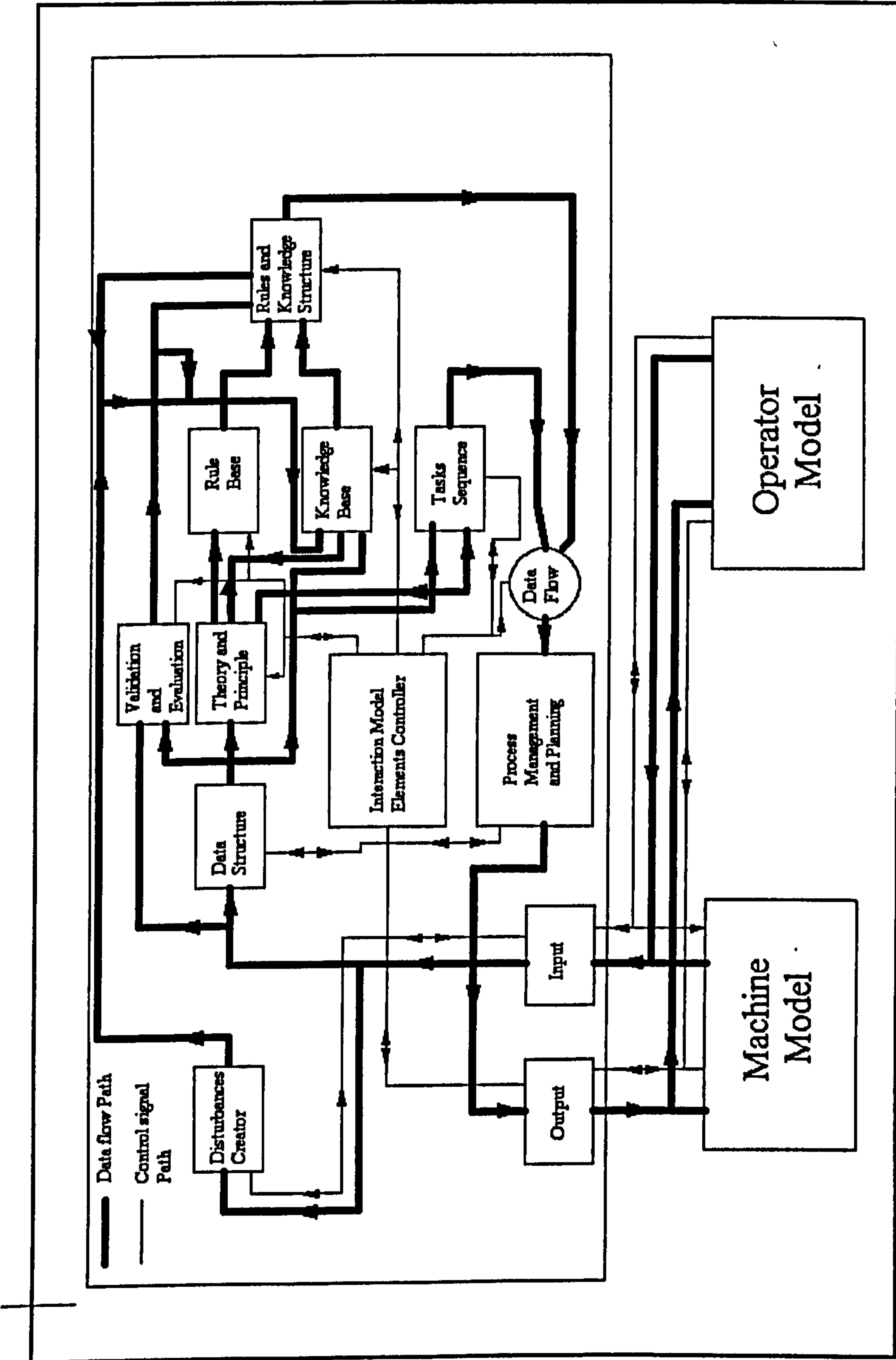


Fig 5.3. The architecture of the interaction module.

5.4 The Theory and Principle Element

The theory and principle element is depicted in Fig. 5.4. It includes various mathematical techniques required to carry out the tasks of the interaction. The mathematical techniques are used to represent the behaviour of the operational personnel and cluster process operational data, and identify the number of regions of operation. The mathematical techniques are organised as a number of computational function blocks, which are dynamically linked according to the tasks that have to be executed. For example, if data has to be classified into regions, a PCA model will be first used and then the PCA result is passed to the fuzzy *c*-means clustering block to classify the operational regions. During this process the dynamic link is established between the dynamic memory, PCA and fuzzy *c*-means clustering blocks. Similarly, if a graphical data representation is required, the dynamic link will be established between the associated including PCA, fuzzy *c*-means and fuzzy digraphs.

The element of the rule and knowledge bases also contains rules for carrying out the task of time management and dynamic reliability analysis. The rules represent a repository of structured expertise gained during continuous simulation of the joint process-operator interaction system. The disturbance creator element dynamically produces disturbances representing operator errors and external disturbances influencing the process and operator's behaviour. The element contains statistical methods such as normal distributions, which can be used to systematically generate disturbances.

A very important part of the theory and principle element is a fuzzy causal network system, which is developed for combined qualitative/quantitative simulation of the temporal behaviour of the joint process-operator interaction system. Chapters 6 and 7 will summarise the procedure of applying the fuzzy causal network as well as the mathematical methods using the directed blocks. The procedure involves processing dynamic trend signals using principal component analysis and fuzzy *c*-means clustering for the purpose of qualitative interpretation of dynamic trend signals, and sectioning the clusters for more accurate interpretation, and generation of rules for qualitative reasoning.

5.5 The Graphical User Interface (GUI) of the Interaction Module

The GUI represents a very important part of the interaction module because it is a monitoring and displaying system for all operations on the joint operator-process interaction system. Fig. 5.5 shows a screenshot of the GUI. The qualitative values of process variables

and the set points of controllers are shown at the top-left corner of the window. Below the set points are data on sampling periods in seconds, sampling counter, the number of samples in each file saved, and the number of clusters. The start and stop buttons of the simulation are at the bottom of the window. On the right hand side of the window, there are three display boxes. The top one shows the operational state spaces of the process, which are represented by the zones covered with small circles of different colours. A dark asterisk indicates the present operational location. The two smaller display boxes underneath show the variability of the variables responsible for the location of the present operation, i.e., T_{out} and CA_{out} , respectively.

Fig. 5.6 shows the operational procedure of the joint operator–process interaction simulation system and data generation. The steps can be summarised as follows:

- (1) Load the PCA module and relevant data such as mean, standard deviation and loading matrix. The PCA model is developed previously from historical data.
- (2) Initialise all parameters, variables and graphics object handlers with values at normal steady state operation. If the process is initially not at normal steady state operation, the system can be directed to return to normal operation.
- (3) Acquire all data from the process simulator and convert them to the format required for the GUI display. The data structure is also changed so that it can be easily accessed by other elements in the integrated system.
- (4) Check if new disturbances are initiated. If true, the new disturbances will be imposed onto the process system. At the same time, the counter is set to one and data recording starts. If false, the system proceeds to the next step.
- (5) Predict and display the current operational location in the PC1 and PC2 state space plane.
- (6) Determine the variables accountable for the current location of the operational region and then plot them in the appropriate boxes.
- (7) If the counter number reaches a predefined number, say ninety, the data is saved. A new disturbance can be initiated and a new cycle begins. This process can be terminated at any time by executing the stop command.

Figs. 5.7 to 5.9 show three operational scenarios of the process subjected to disturbance in cooling water inlet temperature (T_{win}), and the corresponding responses due to no operator intervention (Fig. 5.7), intervention by an inexperienced Operator A (Fig. 5.8), and intervention by an experienced Operator B (Fig. 5.9), respectively. The directed digraphs show the disturbances represented by red circles, the controlled variables represented by the green circles, and the other variables represented by dark circles. The dark arrows represent the present operational status and the relationships between variables.

In Fig. 5.7 the initial and final locations of the operational point are clearly marked. A series of dark asterisk indicate the trajectory of the process evolution when T_{win} changes and there is no intervention from operators. This casual digraph reveals that the disturbance T_{win} influences T_{out} , and T_{out} influences C_{out} , while T_{out} and F_{win} influence each other until the process reaches a new steady state after fifty-nine samples.

Fig. 5.8 shows a different path of evolution under the influence of the same T_{win} disturbance, but with the intervention of the inexperienced Operator A, who changed the set point of the feed flow (F_{in}). The operator brought the process to a steady state after fifty-six samples. The figure also shows that at some instants, Operator A was confused and uncertain about the overall conditions of the process operation. However, Operator A realised that the process had to stop at one point because it might become uncontrollable. This is indicated by the final position of the dark asterisk, which shows that if the operator had continued to intervene in the process operation, it would go beyond the normal operational region.

Figure 5.9 shows the path of the evolution under the influence of the same T_{win} disturbance, but with the intervention of the confident Operator B in the F_{in} set point. This operation reveals that the operator let the process to take control first and then intervened. This is indicated by the direction of the first two samples in the digraph. However, the above behaviour can be interpreted in different ways. Operator B might not acknowledge the change in the process operation, might be slowly to response initially, or might be intentionally not to intervene at the initial stage because of confidence and skill. The most likely answer is that the Operator B was confident because the process became steady after thirty-three samples.

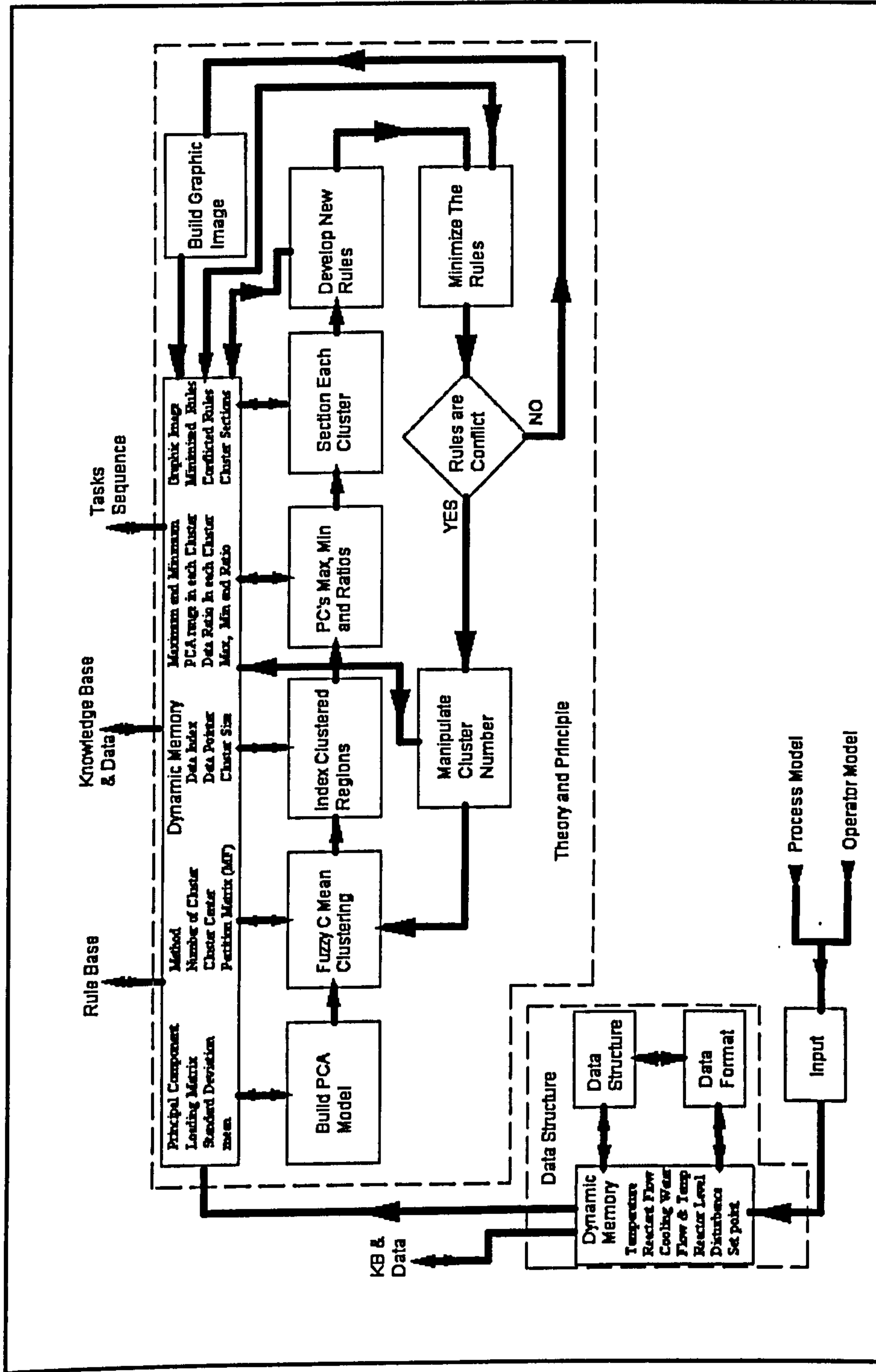


Fig 5.4. The theory and principle element.

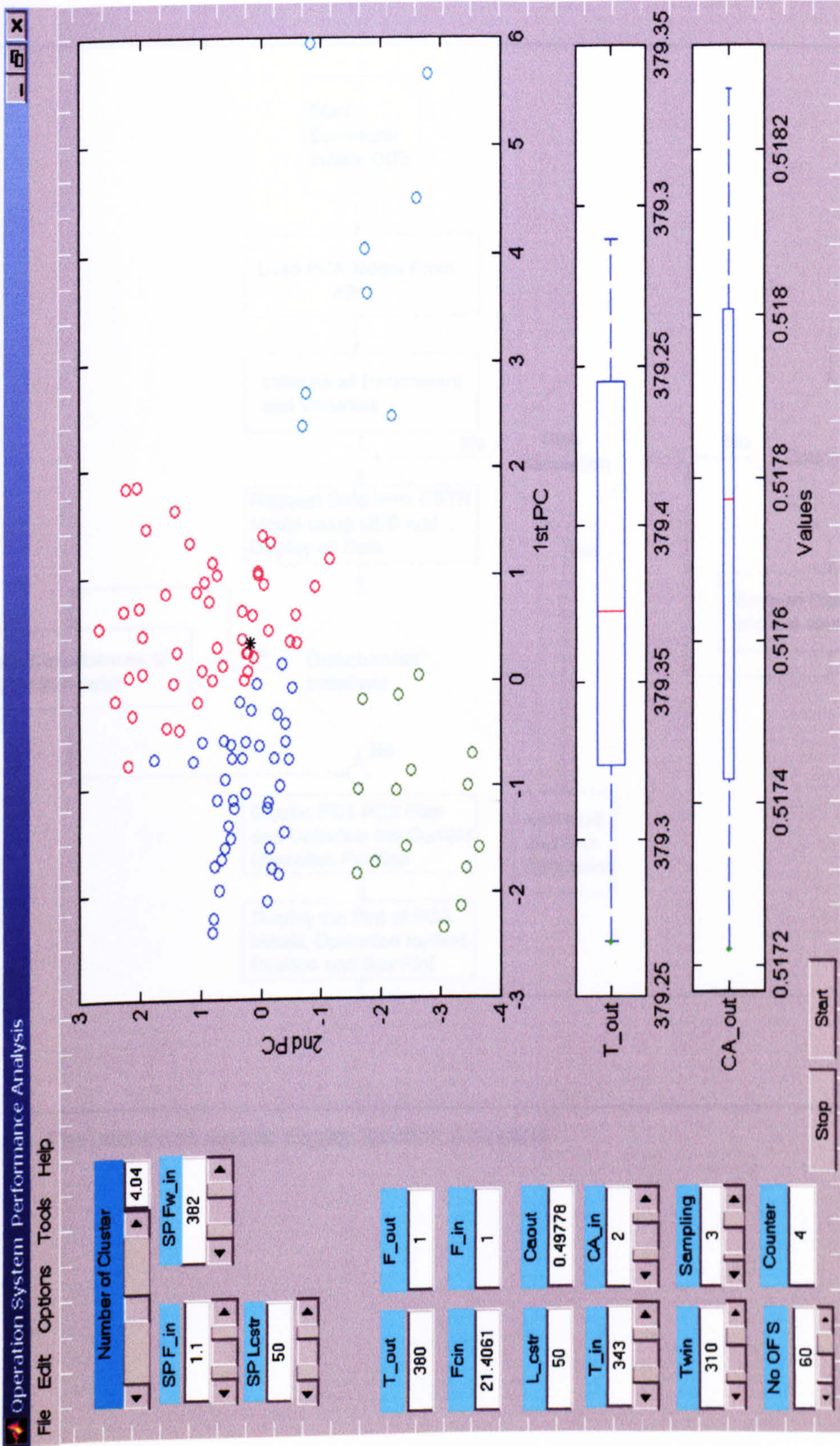


Fig 5.5. The interaction model graphical user interface.

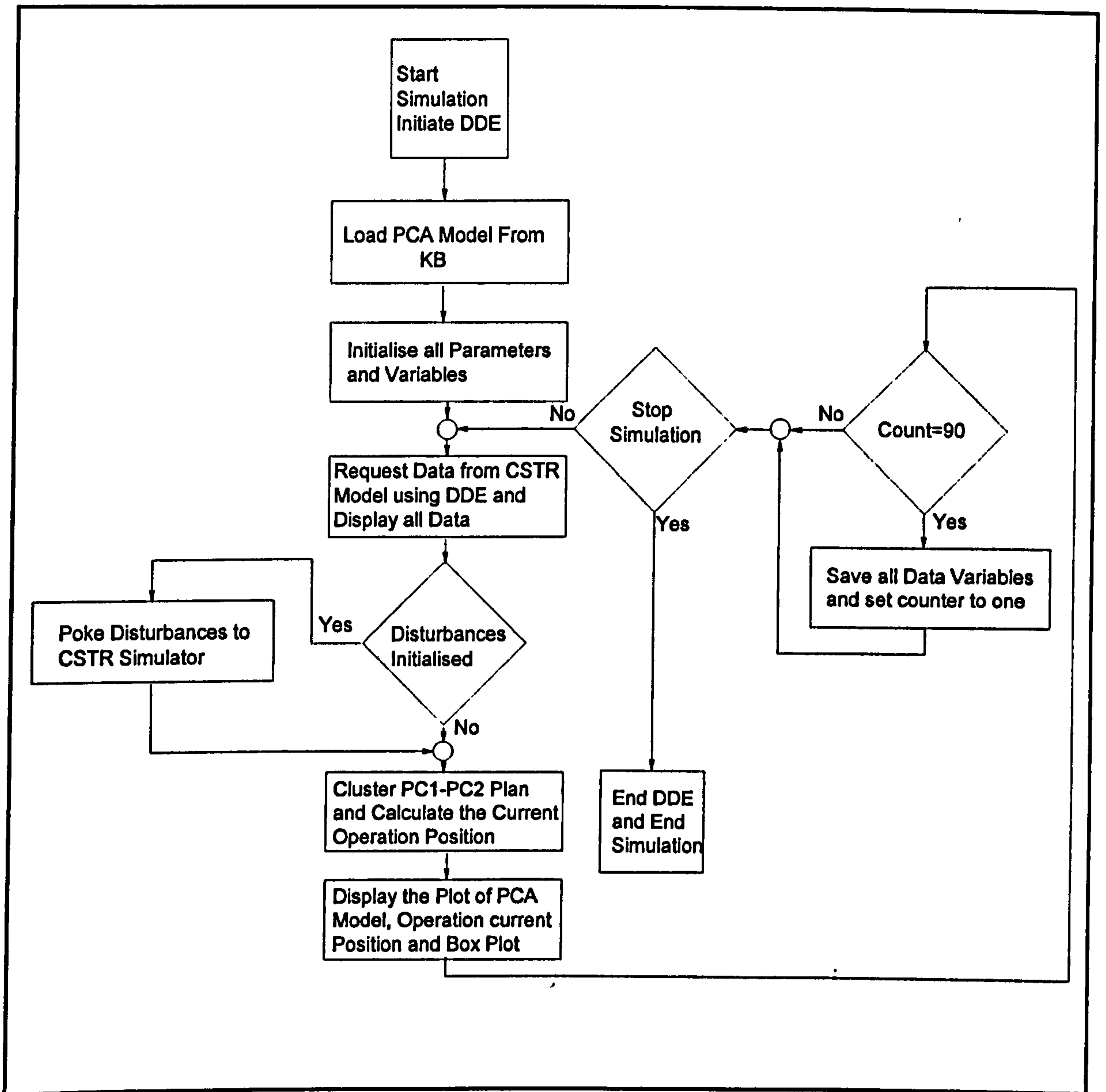


Fig. 5.6. The interaction module display function flow chart.

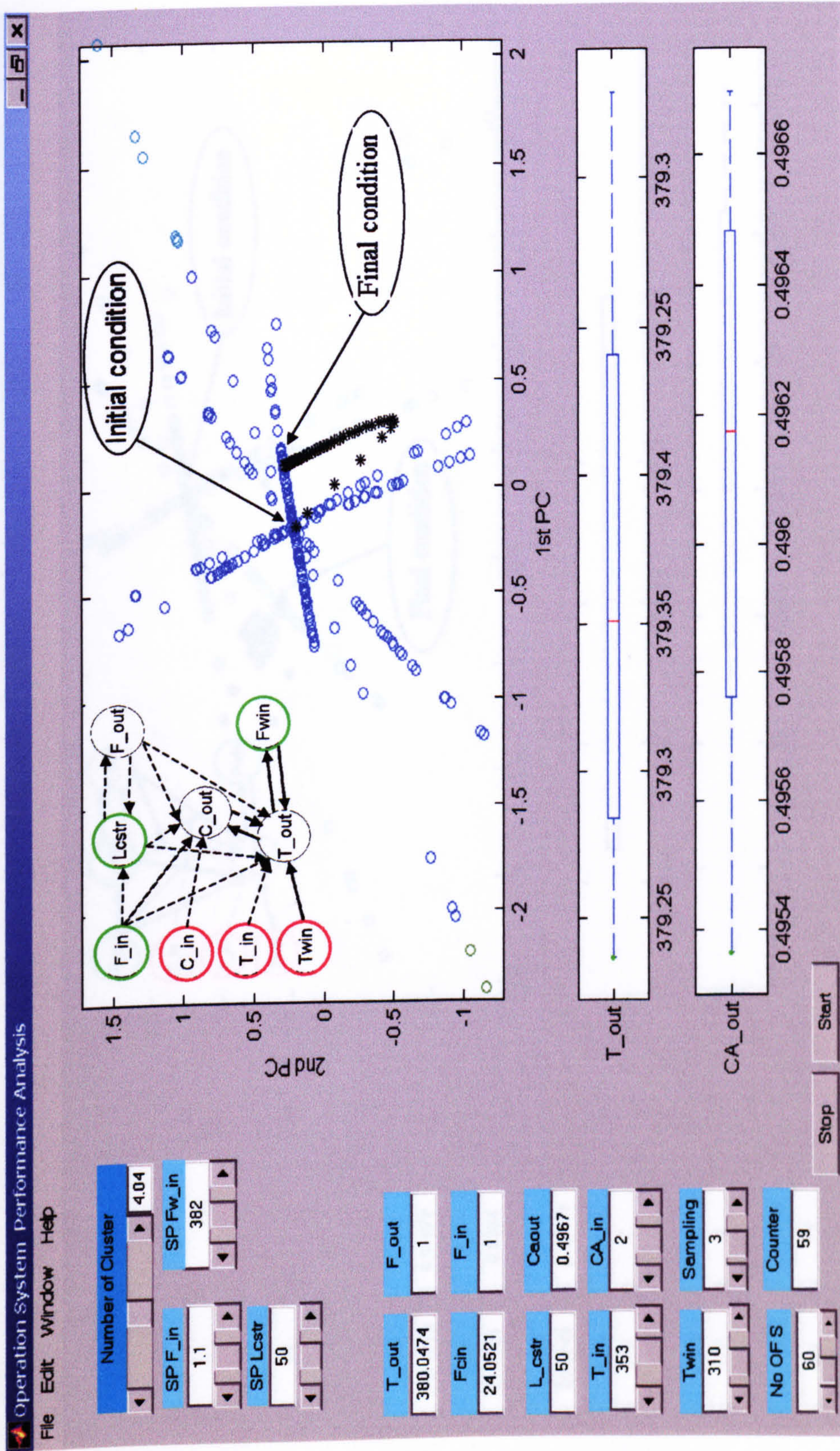


Fig. 5.7. Operation path represented by the dark asterisks (No operator intervention).

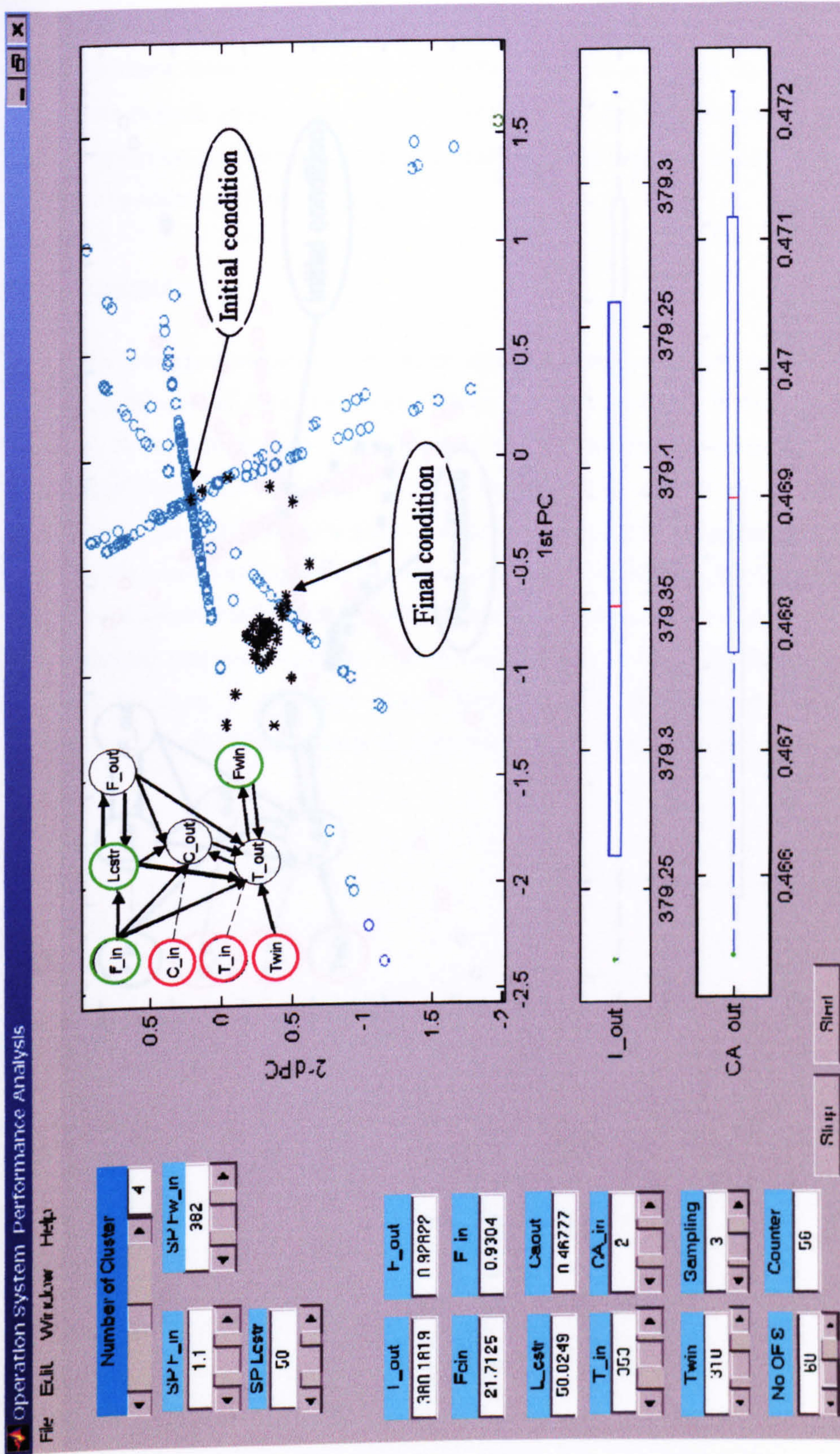


Fig. 5.8. Operation path represented by the dark asterisks (Operator A intervention).

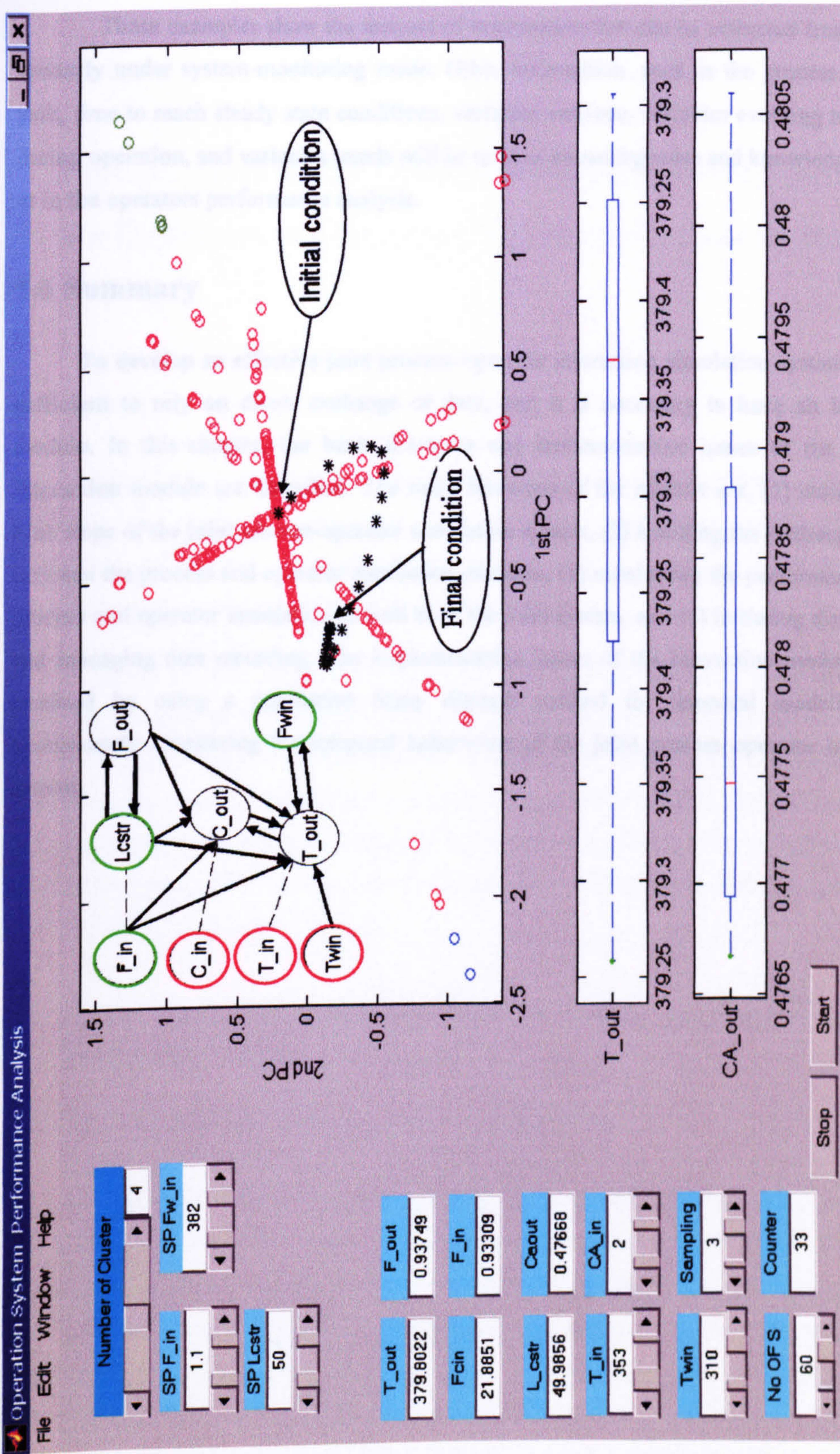


Fig. 5.9. Operation path represented by the dark asterisk (Operator B intervention).

These examples show the amount of information that can be extracted from the GUI instantly under system-monitoring mode. Other information, such as the process operation path, time to reach steady state conditions, variables variance, variables evolving trajectories during operation, and variables trends will be used in extracting rules and knowledge, as well as in the operators performance analysis.

5.6 Summary

To develop an effective joint process–operator interaction simulation system, it is not sufficient to rely on direct exchange of data, and it is necessary to have an interaction module. In this chapter, the basic functions and implementation issues of the proposed interaction module are described. The main functions of the module are, (1) managing the time steps of the joint process-operator simulation system, (2) handling the exchange of data between the process and operator simulation modules, (3) monitoring the performance of the process and operator simulation as well as of the joint system, and (4) initiating disturbances and managing data recording. The implementation issues of the interaction module can be resolved by using a qualitative fuzzy digraph method for temporal modelling, and continuously monitoring the temporal behaviours of the joint process–operator interaction system.

Chapter 6

A Digraph Method for Qualitative/ Quantitative Modelling of the Dynamics of Combined Operator-Process Systems

6.1 Introduction

Qualitative models have in recent years attracted much attention in process fault diagnosis and behaviour description. This is because qualitative models can handle incomplete information, function with incomplete data, and most importantly, provide transparent and causal explanations of systems behaviour.

In this chapter, previous work on qualitative process modelling is reviewed and a new digraph method is developed for quantitative/qualitative modelling of the temporal behaviour of joint operator-process systems. Section 6.2 provides a state-of-the-art review of qualitative reasoning for fault diagnosis using signed digraphs (SDG), and the progress on applying digraphs to model the temporal behaviour of processes. Some observations are made in Section 6.3. The proposed method is presented in Sections 6.4 and 6.5. Conclusions will be made in Section 6.6.

6.2 Signed Digraph for Process Fault Detection and Diagnosis: A Literature Review

6.2.1 The Original Signed Digraph for Fault Diagnosis

Iri et al. (1979) first proposed the idea of applying signed digraph (SDG) to process failure diagnosis. Since then, most works have been based on the modification of this idea, therefore it is useful to briefly introduce the method. A SDG graph is a network of nodes and directed arcs. A node represents a variable, and an arc indicates the cause-effect (CE) relationship of variables. A sign of either “+” or “-” is attached to each arch representing a positive or negative effect. A node takes values from a qualitative value space, such as high, low and normal. For example, Fig. 6.1 shows a buffer tank configuration and Fig. 6.2 is its schematic representation of SDG digraph.

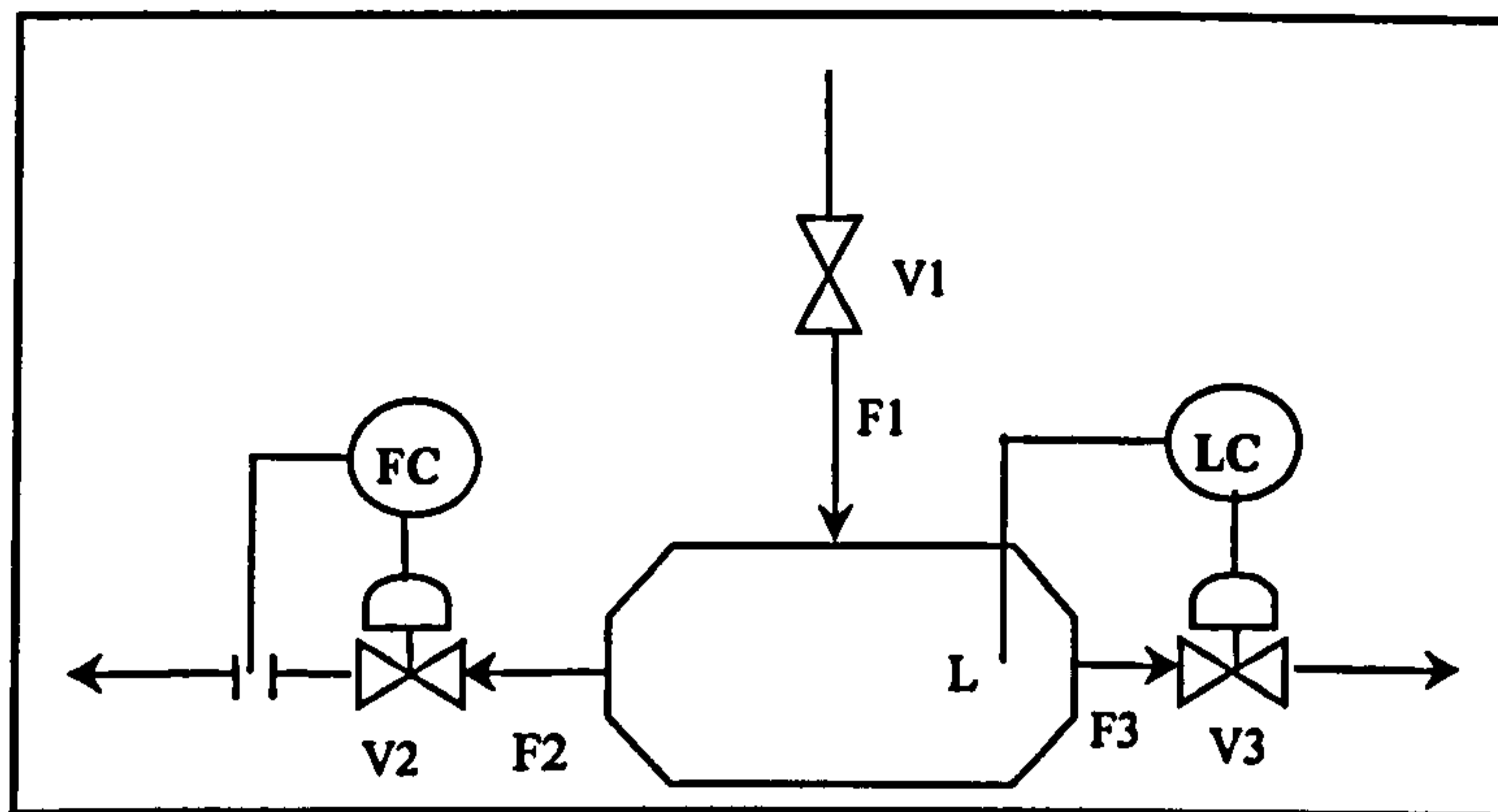


Fig. 6.1. The buffer tank (Iri et al., 1979).

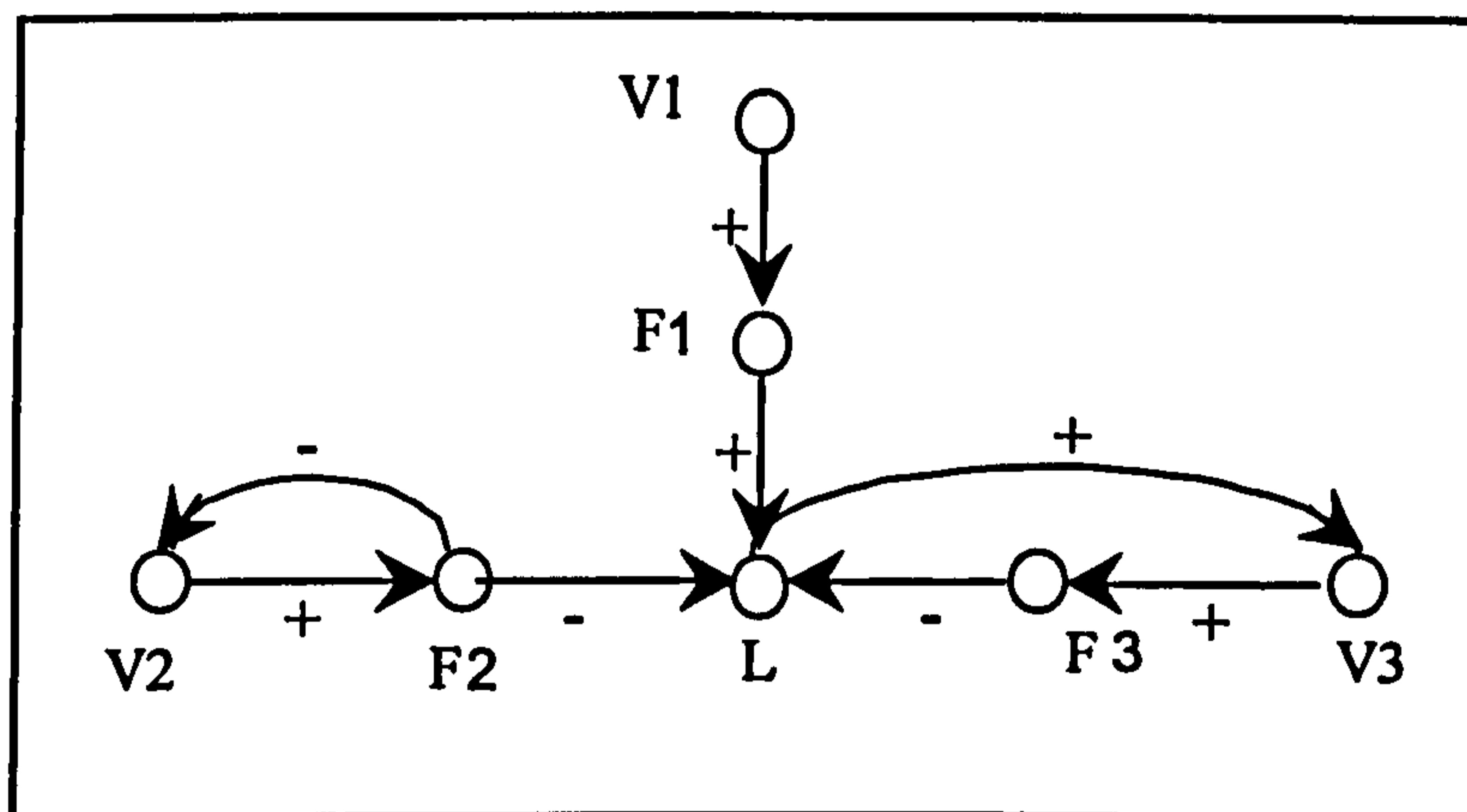


Fig. 6.2. The SDG digraph for the buffer tank (Iri et al., 1979).

Iri et al. (1979) have also developed a combined origin-searching and depth-first reasoning algorithm, specifically for the purpose of process fault diagnosis. The method can be illustrated by reference to Figs. 6.1 and 6.2, and consists of the following steps.

- (1) According to the observed variables, the original values of nodes are given in Table 6.1. In this partial pattern, F1, F2 and F3 are the values of flow, which can be observed on the monitor, and L is the controlled variable.
- (2) Assume a sign for an unknown node and expand the partial pattern by adding a sign. To judge the sign of V3, three scenarios are possible.
- (3) Decompose a quasi-CE graph for the partial pattern into strongly-connected components and determine the partial order among them, as shown in Figs. 6.3a, b, & c.
- (4) Repeat Step 2 until all nodes are determined.

Table 6.1. The original values of nodes.

F1	V1	L	V2	F2	V3	F3
0		+		-		+

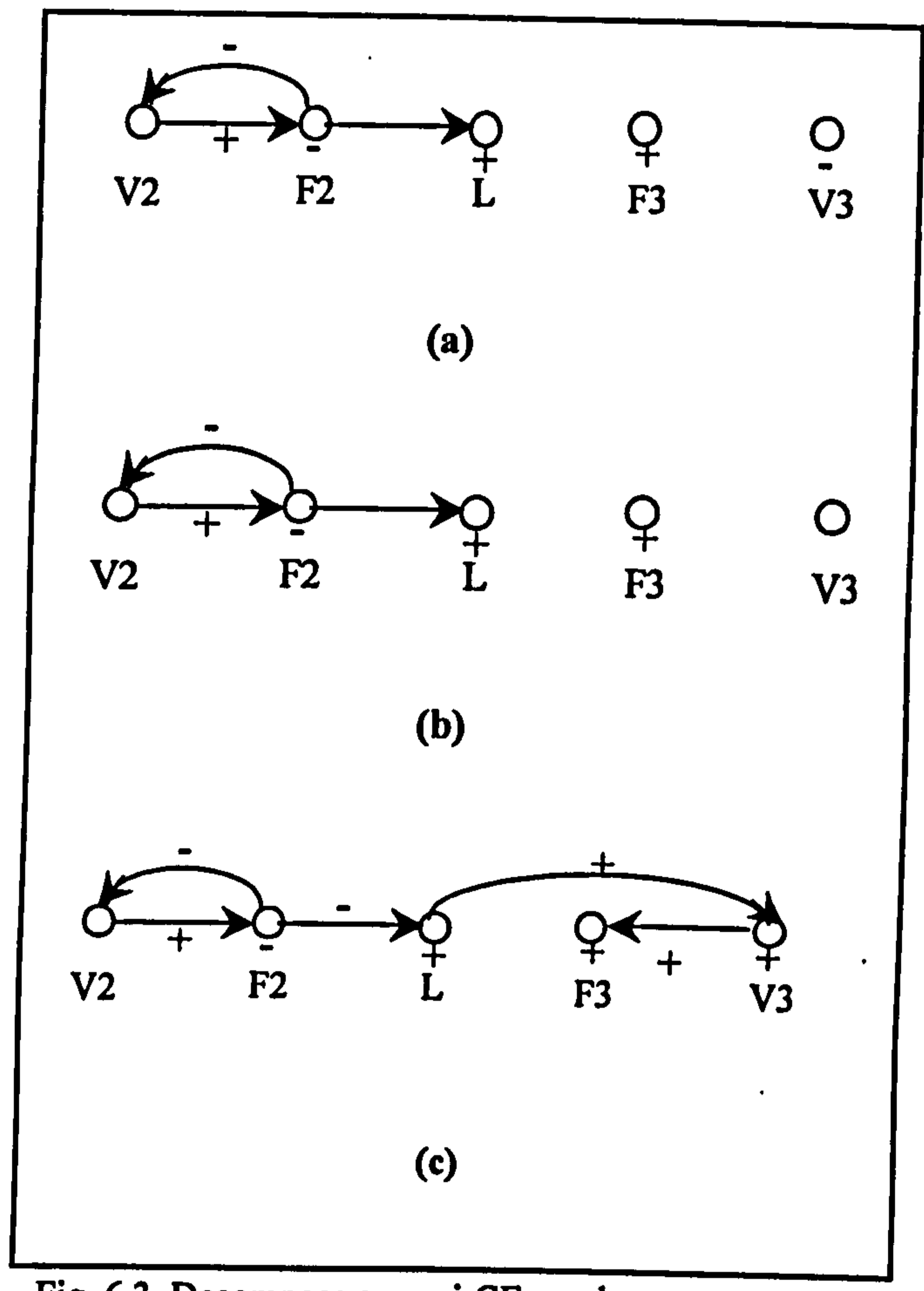


Fig. 6.3. Decompose a quasi-CE graph.

6.2.2 Development of SDG

The original SDG proposed by Iri et al. (1979) is not a very efficient method due to some limitations. Consequently, new approaches have been developed by other researchers to improve it. The limitations of the original SDG can be summarised as follows:

- (1) In the original SDG and many later versions of it, each node or variable can take values only from the value space of $(-, 0, +)$, which is clearly insufficiently precise for many reasoning tasks.
- (2) Reasoning tasks can be classified into several categories such as *fault diagnosis*, *operational supervision* and *simulation of behaviour*. The reasoning algorithm of Iri et al. (1979) is only applicable to fault diagnosis. Complications arise in the later two occasions because ambiguous solutions can occur. This can be clearly illustrated with reference to the buffer tank problem of Iri et al. (1979), as shown in Figs. 6.1 and 6.2. When FC and LC controllers are in manual status, V1 increases moderately, and V2 and V3 increase slightly, what direction will L move? From the SDG of Fig. 6.2, an ambiguous solution arises, as L is an uncertain value (i.e. the rate of change of L will be unknown). This can be seen more clearly in Fig. 6.4, where reasoning is in the direction of the arrows, when X2 is + and X3 is -.

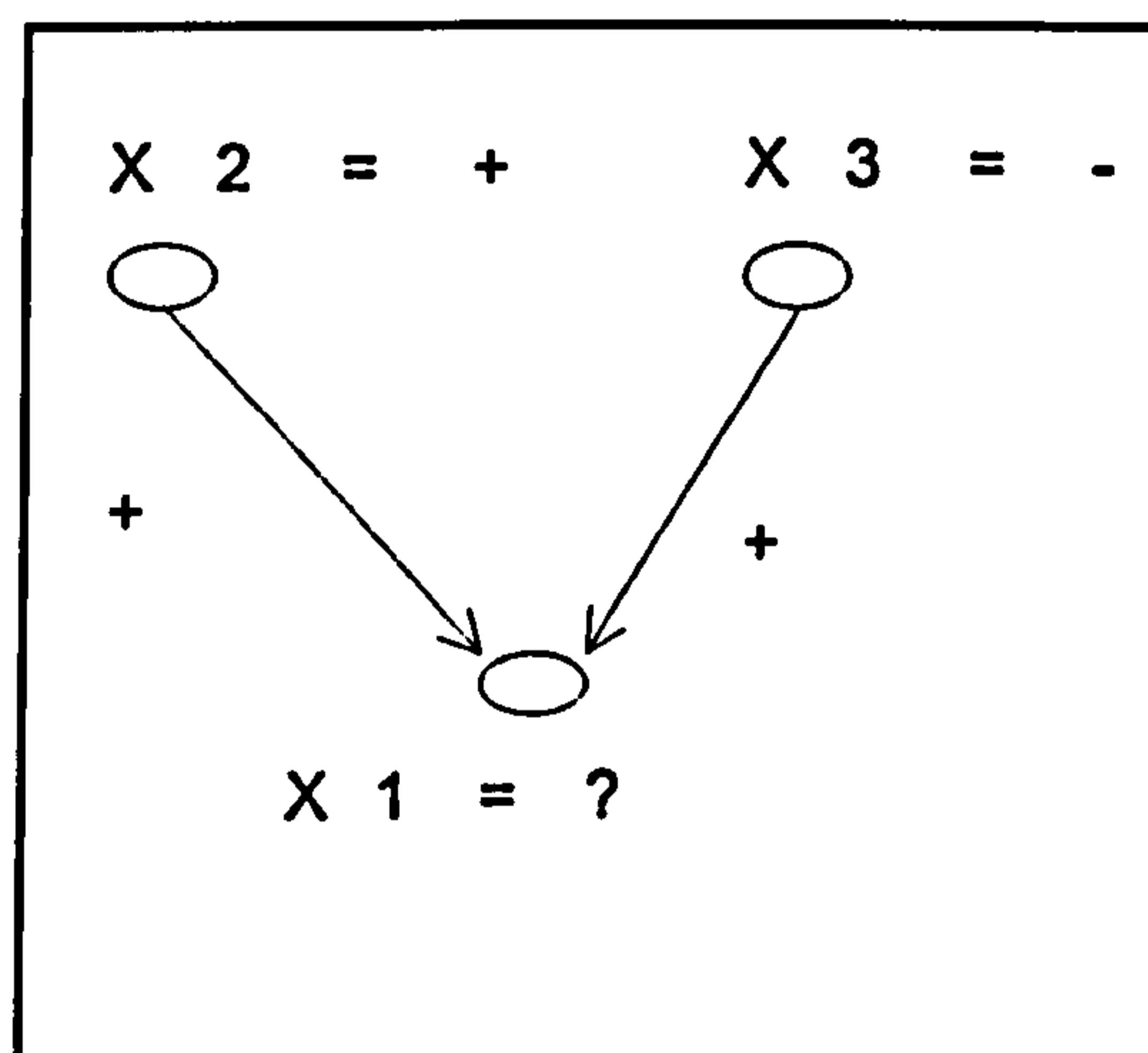


Fig. 6.4. An ambiguous solution.

- (3) While the reasoning algorithm can be computerised, the conversion of variable values to qualitative values of $+$, 0 or $-$ is a manual operation. In fact, the original SDG and many later versions of it are only suitable as an analytical tool that can

help tracing up and down the network for problem analysis. There is a clear need to convert numerical data into qualitative expressions automatically.

- (4) Most SDG models are unable to deal simultaneously with the uncertainty in data and in reasoning.
- (5) The original SDG and many later versions are not capable in handling interacting and recycle nodes, which arise due to control loops, recycle streams and inherent interaction of variables in processes.
- (6) The original and many later versions of SDG are only applicable to steady state processes. Some SDG extension methods have been proposed to deal with dynamics, but most are still not satisfactory.
- (7) In practice, drawing the digraph can be a very daunting task, particularly when the process is complex and interactions between variables are strong but only partially unknown. Most previous studies on SDG have also overlooked this issue.

Despite the aforementioned limitations, SDG has still attracted considerable attention because it can handle incomplete models, functions with incomplete data, and most importantly, provide transparent and causal explanations to systems behaviour and make complex systems traceable. In fact, these limitations also provide the room for many continuous improvements.

6.2.3 The Extended SDG

Oyeleye and Kramer (1989) and Rose (1990) presented an Extended Signed Directed Graph (ESDG) for malfunction diagnosis in continuous processes. In an ESDG, certain non-physical feed forward paths can be included in the network that can explain inverse response and compensatory response in negative feedback loops. To develop an ESDG, quantitative models need to be converted to qualitative expressions. The ESDG method can only be applicable to processes at steady state.

Ouassir and Melin (1997) have improved the ESDG method further by including all possible fault origins to the ESDG, which originally only represents the cause-effect relationships of variables. An example is represented in Fig. 6.5 and Eqns. (6.1) to (6.3).

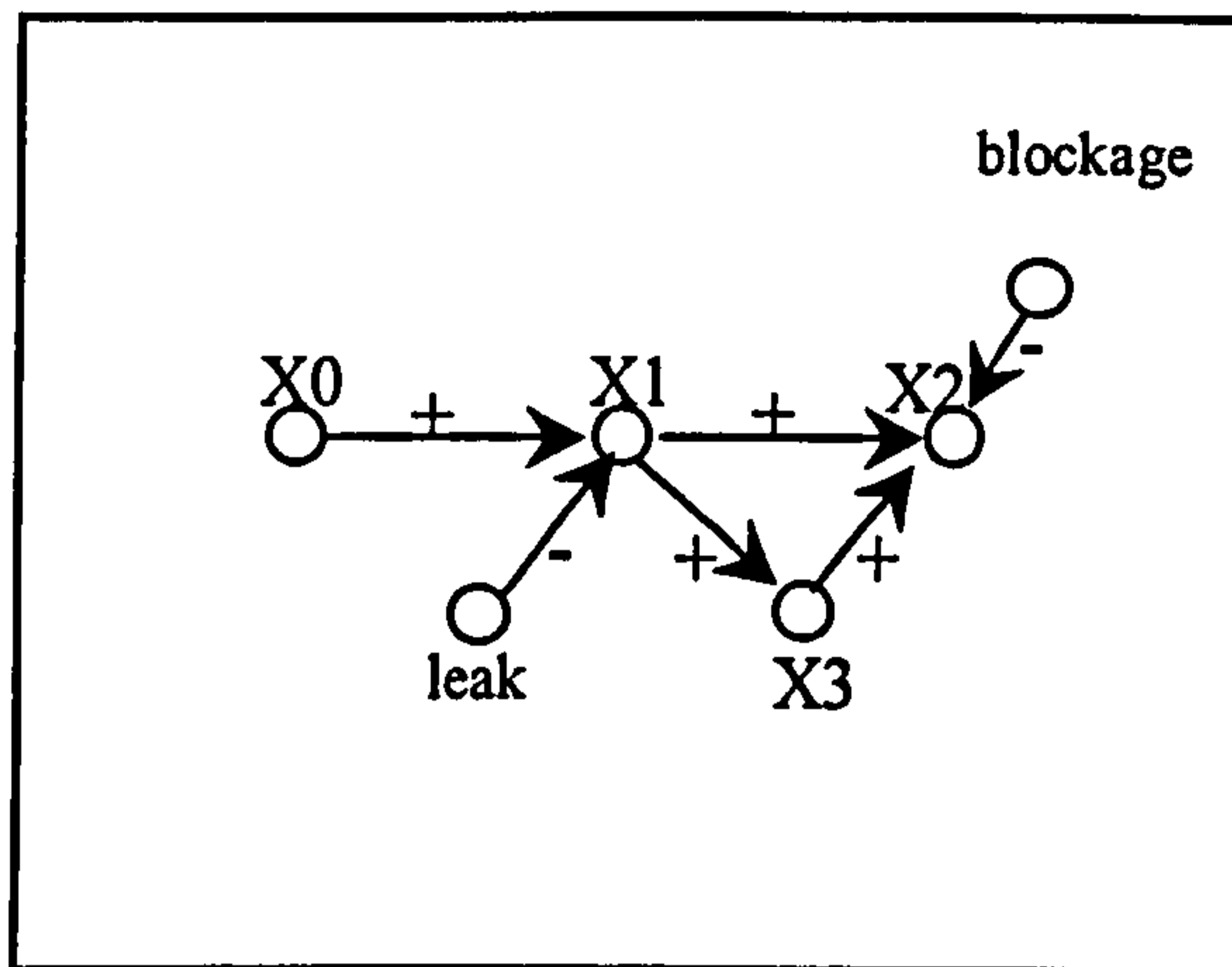


Fig. 6.5. SDG with nodes representing faults.

$$[x1] = -[x2] + [x0] - [leak] \quad (6.1)$$

$$[x2] = [x1] + [x3] - [blockage] \quad (6.2)$$

$$[x3] = [x1] \quad (6.3)$$

6.2.4 Possible Cause – Effect Diagrams

Wilcox and Himmelblau (1994) developed the possible cause–effect graph (PCEG) method. The main difference of PCEG from SDG is that in PCEG a node represents an event, instead of a variable. Fig. 6.6 shows a simple example, which indicates a set of abnormal statements, such as T1 being H (high) and L (low), and T1 reading being H (high) and L (low). A causal description for Fig. 6.6 is that T1 reading being H can cause T1 being H (other factors can also cause T1 being H, T1 Reading being H is just one of the possible factors leading to T1 being H). It seems that the major drawback of the PCED method is that the digraph is often very congested and complex, because each variable can be expanded into a number of nodes. In comparison, a SDG digraph is simpler and more readable.

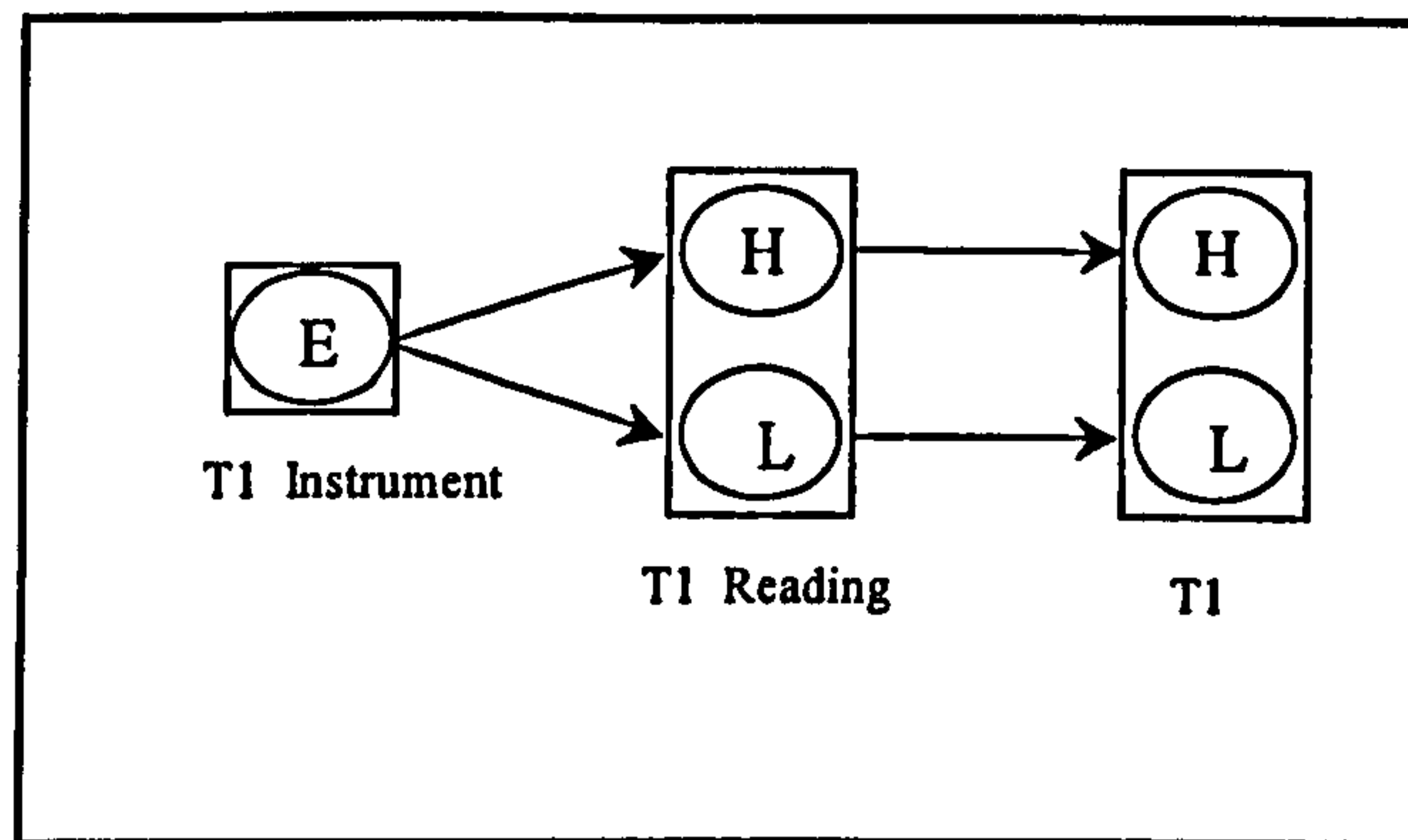


Fig. 6.6. A simple example of part of a PCED.

6.2.5 Fuzzy SDG

Yu and Lee (1991) have indicated that (+, 0 and -) are not sufficient in describing the relationship between two connected nodes and therefore introduced fuzzy membership functions into the branches so that the qualitative and quantitative reasoning can be combined. However, no such improvement has been made for the nodes. Gujima et al. (1993) introduced more than three values in the nodes in order to improve the accuracy in fault diagnosis, though fuzzy concepts were not used. The application of fuzzy concepts by Han et al. (1994) and Shih and Lee (1995) only have enabled the input nodes to convert numerical data to qualitative expression but the graph as a whole, is still a crisp one. Wang et al., (1995) have developed the most comprehensive method of fuzzy digraph, which takes the crisp SDG as a specific instance but it has far more features to overcome many of the limitations of a crisp SDG.

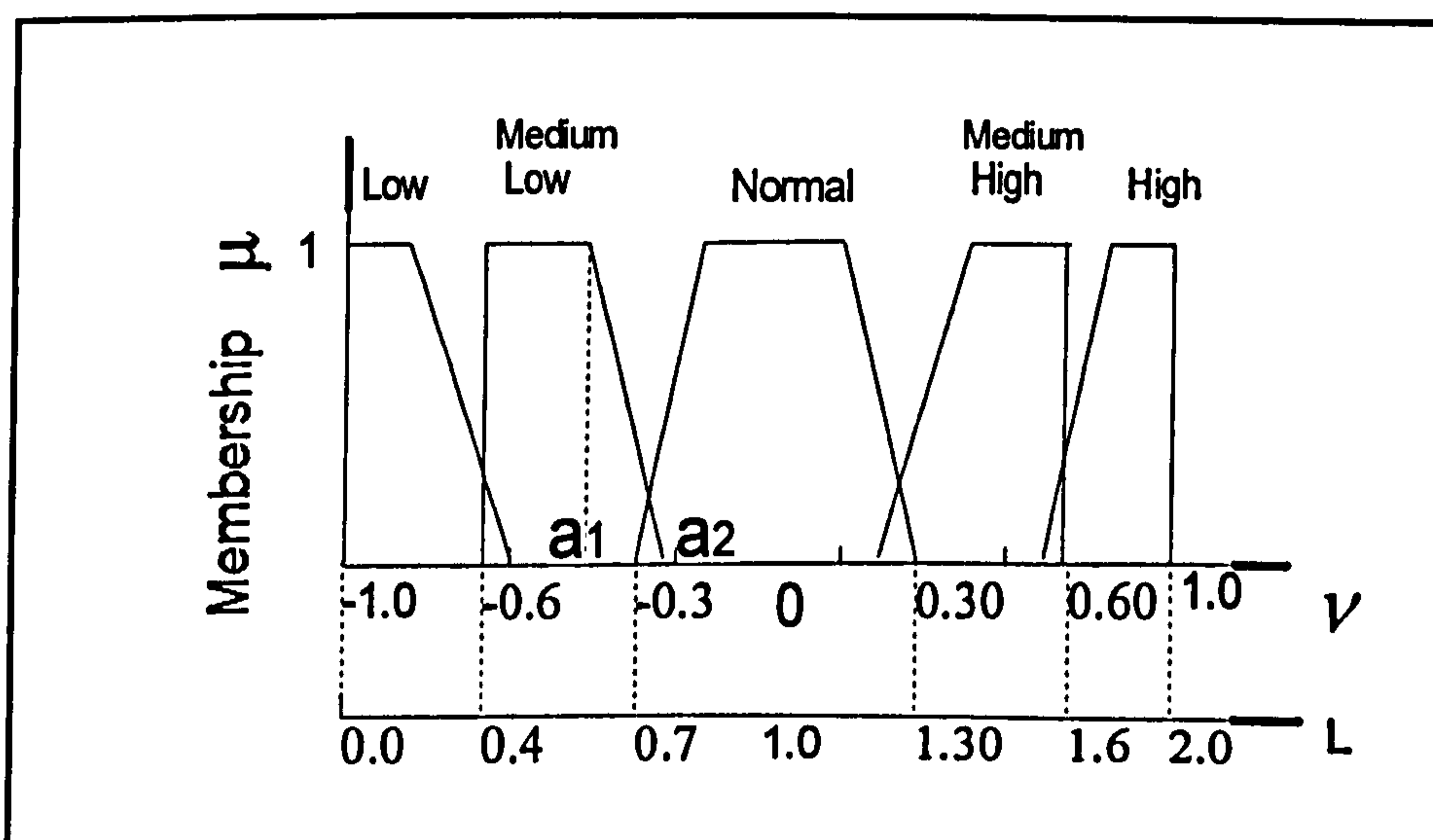


Fig 6.7. An example of the fuzzy value space definition of a fuzzy variable (Wang et al., 1995).

Each node in a fuzzy-SDG is represented by a fuzzy variable. An example of the value space of a node is shown in Fig. 6.7. The number of fuzzy values covered by the fuzzy value space is determined by the problem requirement. It is worth noting that the method is not restricted to a three values pattern (-, 0, +). Every legal value of a node variable, such as high or medium high shown in Fig. 6.7 is a fuzzy set \bar{m} defined by Eqn. (6.4). In Eqn. (6.4), x is an element of M and μ is the membership function. M is therefore, represented by its membership function, μ , such that the value of μ illustrates the degree of membership of the element x belonging to M . Whether a value of x belongs to M depends on both the value of μ and the λ cut-value of M . The membership function, may take various shapes but the most common is the triangular and trapezoidal representation. Fig. 6.7 is a half-decline trapezoidal form. For the medium low in this figure, the membership value is calculated by Eqn. (6.5).

$$M = \{x, \mu\}, \quad \mu = [0,1] \quad (6.4)$$

$$m = \begin{cases} 1 & 0.6 \leq v < a_1 \\ \frac{a_2 - v}{a_2 - a_1} & a_1 \leq v \leq a_2 \\ 0 & v > a \text{ or } v < 0.6 \end{cases} \quad (6.5)$$

$$e(x_{j+1} \rightarrow x_j) = S_{j,j+1} \frac{R_{x_{j+1}}}{R_{x_j}} \quad (6.6)$$

$$S_{j,j+1} = \frac{\partial x_j}{\partial x_{j+1}} \quad (6.7)$$

$$S_{j,j+1} = \frac{\partial(dx_j/dt)}{\partial x_{j+1}} \quad (6.8)$$

A branch in a fuzzy digraph is defined by the direction of the arrow and the effect strength. Suppose that x_{j+1} and x_j are two nodes linked by a branch directed from x_{j+1} to x_j , then the effect strength of x_{j+1} on x_j is determined by Eqn. (6.6), in which $R_{x_{j+1}}$ and R_{x_j} are the operational range of node x_{j+1} and x_j , respectively, and $S_{j,j+1}$ is the sensitivity of x_j to x_{j+1} , determined by Eqn. (6.7). The operational range for a node consists of positive and negative ranges, corresponding to fuzzy values, v in the range $[0, 1]$ and $[-1, 0]$. Obviously, the larger the value of $e(x_{j+1} \rightarrow x_j)$, the stronger the effect of x_{j+1} on x_j . If the relationship

uses a time derivative to account for the dynamics, this can be approximated using a backward difference. The sensitivity will be derived from the partial derivative estimated using the partial differential operator, with respect to the rate of change of the quantity as shown by Eqn. (6.8). In many situations the relationship between x_{j+1} and x_j is non-linear, while the partial derivatives are estimated by linear approximations.

Since the publication of the method (Wang et al. 1995), it has further evolved over the years (Wang et al., 1996a, 1996b, 1997; Huang and Wang, 1999). The advantages are that this approach generates fewer ambiguous solutions. It can provide a more precise description of the variables than (-, 0 +), and produce a causal explanation. In particular, it allows reasoning in both arrow to and arrow from directions so that it can be used for different reasoning tasks, such as single and multiple fault diagnosis, operational supervision and simulation of operations.

6.2.6 Digraphs for Modelling Dynamic Behaviour

Most studies on SDG have focused on processes at steady state. In applying SDG to modelling dynamic behaviour of a process, it is recognised that the most critical issue is to find a way to qualitatively represent a segment or a window of a dynamic trend (Fig. 6.8).

In the early work of expert systems such as G2 (Moore and Kramer, 1986), simple descriptors were employed to describe dynamic trends, such as temperature *increase* or *decrease*. Later, other approaches were proposed for qualitative interpretation including the threshold value method (Lee et al., 1999), the episodes (Cheung and Stephanopoulos, 1990a, 1990b; Bakshi and Stephanopoulos, 1994a, 1994b; Janusz and Venkatasubramanian, 1991) and the principal component analysis (Li and Wang, 2001). Fig. 6.9 illustrates the threshold method. Clearly, it is a relatively simple method but important information can be missing.

Janusz and Venkatasubramanian (1991) used nine primitives to represent any plots of a function. The method was further evolved to seven episodes as shown in Fig. 6.10. A dynamic trend of a variable in a windowed time scale is a series of episodes when grouped together so that they can capture the feature of the trend. Cheung and Stephanopoulos (1990a, 1990b) developed a similar approach, which makes use of seven primitive triangles to describe a trend.

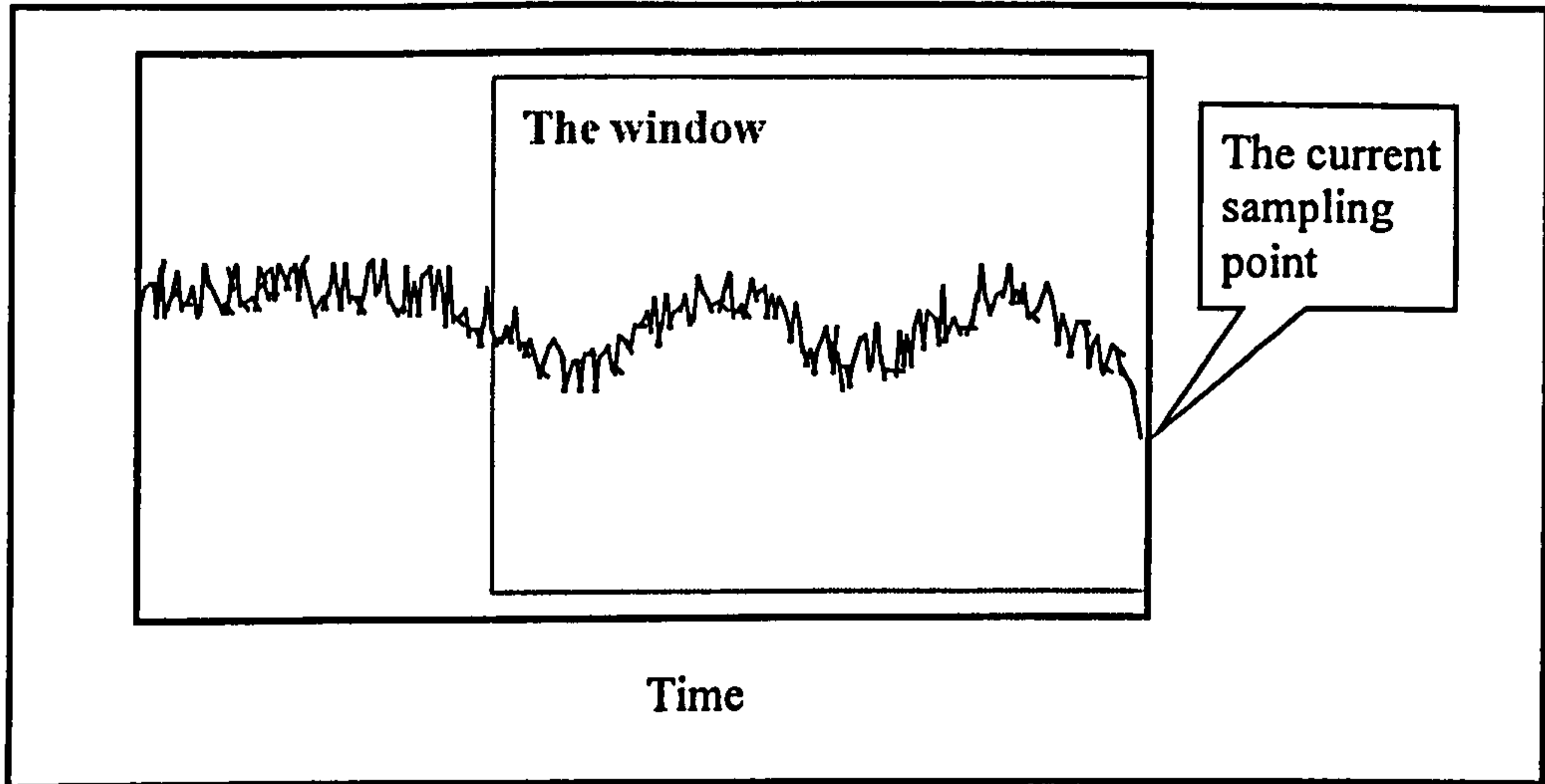


Fig. 6.8. The temporal behaviour (i.e., trend) of a variable in a window time scale.

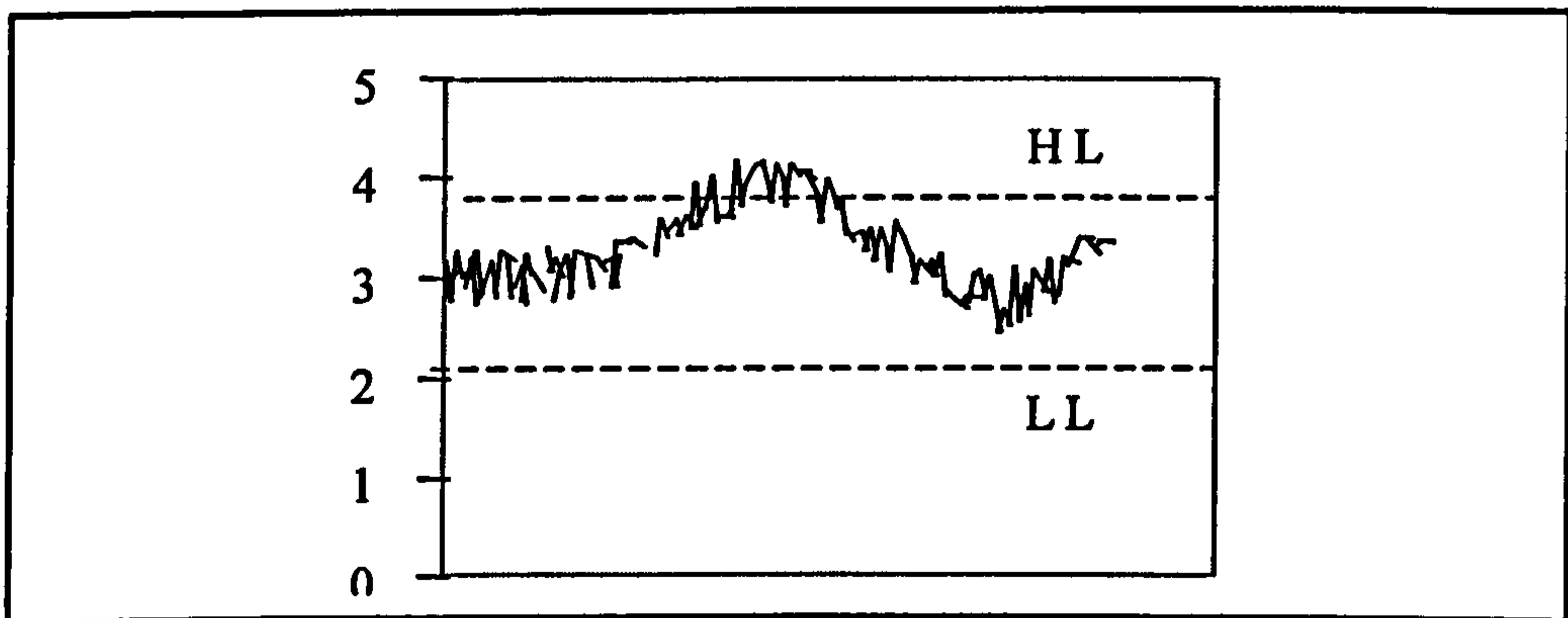


Fig. 6.9. Illustration of threshold method for qualitative interpretation of dynamic trends. HL – high limit, LL – low limit.

These original episode based methods suffer from being weak in dealing with the adverse effect of noises. As a result, Bakshi and Stephanopoulos (1994a,b) further developed the triangular approach by introducing the wavelets based multi-scale signal analysis technique. Wavelets multi-scale analysis is able to eliminate the noise components, and at the same time, automatically identify the inflection points of a trend signal. An inflection point is considered as the connection of two episodes. For example, the three trends in Fig. 6.11 can be converted to:

$$x_1 = [B \ CD \ A \ D \ AB \ C]$$

$$x_2 = [B \ CD \ AB \ CD \ AB \ C]$$

$$x_3 = [B \ CD \ A \ D \ AB \ C]$$

(6.9)

In addition, the discrimination and clustering of trends is not straightforward. The triangular episode representation is further used to develop inductive rules for product quality monitoring. An example of such rules is “if the trend follows {... AB CD A D AB ...}, the batch run is likely to be bad”, where AB, CD, A, D and AB are different episodes. It is clear that the level of cognition of such a description is still not very high. Furthermore, the episode method has never been applied to SDG.

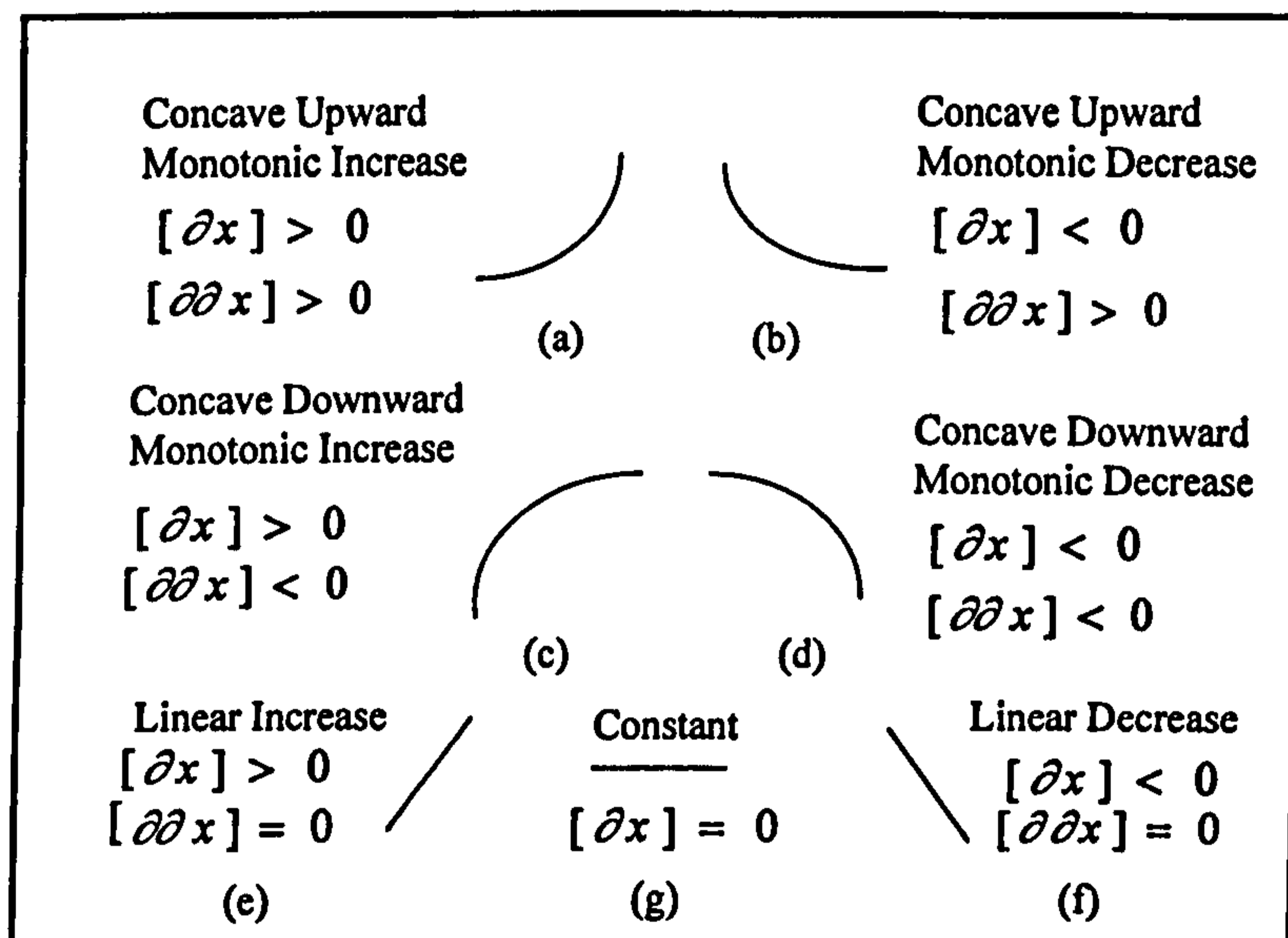


Fig. 6.10 The seven episodes.

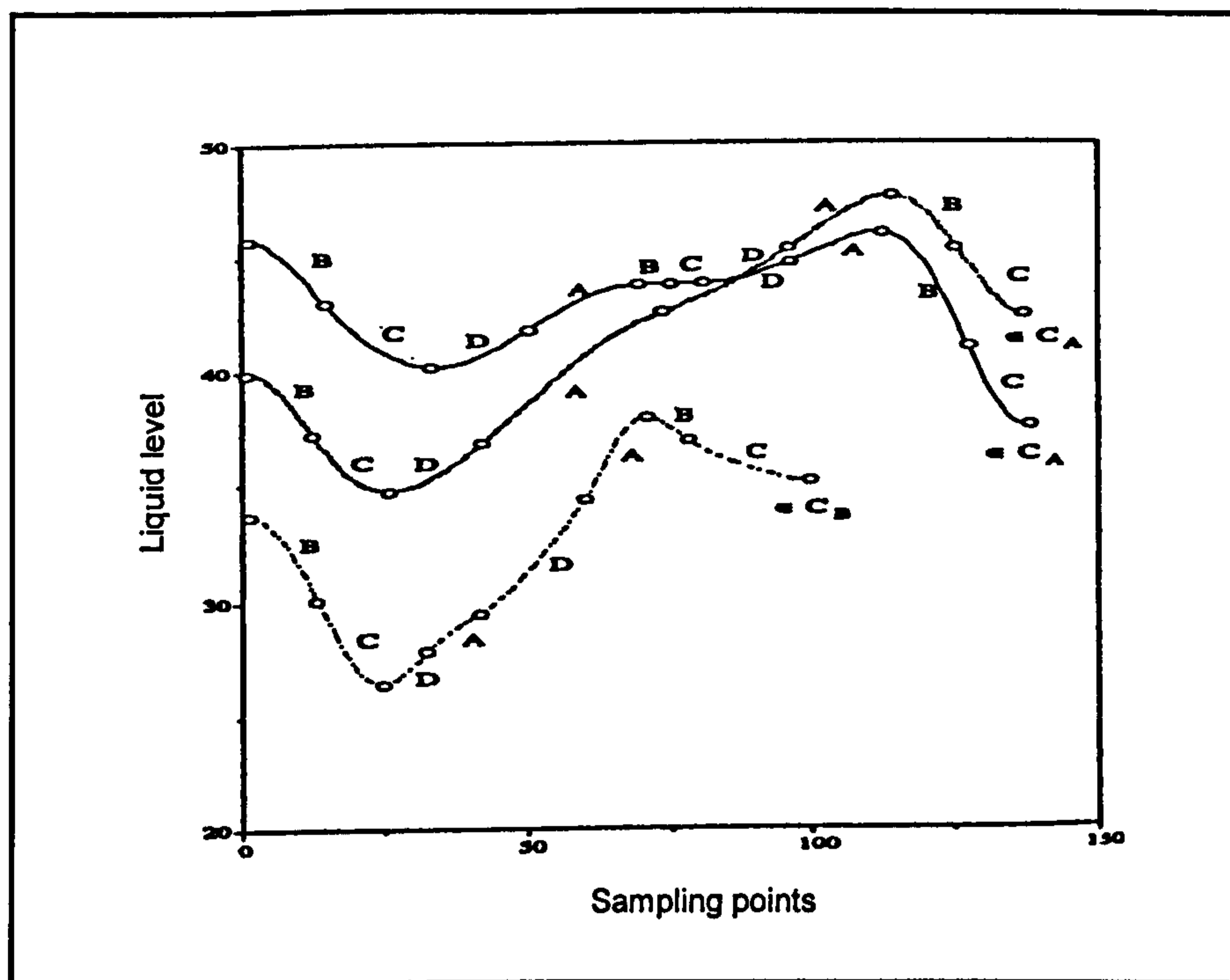


Fig. 6.11 Three trends and their episodes.

Li and Wang (2001) developed a fuzzy clustered method for qualitative modelling of process temporal behaviour. A new method for qualitative interpretation of dynamic trends was also proposed, which was based on PCA. The method can be illustrated using Fig. 6.12.

The 75 process variable trends in a wide time scale of a size of 80 sampling points is used to form a matrix of 75×80 . The method involves processing the data matrix using principal component analysis (PCA). Plotting the first two principal components gives three clusters, i.e., A, B and C (Fig. 6.12). Similarly, for the variable L, the dynamic trends are also grouped into three clusters, i.e. D, E and F in the PC1-PC2 plan. Rules can be easily generated for this simple case,

IF $F_i = A$ THEN $L = D$

IF $F_i = B$ THEN $L = E$

IF $F_i = C$ THEN $L = F$

Comparing to previous methods, the approach of Li and Wang (2001) allows simple but rigorous qualitative/quantitative representation of the temporal trends of individual variables.

In addition to the qualitative representation of dynamic trend signals, another challenge to qualitative dynamic simulation of process temporal behaviour is how to perform

reasoning when there are interacting and recycle nodes in a digraph. Wang and Li (2001) have solved the problem using a concept of the node clusters, i.e., to treat a cluster of interacting or/and recycle nodes as a single node in the reasoning. This can be illustrated using Fig. 6.13 and Table 6.2. As an example, the reasoning rules generated from the digraph of Fig. 6.13 and the data set 1 of Table 6.2 are

IF $X_1=A$ and $X_6=A$ THEN ($X_2=B$ and $X_3=A$ and $X_4=C$)

IF $X_2 = B$ THEN $X_3 = C$

Li and Wang (2001) also introduced fuzzy concept to the fuzzy digraph so that it can be used for combined qualitative/quantitative temporal reasoning.

Table 6.2 An Example Data Collection for Illustrating the Reasoning Mechanism.

Data case	X_1	X_2	X_3	X_4	X_5	X_6
1	A	B	A	C	C	A
2	B	A	B	B	A	C
3	C	C	C	A	B	B

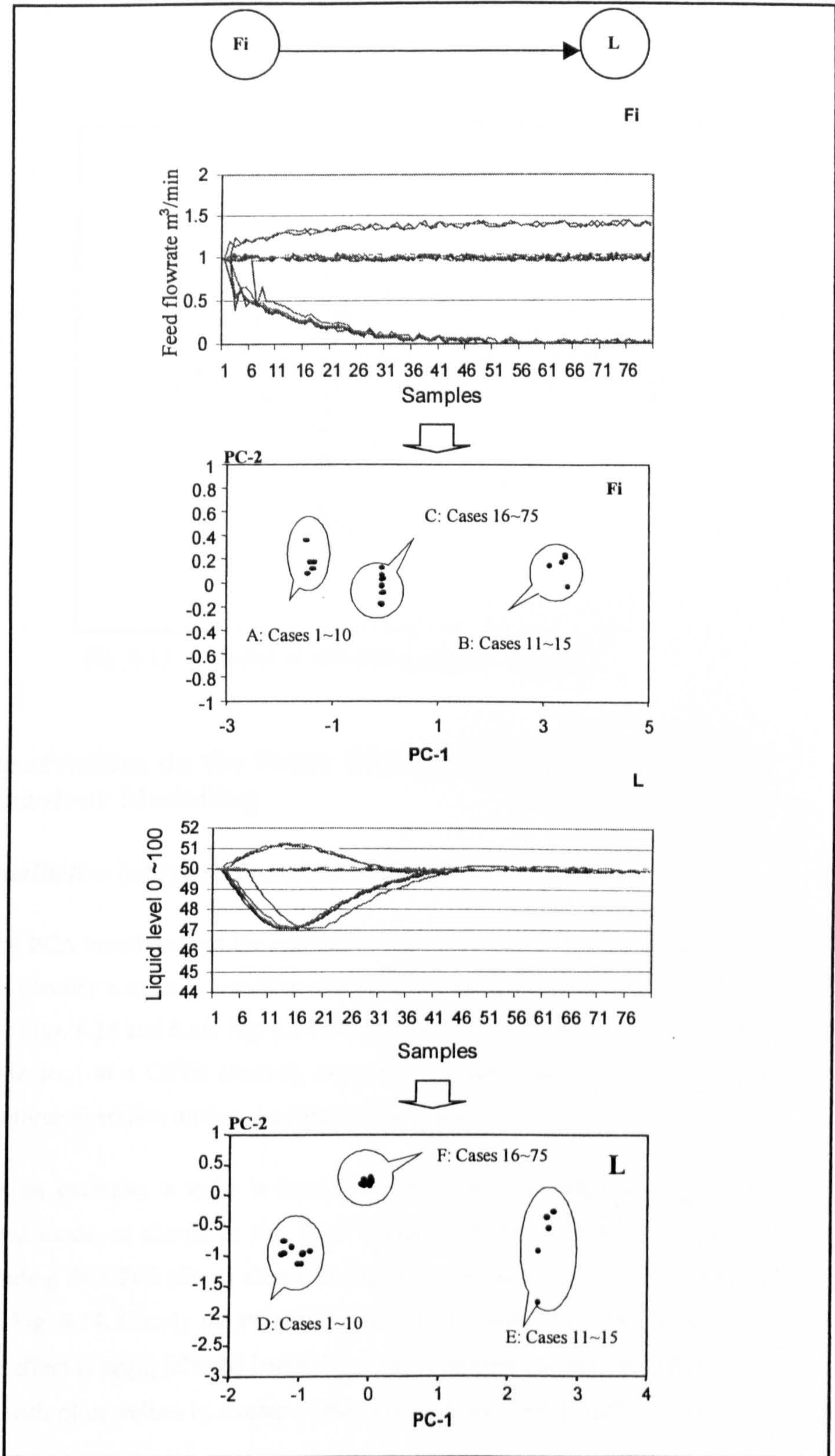


Fig 6.12. Categorical characterisation of dynamic trends using PCA.

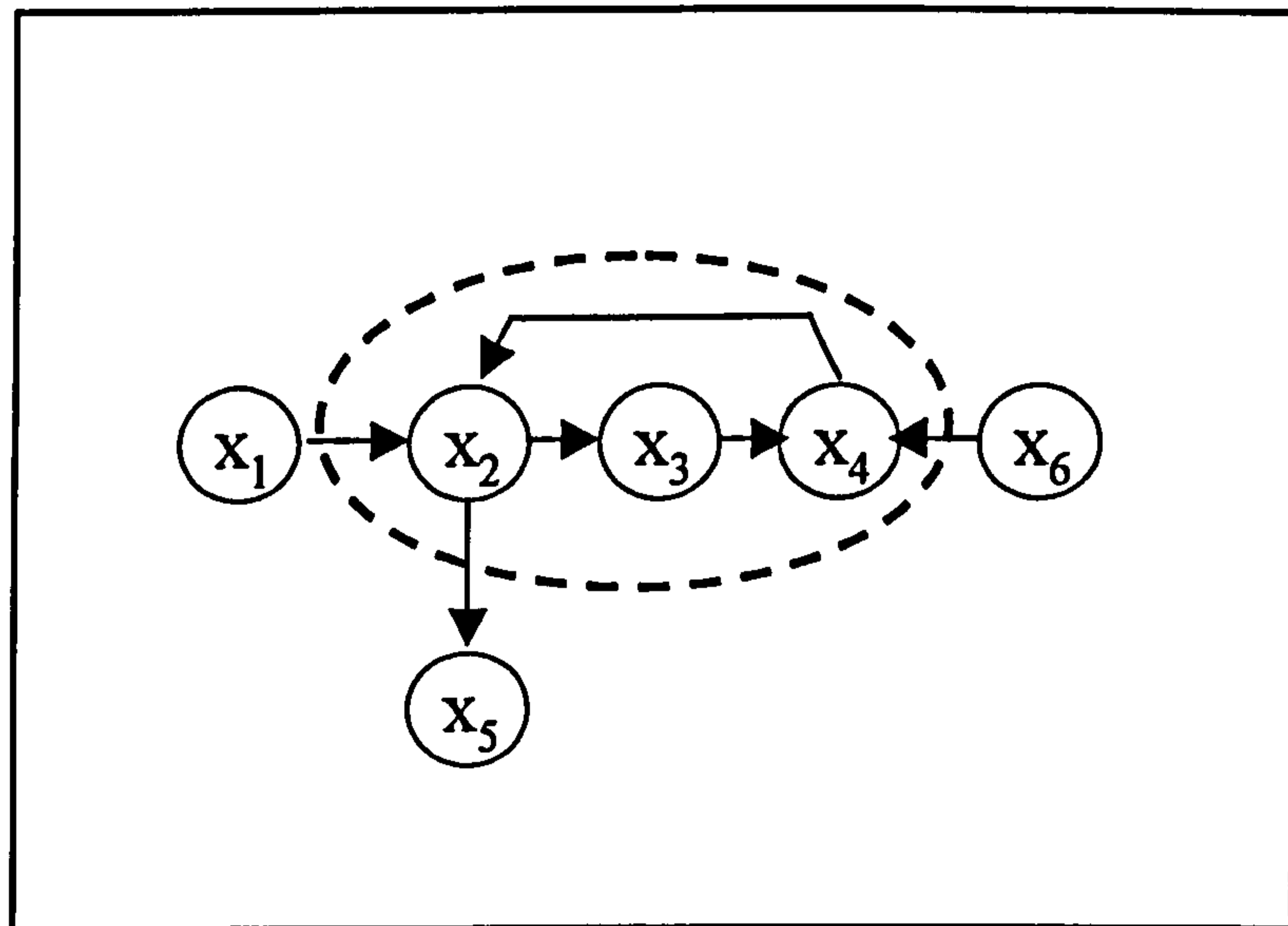


Fig. 6.13. A cluster of interacting and recycle nodes.

6.3 Observations on the Fuzzy Digraph Method for Temporal Behaviour Modelling

6.3.1 Qualitative Interpretation of Dynamic Trends

The PCA based method for qualitative interpretation of dynamic trends is found to be unable to identify a spike or a sudden change in the dynamic trend. This can be shown with the aid of Figs. 6.14 and 6.15. Fig. 6.14 shows 75 dynamic trend cases of a variable (the flow rate of the feed to a CSTR reactor), each with 80 sampling points. These trends clearly represent three operation modes, denoted by b, c and a.

As an example, a spike is introduced into one case (data case no. 25) of the c operational mode, as shown in Fig. 6.14. Using the method of Li and Wang (2001), the corresponding PC1-PC2 plot is shown in Fig. 6.15. Clusters b, c, and a, correspond to b, c and a, in Fig. 6.14. Clearly the PC1-PC2 plot does not show any trace of the spike because the spike affect is negligible and buried by other values affects. The spike sample is grouped together with other values in cluster c (the spike sample is represented as red colour in the green cluster c).

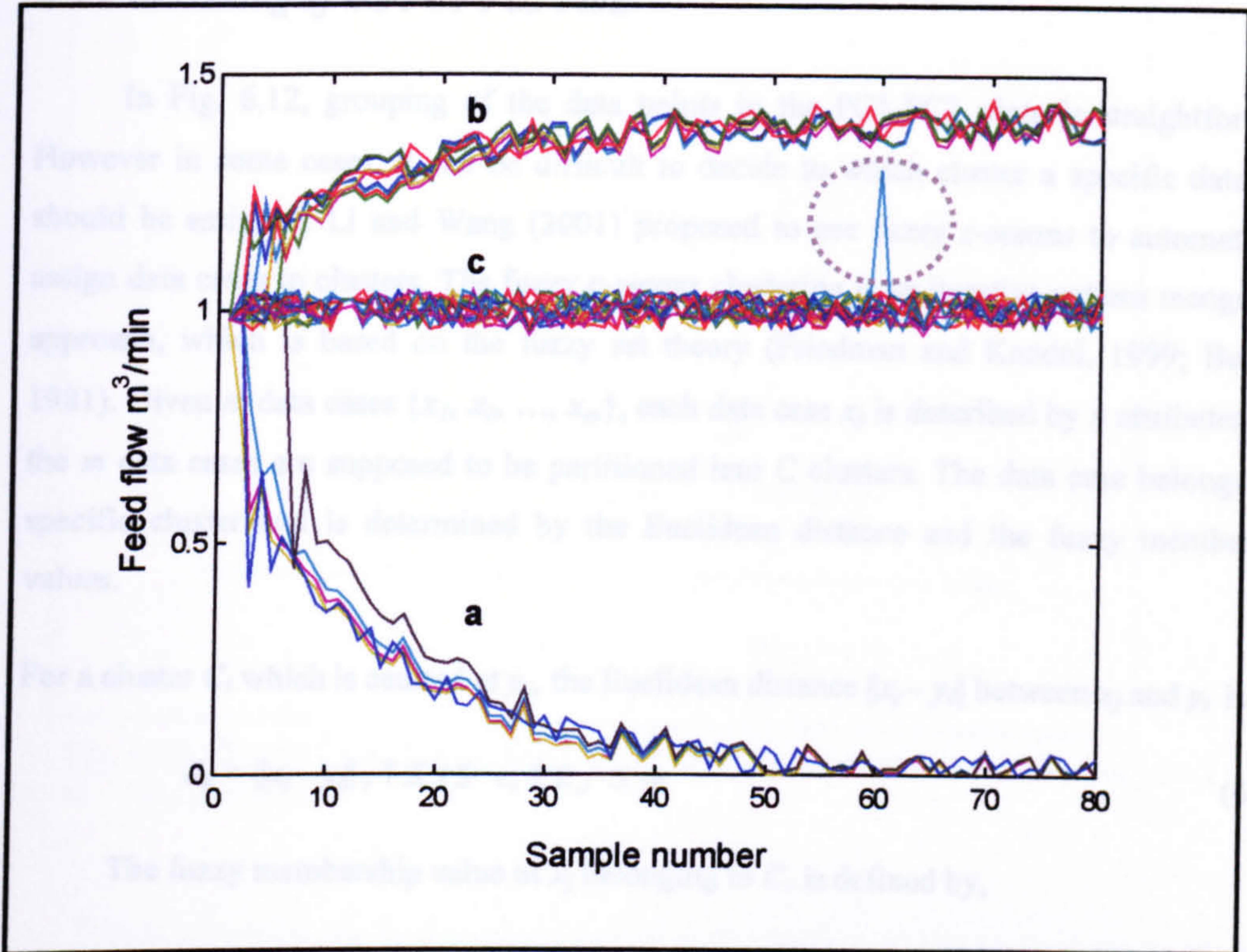


Fig. 6.14 CSTR feed dynamic trends with a spike introduced in case 25.

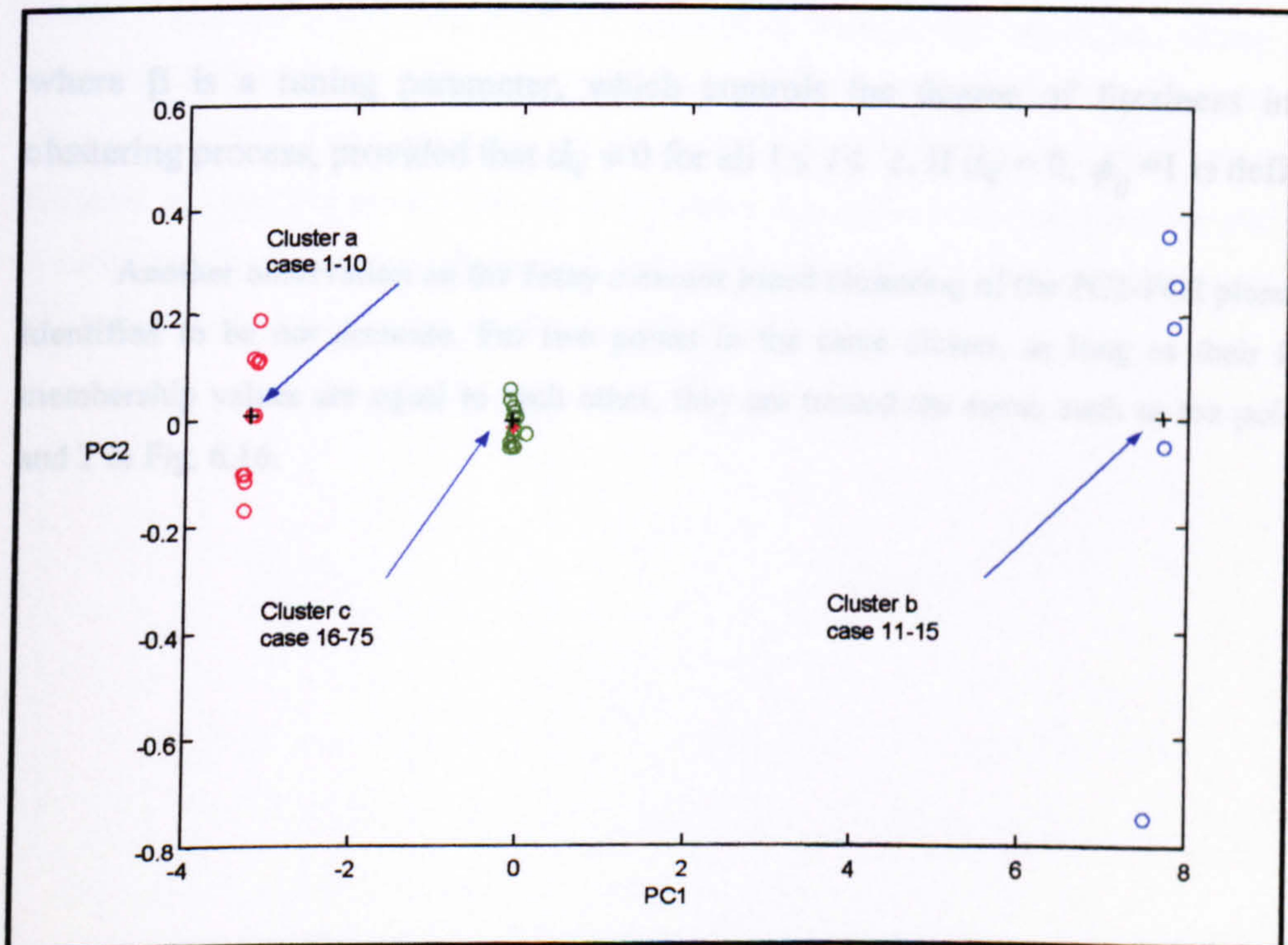


Fig. 6.15 PC1-PC2 plan plot of the dynamic trends of Fig. 6.14.

6.3.2 Clustering of the PC1-PC2 Plots

In Fig. 6.12, grouping of the data points in the PC1-PC2 plots is straightforward. However in some cases, it can be difficult to decide to which cluster a specific data case should be assigned. Li and Wang (2001) proposed to use fuzzy *c-means* to automatically assign data cases to clusters. The fuzzy *c-means* clustering is an iterative pattern recognition approach, which is based on the fuzzy set theory (Friedman and Kandel, 1999; Bezdek, 1981). Given m data cases $\{x_1, x_2, \dots, x_m\}$, each data case x_j is described by n attributes, and the m data cases are supposed to be partitioned into C clusters. The data case belongs to a specific cluster and is determined by the Euclidean distance and the fuzzy membership values.

For a cluster C_i which is centred at y_i , the Euclidean distance $\|x_j - y_i\|$ between x_j and y_i is

$$d_{ij} = \|x_j - y_i\|, 1 \leq i \leq c, 1 \leq j \leq m \quad (6.10)$$

The fuzzy membership value of x_j belonging to C_i is defined by,

$$\phi_{ij} = \left[\sum_{k=1}^c \left(\frac{d_{ij}}{d_{kj}} \right)^{2/(\beta-1)} \right]^{-1}, 1 \leq i \leq c, 1 \leq j \leq m \quad (6.11)$$

where β is a tuning parameter, which controls the degree of fuzziness in the clustering process, provided that $d_{kj} \neq 0$ for all $1 \leq i \leq c$. If $d_{kj} = 0$, $\phi_{ij} = 1$ is defined.

Another observation on the fuzzy *c-means* based clustering of the PC1-PC2 plane was identified to be not accurate. For two points in the same cluster, as long as their fuzzy membership values are equal to each other, they are treated the same, such as the points 1 and 2 in Fig. 6.16.

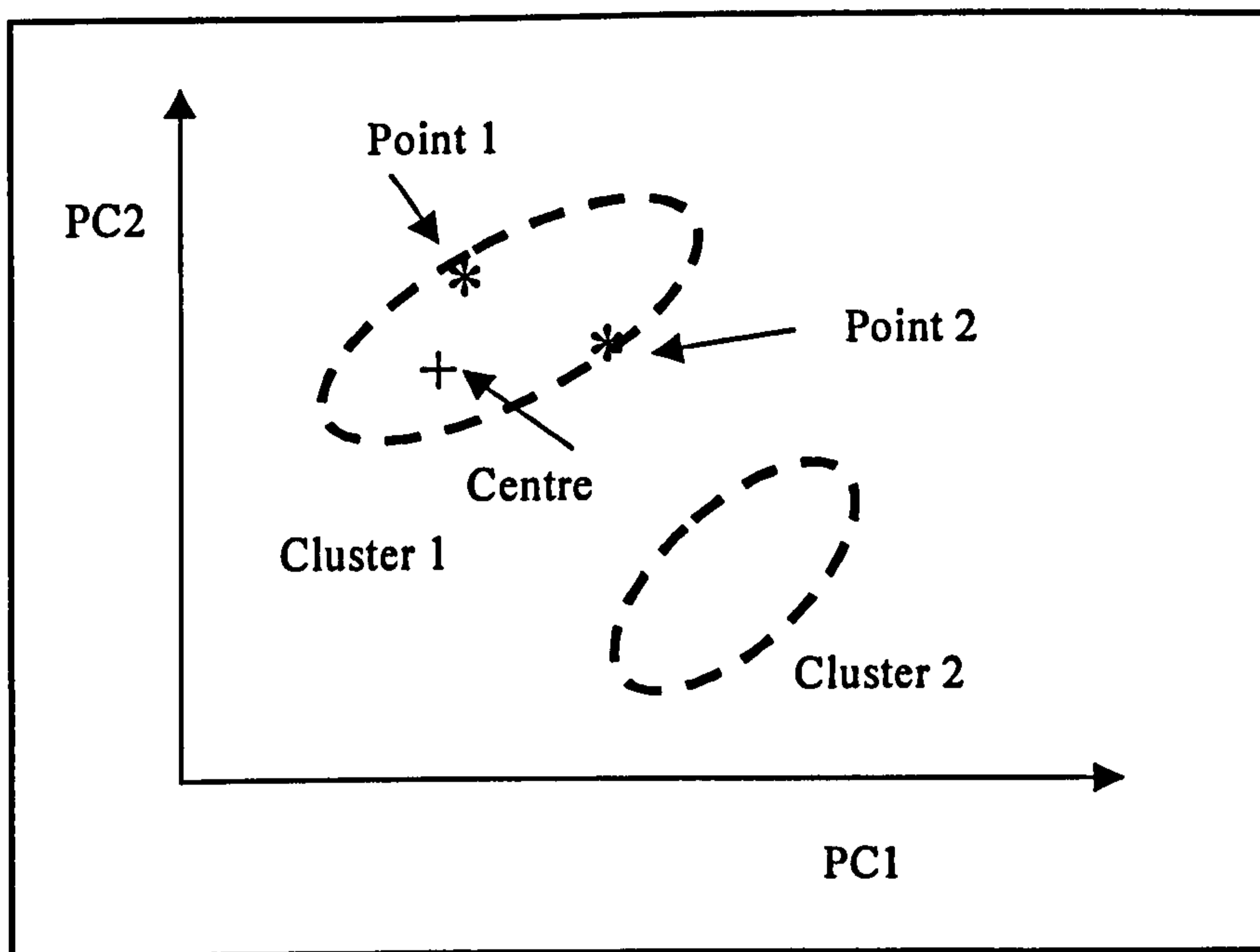


Fig. 6.16. Points 1 and 2 have equal value of fuzzy membership and belong to the same cluster.

This argument can be illustrated further with reference to the particular case study of the CSTR reactor. Fig. 6.17 shows the PC1-PC2 plot of the CSTR reactant feed flow transients. The plot shows that there are four clusters. Both samples 364 and 370 belong to cluster 3 (the red cluster) and have very close fuzzy membership values, i.e., almost equal distances to the cluster centre. However, their relative positions are important. Fig. 6.18 shows the PC1-PC2 plot when the process reached new steady states. It clearly shows that Samples 364 and 370 are in different steady states. It is also a clear indication that the fuzzy c-means approach gives insufficient information. Consequently, a new method using the idea of sectioning is needed and its development is given in Section 6.4.

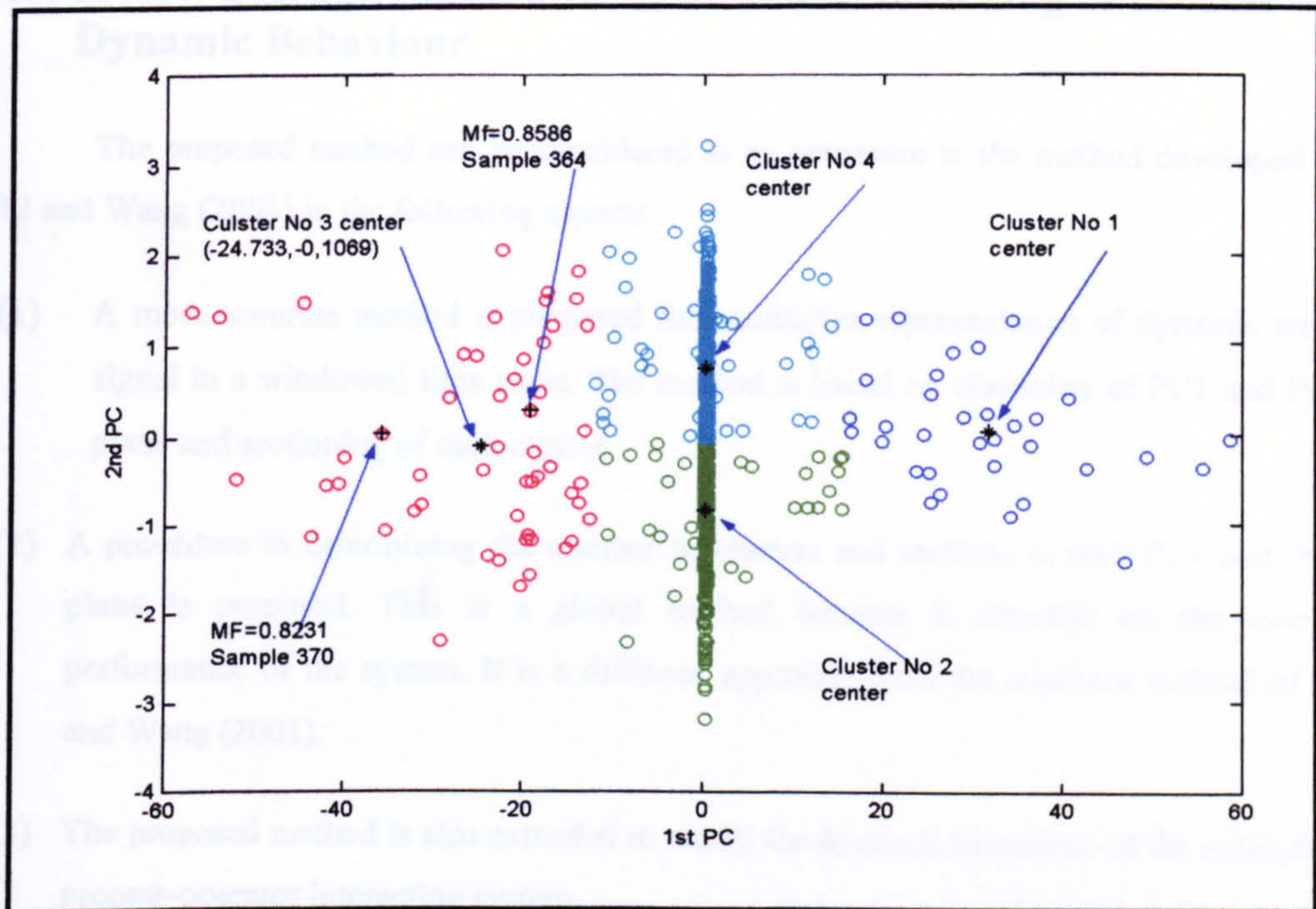


Fig. 6.17 PC's plot of dynamic trend reactant feed flow in CSTR process.

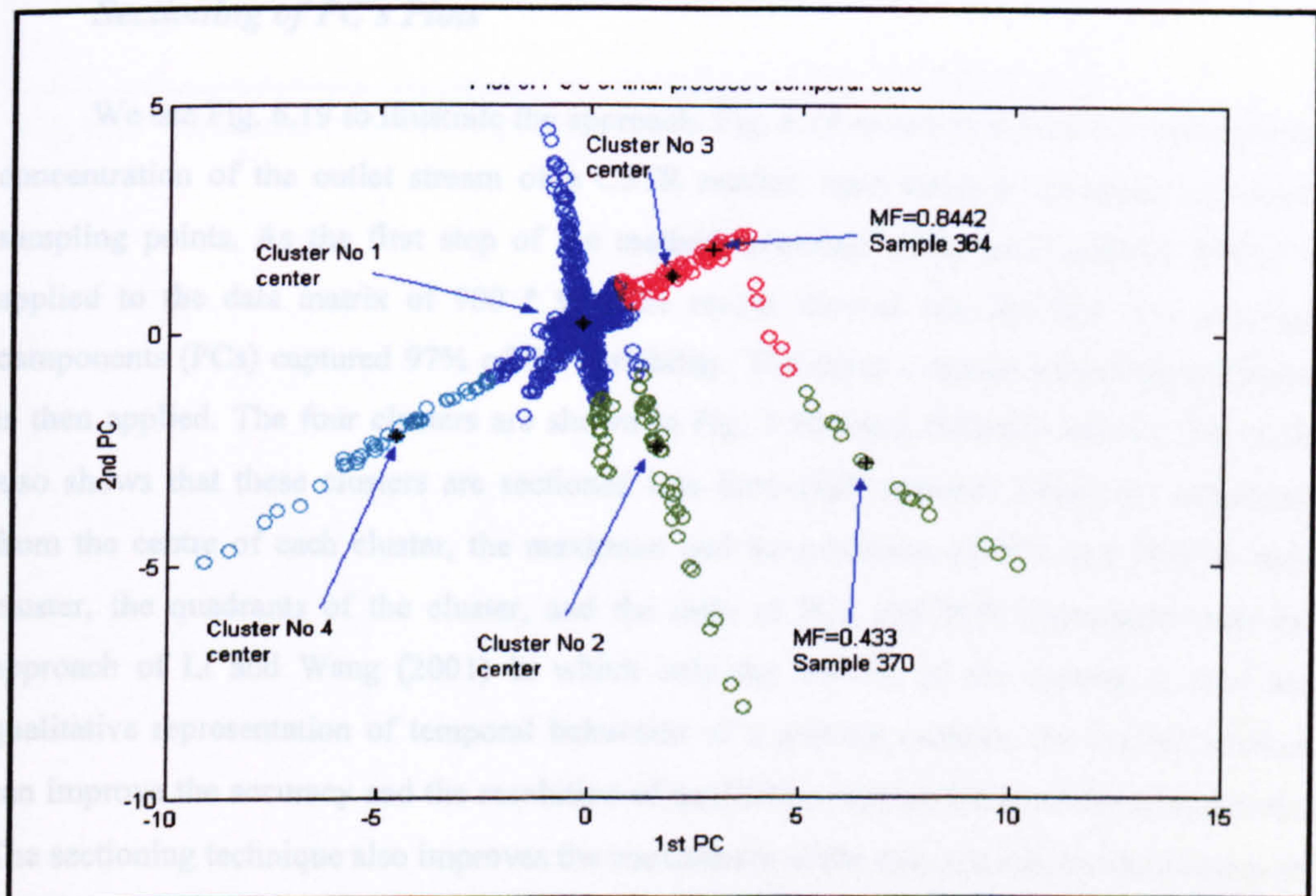


Fig. 6.18 PC's plot of final steady state temporal behaviour of the process.

6.4 A New Digraph Method for Qualitative Modelling of Process Dynamic Behaviour

The proposed method can be considered as an extension to the method developed by Li and Wang (2001) in the following aspects.

- (1) A more accurate method is proposed for qualitative representation of dynamic trend signal in a windowed time scale. The method is based on clustering of PC1 and PC2 plane and sectioning of each cluster.
- (2) A procedure in determining the number of clusters and sections in each PC1 and PC2 plane is proposed. This is a global method because it depends on the overall performance of the system. It is a different approach from the localised method of Li and Wang (2001).
- (3) The proposed method is also extended to model the dynamic behaviour of the combined process-operator interacting system.

6.4.1 Qualitative Representation of the Dynamic Trends Based on Clustering and Sectioning of PC's Plots

We use Fig. 6.19 to illustrate the approach. Fig. 6.19 shows nine hundred trends of the concentration of the outlet stream of a CSTR reactor, each trend is composed of ninety sampling points. As the first step of the method, principal component analysis (PCA) is applied to the data matrix of 900×90 . The results showed that the first two principal components (PCs) captured 97% of the variability. The fuzzy *c*-means clustering technique is then applied. The four clusters are shown in Fig. 6.20 using different colours. Fig. 6.20 also shows that these clusters are sectioned into forty-eight sections. These are calculated from the centre of each cluster, the maximum and the minimum of PC1 and PC2 of each cluster, the quadrants of the cluster, and the ratio of PC1 and PC2. Compared with the approach of Li and Wang (2001) in which only the number of the clusters is used for qualitative representation of temporal behaviour of a process variable, the current method can improve the accuracy and the resolution of qualitative representation of dynamic trends. The sectioning technique also improves the consistency of the data and minimises chances of rules conflict.

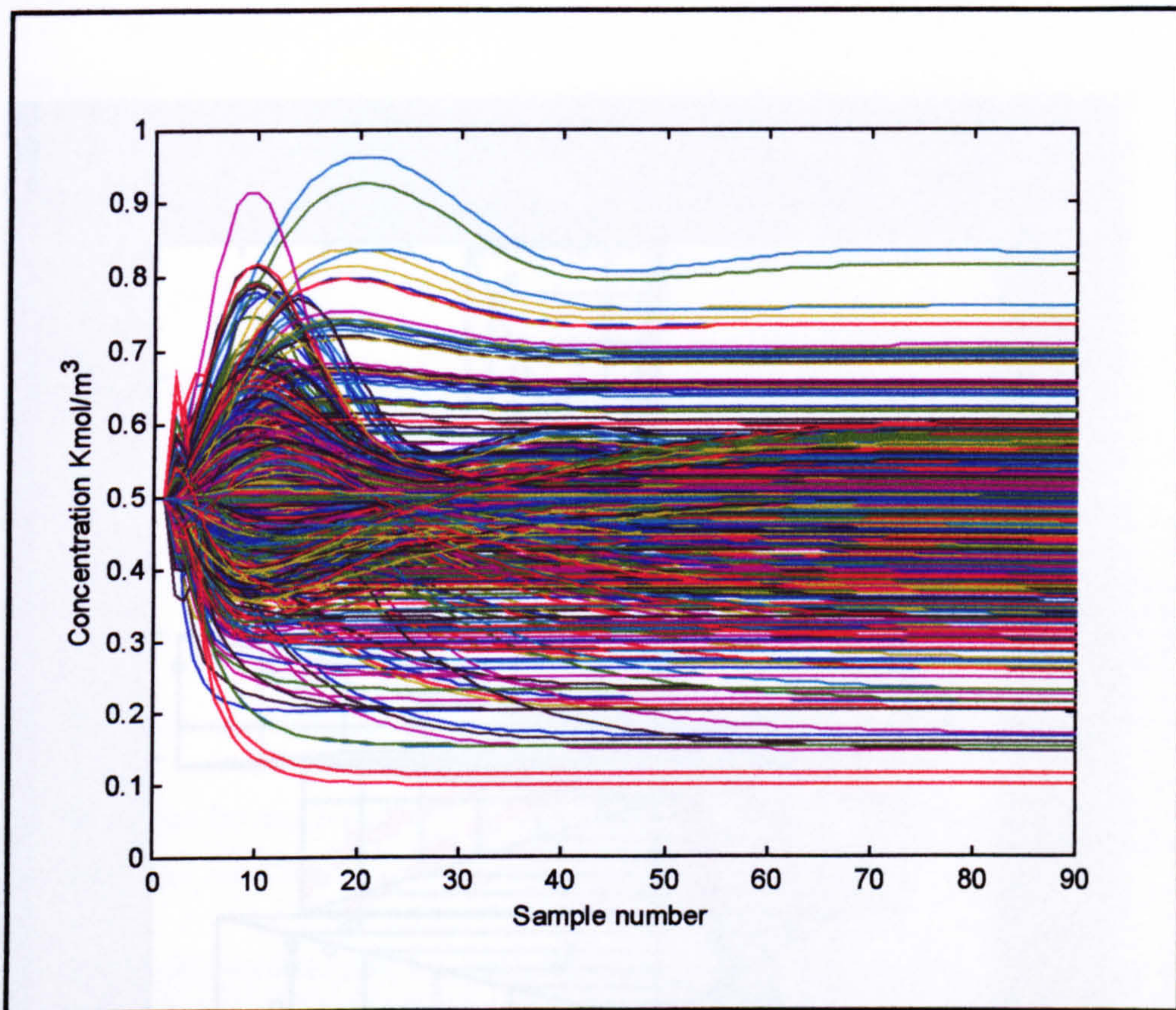


Fig. 6.19 Concentration of the output stream of the CSTR reactor.

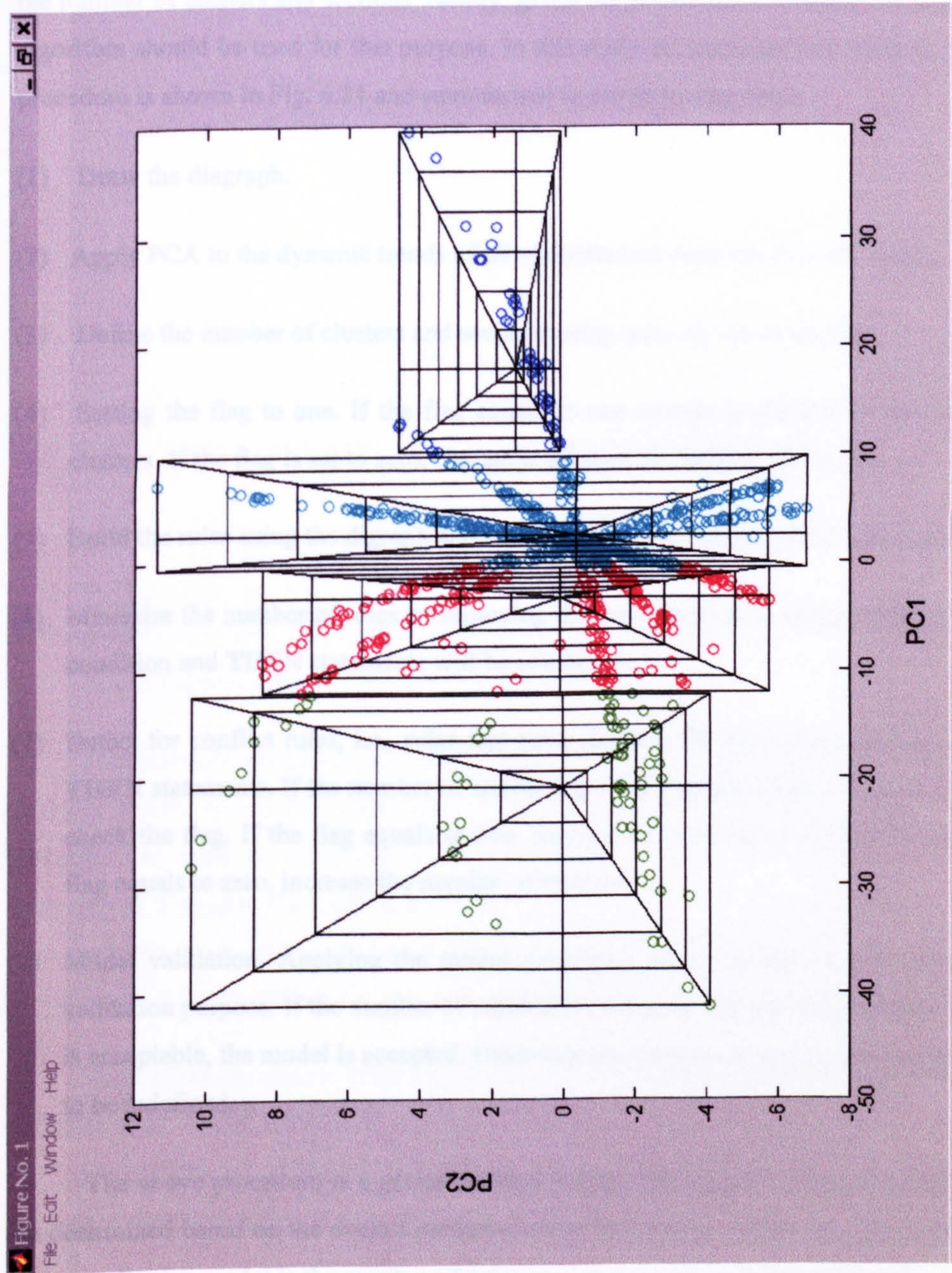


Fig 6.20. PC1 and PC2 plane of figure 6.19 trends clustered and sectioned to 4 clusters and 48 sections.

6.4.2 Number of Clusters and Sections

The method for qualitative representation of dynamic trends requires determination of the number of clusters and sections. Ideally, given the performance measure, an optimisation algorithm should be used for this purpose. In this study an empirical procedure is used. The procedure is shown in Fig. 6.21 and summarised in the following steps:

- (1) Draw the digraph.
- (2) Apply PCA to the dynamic trends of all variables and draw the PC1-PC2 plots.
- (3) Define the number of clusters and sections using rules-of-thumb method.
- (4) Setting the flag to one. If the flag equals to one change is allowed on the number of clusters. If the flag is set to zero, change is allowed on number of sections.
- (5) Build the rules using the digraph and PC1-PC2 plots and their clusters and sections.
- (6) Minimise the number of rules by removing the duplicated rules. Rules with the same **IF** condition and **THEN** statements will be combined.
- (7) Detect for conflict rules, i.e., rules that have identical **IF** condition parts, but different **THEN** statements. If the number of conflicting rules is greater than an acceptable value, check the flag. If the flag equals to one, increase the number of clusters by one. If the flag equals to zero, increase the number of sections.
- (8) Model validation. Applying the model developed from training data to test data for validation purpose. If the number of validation data cases that can be predicted correctly is acceptable, the model is accepted. Otherwise the number of clusters and sections need to be redefined.

The above procedure is a *global* method because the number of clusters and sections are determined based on the overall performance of the system. In this case the performance of the qualitative model is the number of data cases that can be correctly predicted.

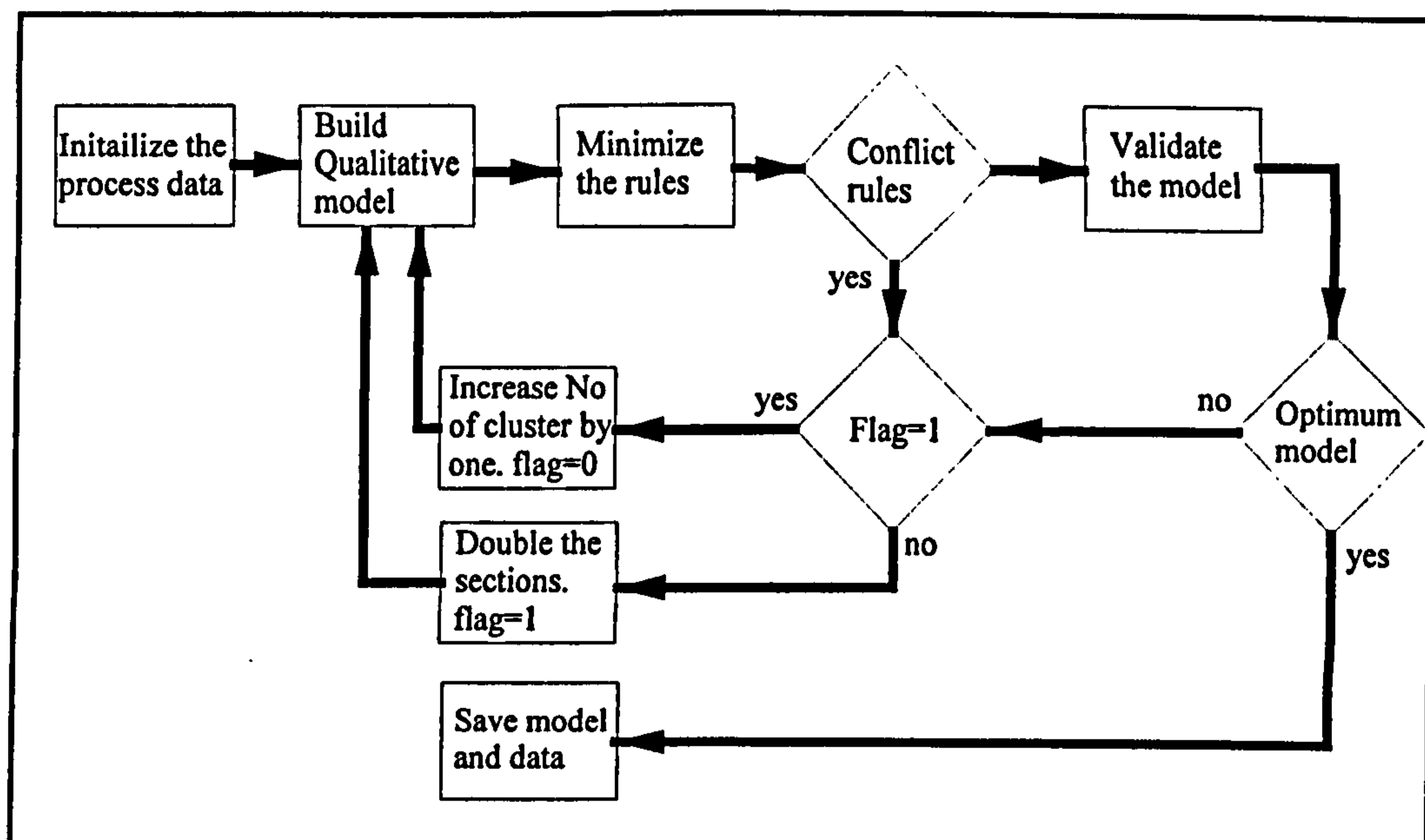


Fig. 6.21 The Procedure for selecting the numbers of clusters and sections.

6.4.3 Modelling the Dynamic Behaviour of a Combined Process-Operator Interaction System

The proposed method is applied to model the dynamic behaviour of the joint process-operator system of a CSTR operation (the CSTR flow sheet is shown in Fig. 3.5). Three variables are used as disturbances, including the feed concentration Ca_{in} , the feed temperature T_{in} and the cooling water temperature T_{win} . Six variables were recorded as state variables, including feed flow rate F_{in} , product flow rate F_{out} , product temperature T_{out} , product concentration Ca_{out} , reactor level L_{cstr} and cooling water flow rate F_{win} .

The qualitative interpretation approach of dynamic trends was applied to the six state variables F_{in} , F_{out} , Ca_{out} , T_{out} , L_{cstr} and F_{win} . As an example, the PC1-PC2 plots for T_{out} and Ca_{out} shown in Fig. 6.22 (a) & (b). The PC1-PC2 plots T_{out} and Ca_{out} are each divided into three clusters and forty-eight sections.

When the operators stop intervention and the process reaches the new steady state, the steady state values of the six state variables, F_{in} , F_{out} , Ca_{out} , T_{out} , L_{cstr} and F_{win} are processed by PCA to get the operational states of the process, as plotted in Fig. 6.22 (c). It also shows three clusters and forty-eight sections. Using inductive learning, a rule can be obtained as follows:

```

IF F_in( cluster = ?, section = ? )
and F_out( cluster = ?, section = ? )
.
.
and C_out( cluster = ?, section = ? )

THEN Process_Operation_State( cluster = ?, section = ? )

```

Purely for illustrative purpose, we only considered T_{out} and C_{out} in the IF part of the rules. Then the rules can be summarised as in Table 6.3. The first rule in Table 6.3 in Prolog format is:

```

Rule(1,43,2,41):-
End_clust=3, End_sec=33,
Output_Result(End_clust, End_esct).

```

In plain English the rule is:

```

IF T_out( cluster = 1, section = 43)
and Ca_out( cluster = 2, section = 41)

THEN Process_End_State( cluster = 3, section = 33).

```

Where the last statement indicates the process steady state location in term of the cluster and the section.

The three disturbances Ca_{in}, T_{in} and T_{in} are changed independently as well as in combination, and not all the changes are step changes. Therefore in order to derive rules to identify the disturbances from the qualitative values of the state variables, clustering of the disturbances is also necessary, Fig. 6.22 (d) shows the clustering of the three disturbances, in three clusters and forty-eight sections. According to Table 6.3, the first rule to identify the location of disturbances is, in Prolog format,

```

Rule(1,43,2,41):-

```

Dist_clust = 1, Dist_sect = 17,

Outprut_result(Dist_clust, Dist_sect).

or IF T_out(cluster = 1, section = 43)

and Ca_out(cluster = 2, section = 41)

THEN Disturbance(cluster = 1, section = 17).

The last statement is the output of the disturbance location.

The quantitative data of process variables for a particular process state or behaviour can also be calculated from the loading matrix and the sections coordinates (Table 6.4). Hence, this method allows reconstruction of the process variables values.

Table 6.3. Clusters and sections of the first 8 cases.

T_out		Ca_out		End_c		Dist_c	
Cluster Number	Section Number	Cluster Number	Section Number	Cluster Number	Section Number	Cluster Number	Section Number
1	43	2	41	3	33	1	17
1	27	2	26	3	4	1	3
1	32	2	8	3	4	1	47
1	42	2	42	1	12	1	21
1	37	2	38	1	35	1	44
1	43	2	40	3	33	1	16
1	21	2	21	1	11	1	7
1	6	2	8	3	4	1	46

Table 6.4. Section of three coordinate values used as quantitative represent.

Cluster	Section	PC1	PC2	PC1	PC2	PC1	PC2
1	1	2.1820	-2.5993	3.5130	-2.5993	3.5130	-2.0393
1	4	2.1820	-2.5993	3.5130	-2.0393	2.1820	-2.0393
1	7	2.1820	-2.5993	2.1820	-2.0393	1.8585	-2.0393
1	10	2.1820	-2.5993	1.8585	-2.0393	1.8585	-2.5993
1	13	2.1820	-2.5993	1.8585	-2.5993	1.8585	-3.5072
1	16	2.1820	-2.5993	1.8585	-3.5072	2.1820	-3.5072
1	19	2.1820	-2.5993	2.1820	-3.5072	3.5130	-3.5072
1	22	2.1820	-2.5993	3.5130	-3.5072	3.5130	-2.5993
2	1	-0.5683	-0.2620	-0.3837	-0.2620	-0.3837	-0.1582

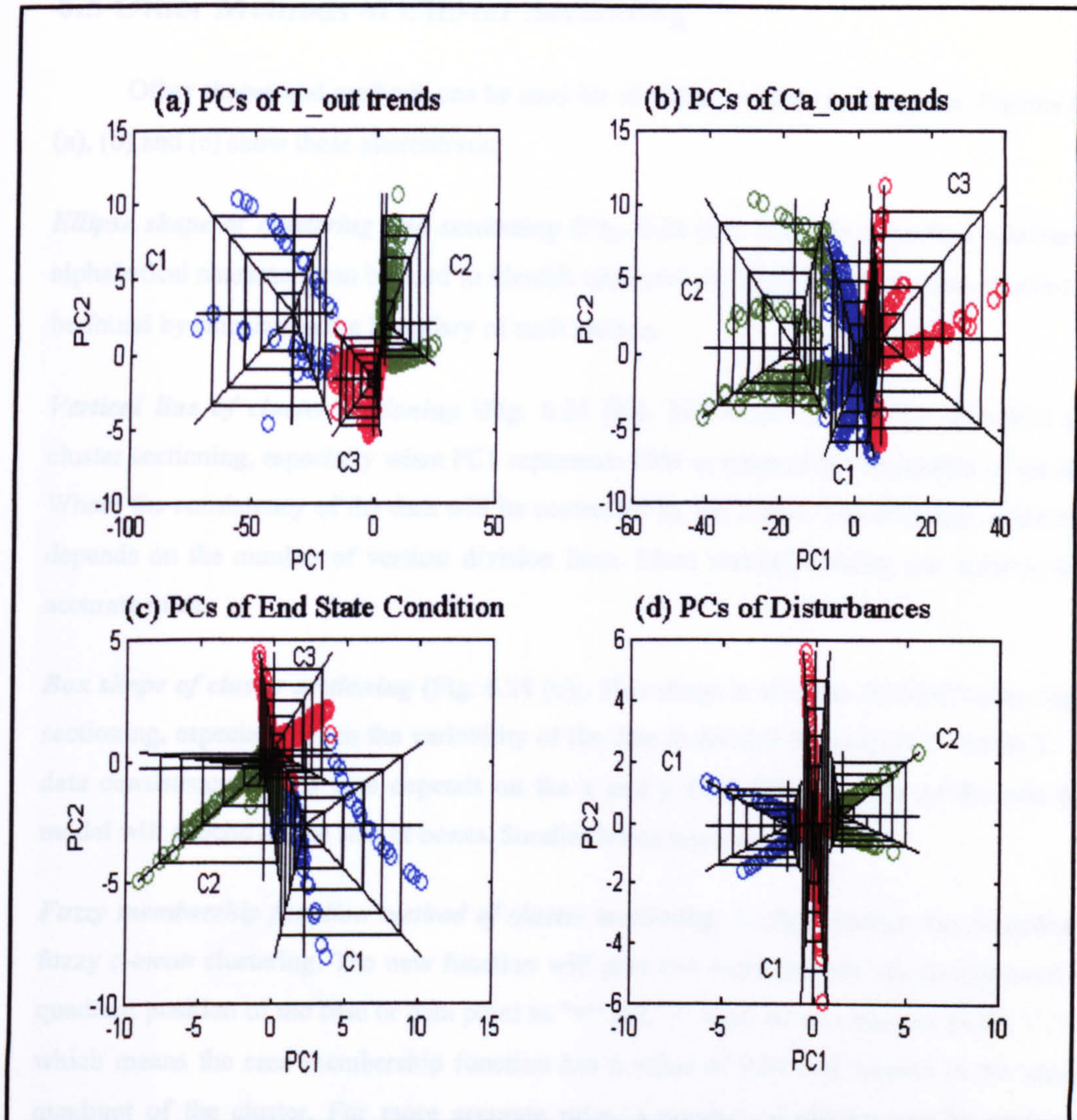


Fig. 6.22 The PC1-PC2 plots the dynamic trends of T_{out} (a) and Ca_{out} (b), the state of the process (c) and the disturbances (d).

Fig. 6.23 shows the screen-shot of the combined process-operator interaction dynamic behaviour simulation. The predicted position of the steady state condition is found in cluster one and section twenty-four, as shown in Fig. 6.23. A digraph of the **If** statement is represented as "clusters and sections of T_{out} and Ca_{in} " and the **Then** condition is represented as "clusters and sections of end condition and disturbances". The present condition of the process operation and the proposed action are shown at the end of the digraph.

6.5 Other Methods of Cluster Sectioning

Other shapes and methods can be used for dividing a cluster into regions. Figures 6.24 (a), (b) and (c) show these alternatives.

Ellipse shape of clustering and sectioning (Fig. 6.24 (a)). Specific numerical numbers or alphabetical characters can be used to identify each section. Each sample or case location can be found by calculating the boundary of each section.

Vertical line of cluster sectioning (Fig. 6.24 (b)). The shape is ideal for PC1-PC2 plan cluster sectioning, especially when PC1 represents 90% or more of the variability of the data. Where the consistency of the data will be controlled by the x-axis. The accuracy of the rules depends on the number of vertical division lines. More vertical division can achieve more accurate rules.

Box shape of cluster sectioning (Fig. 6.24 (c)). This shape is ideal for PC1-PC2 plan cluster sectioning, especially when the variability of the data is divided between PC1 and PC2. The data consistency in this case depends on the x and y axes. The accuracy of the rule base model will depend on the size of boxes. Smaller boxes more accurate rules.

Fuzzy membership function method of cluster sectioning. A slight change can be added to fuzzy *c-mean* clustering. The new function will give two extra outputs, which represent the quadrant position of the case or data point as “+” and “-“ sign. As an example, (0.85, '-', '+'), which means the case membership function has a value of 0.85 and located in the second quadrant of the cluster. For more accurate rules, a number of ellipses can be used as a boundary limit for the membership function. For example, the closest ellipse to the cluster centre represents a 0.9 membership function and the furthest ellipse represents a 0.4 membership function.

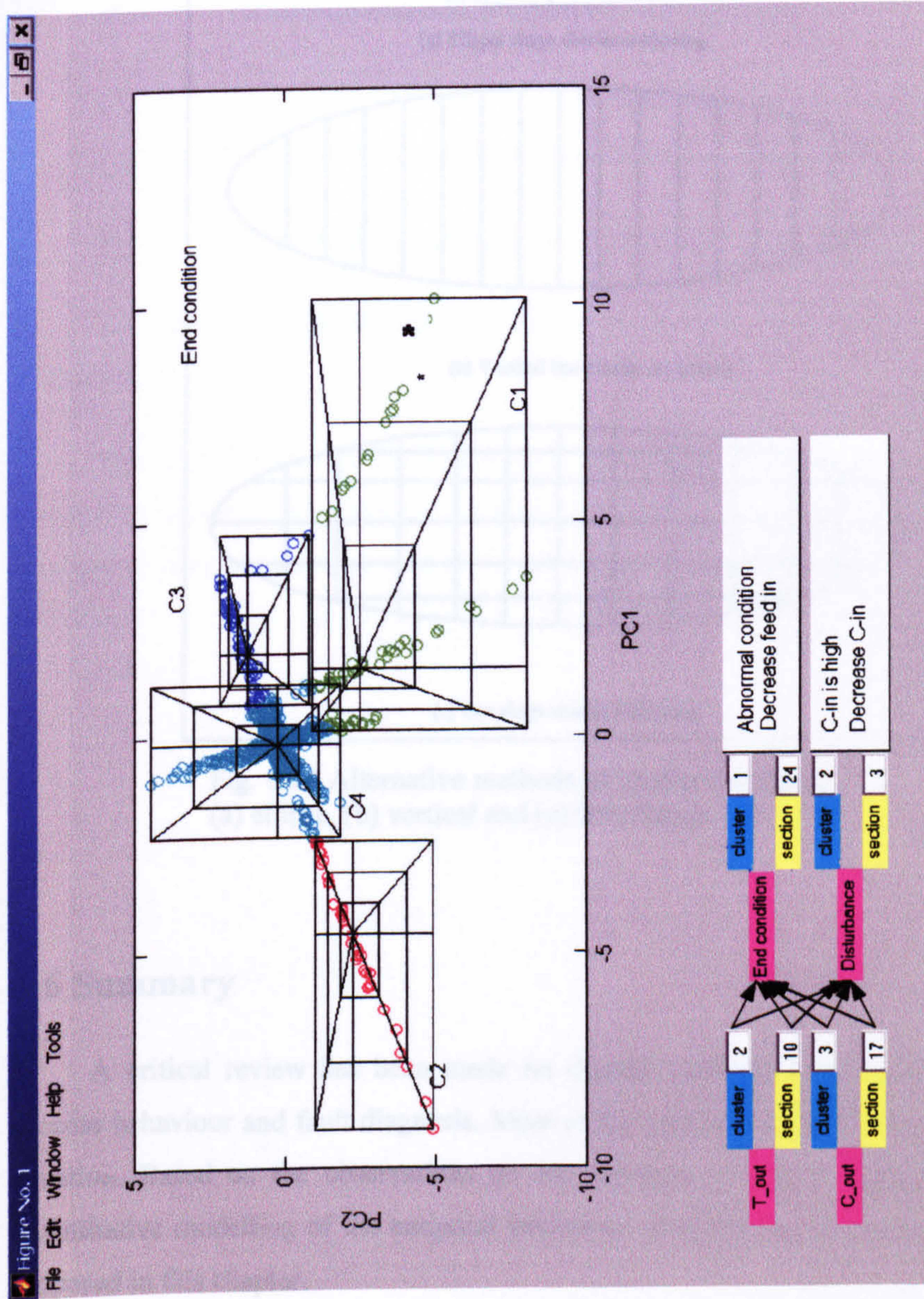


Fig 6.23. Combined process-operator interaction dynamic behaviour simulation.

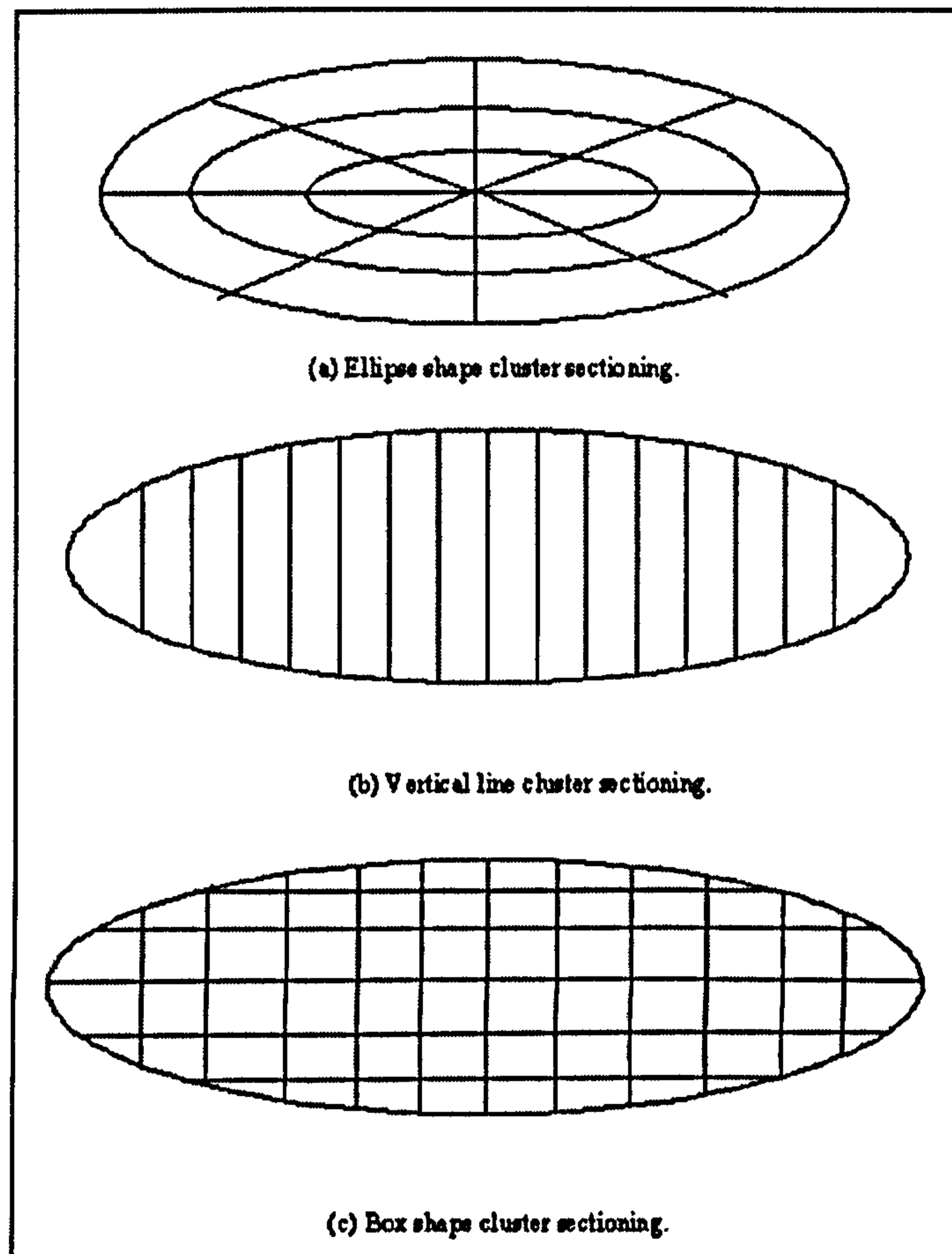


Fig. 6.24 Alternative methods of cluster sectioning, (a) ellipse, (b) vertical and (c) box shapes.

6.6 Summary

A critical review has been made on digraph methods for qualitative modelling of process behaviour and fault diagnosis. Most of the methods were developed for steady-state situation. Based on the observations on the methods of a new approach for qualitative /quantitative modelling of the temporal behaviour of combined operator-process systems is proposed in this chapter.

The method involves the following steps:

- (1) Drawing the digraph based on knowledge of the process.
- (2) Combining statistical techniques with joint operator-process simulation to generate data for model development and validation.

- (3) Qualitative interpretation of the temporal behaviour of all the individual variables using PC1-PC2 plots of principal component analysis. Fuzzy *c*-means is used to cluster the PC1-PC2 plots and each cluster is further sectioned.
- (4) The operational state is also clustered and sectioned.
- (5) Automatic generation of rules describing the reasoning mechanism in the digraph and the conditions leading to abnormal operation regions.
- (6) The method is developed for joint operator-process simulation system.

An iterative procedure for determining the number of clusters and sections is also presented.

The main features of the new method are, (a) the sectioning method overcomes the ambiguity problem of previous methods, (b) the accuracy and the resolution of the qualitative rules is increased, and (c) it can be applied to joint operator-process simulation systems.

Chapter 7

Applications and Case Studies

7.1 Introduction

In this chapter, the method developed in chapter 6 for qualitative/quantitative modelling of process temporal behaviour is applied to the joint operator-process simulation of a CSTR reactor. The purpose is to demonstrate the procedure of model development and validation. As indicated in chapter 6, ideally the numbers of clusters and sections should be calculated using mathematical optimisation. In practice, this is very complicated, therefore an iterative method was proposed. The numbers of clusters and sections were determined by trading-off the global performance measure in terms of accuracy and simplicity of the rules. The models were first developed using training data and then validated using test data. A systematic procedure for validating the model and feedback of the validation result to model revision is described in detail in this chapter.

7.2 Generation of Validation Data

The procedure of generating the training and validation data is shown in Fig. 7.1 and can be summarised in the follow steps:

- (1) Set the initial conditions, such as the mean (μ) and standard deviations (std) for each disturbance. These values can be assigned through the interface of the interaction model. The mean and the standard deviation for the three disturbances of the CSTR reactor, i.e., C_{in} , T_{in} and T_{win} are: $\mu=[2\ 340\ 310]$ and $std=[0.6\ 10\ 10]$.
- (2) Use the mean μ and the standard deviation std to generate disturbances, which will be applied to the CSTR simulator. Using the mean μ and the standard deviation std and a random number generator, ninety disturbances are generated in this study.
- (3) Apply all disturbances to the CSTR reactor simulator. For each data case, the simulator always starts from normal operation.
- (4) Organize the validation data and add white noise. White noise normal distributed with zero mean.

7.3 The Validation Procedure of Qualitative Models

The validation procedure is shown in Fig. 7.2 and summarised in the following steps:

- (1) Load all the data that is obtained in the model training stage and is required for the validation process, including the mean, standard deviations, cluster centres and sections, Max/Min values for PC2 and PC1 ratios, and loading matrices.
- (2) Use the above data obtained in model training stage to process the validation data, and so plot the validation data on the PC1-PC2 planes.
- (3) Check if all the validation data falls within the clusters and sections of the training data. If a validation data case goes outside, it should be removed from the validation data. This consideration is similar to feedforward neural network that can guarantee correctness and accuracy only if the new data falls within the training data space. This limitation can be overcome through extensive training using data covering various scenarios.
- (4) Calculate the distance of all validation data from the cluster centres.
- (5) Also assign validation data cases to specific sections. Construct a matrix to represent the assignments of all validation data cases to clusters and sections.
- (6) Identify the cases of the validation data that can be correctly predicted using the rules obtained at the training stage.
- (7) Check the closeness of the clusters and sections predicted by the rule-based models and the true locations.
- (8) Calculate the quantitative values from the qualitative predictions. This will make use of the section coordinates of PC1 and PC2 and the loading matrix.
- (9) Create a residual error plot (Fig. 7.3) with 95% confidence intervals on the residual errors using the value of the process variables produced in step (8) and the actual values. The outlier cases, which are outside the 95% confidence limits, can be clearly visualised in red colour. The one-way analysis of variance (ANOVA) is carried out for each final temporal state of process variables calculated in step (8) and the actual process variables of the validation data. Then create a box and whisker plot for each variable (Fig. 7.4).

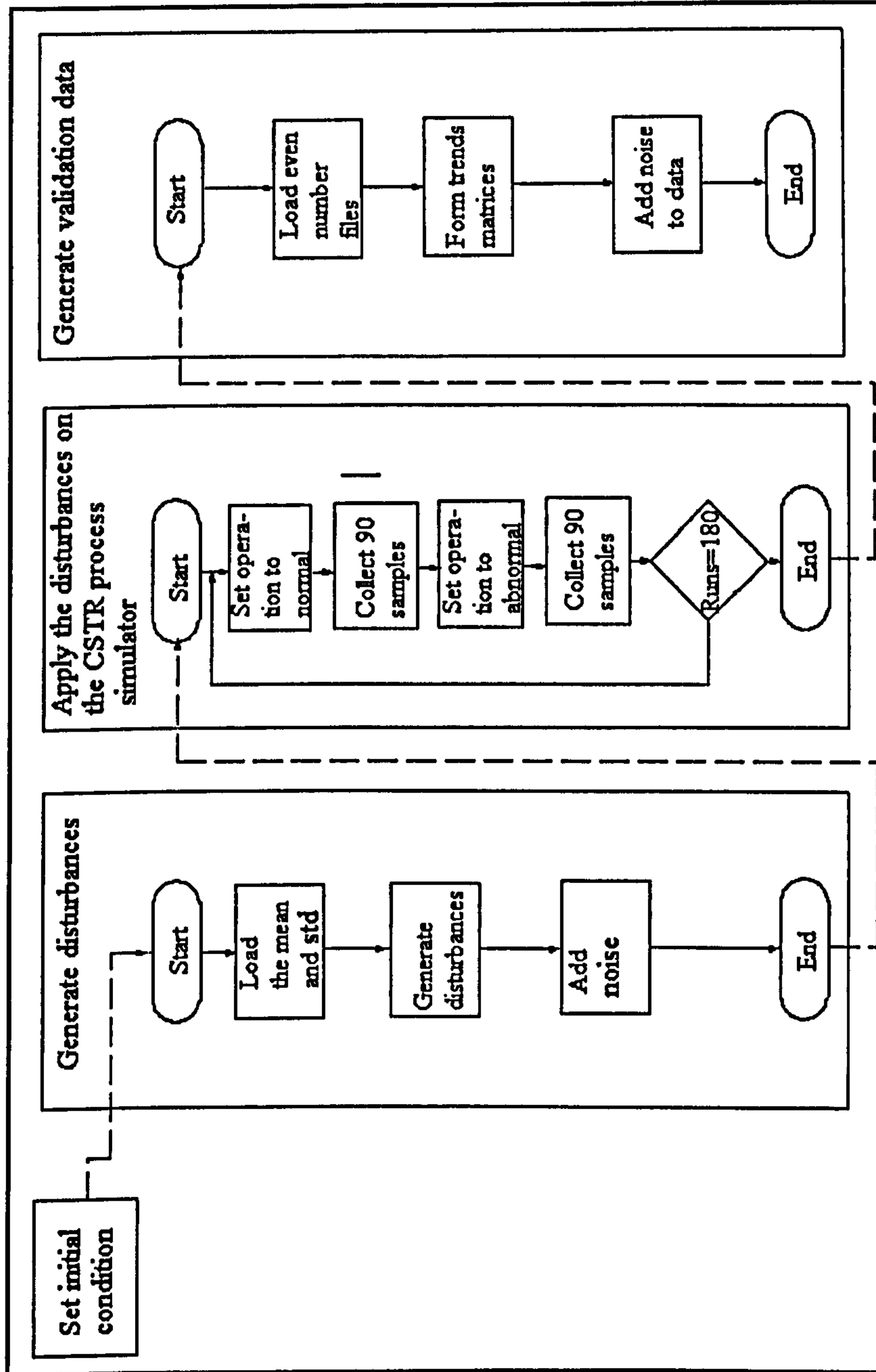


Fig 7.1 Generation of validation data.

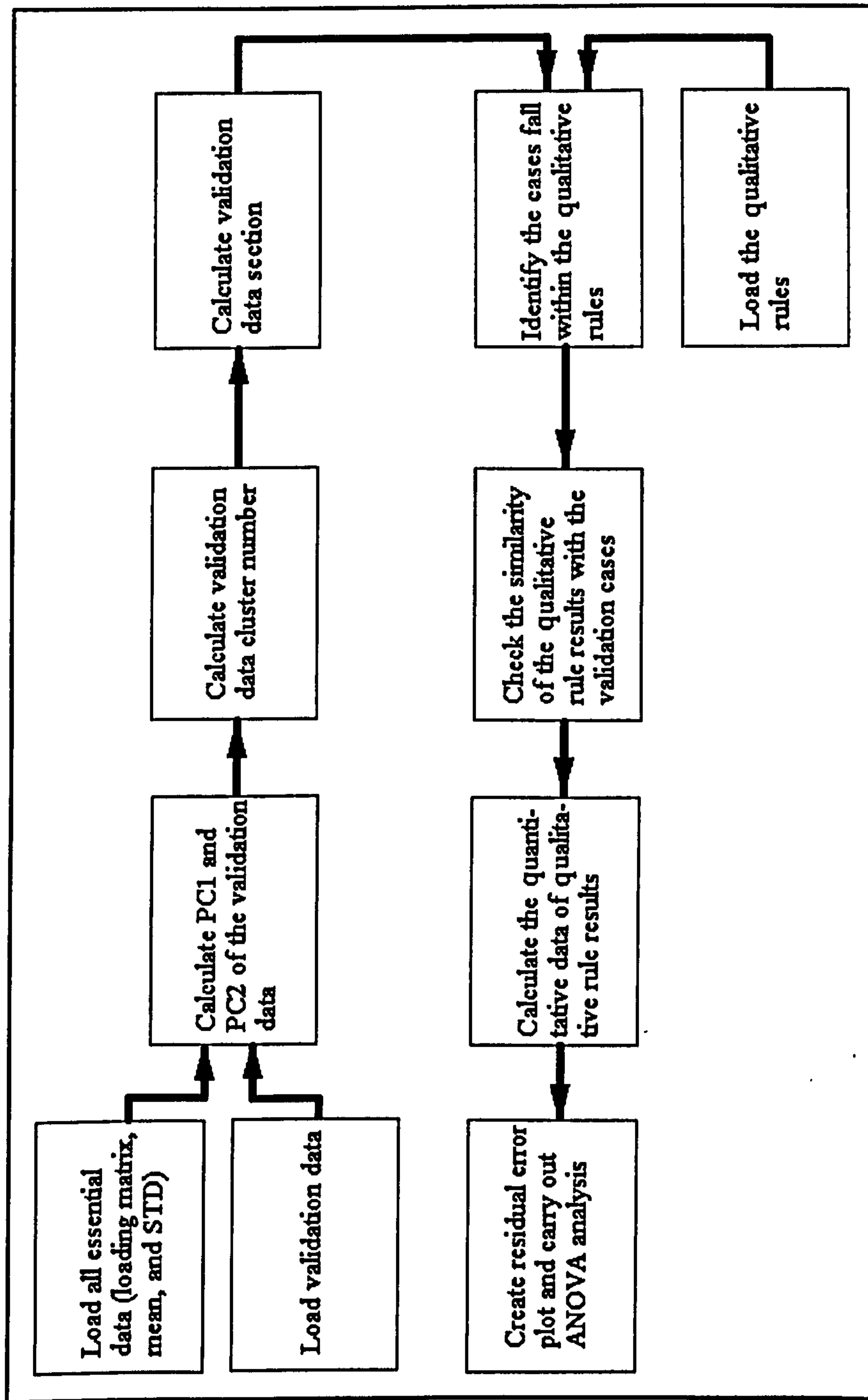


Fig 7.2. The validation procedure of qualitative models.

7.4 One-Way Analysis of Variance (ANOVA)

ANOVA is used to determine if the data from different groups has a common mean or they are actually different in the measured characteristics. ANOVA is a simple but special case of the linear model and has a form of:

$$y_{ij} = \alpha_{.j} + \varepsilon_{ij} \quad (7.1)$$

where y_{ij} is a matrix of observations, $\alpha_{.j}$ is a matrix whose columns are the group means (the 'dot j' notation means that α applies to all rows of the j^{th} column), and ε_{ij} is the matrix of the random disturbances. The value of an element in the column of y is the sum of a constant and a value from a random disturbance.

The results of each case study tabulated in tables are known as ANOVA tables. The construction of an ANOVA table can be demonstrated using Table 7.1, which shows all equations required to carry out ANOVA calculation. \hat{y}_i are the estimated values of the model, y_i are the actual observation values, and \bar{y} are the means of the observation values. The F-Factor is used for null hypothesis test, to see if the means of the columns are identical. A p-value will return by the hypothesis test, which will be examined during the case studies. If a p-value is closed to zero, it is a doubtful case with respect to the null hypothesis and indicates that the means of the columns are different. ANOVA Table divides the variability of the data into two parts. The first part is the variability due to differences among the column means. The second part is the variability due the differences between the data in each column and column mean.

The box plots produced from the ANOVA test are used to confirm the results from the ANOVA tests by displaying the means of the estimated and the observed values, and the data spread from the means. The box has lines showing the lower quartile, median and upper quartile. The whiskers are lines extending from each end of the box to show the extent of the rest of the data. Outliers are data with values beyond the end of the whiskers.

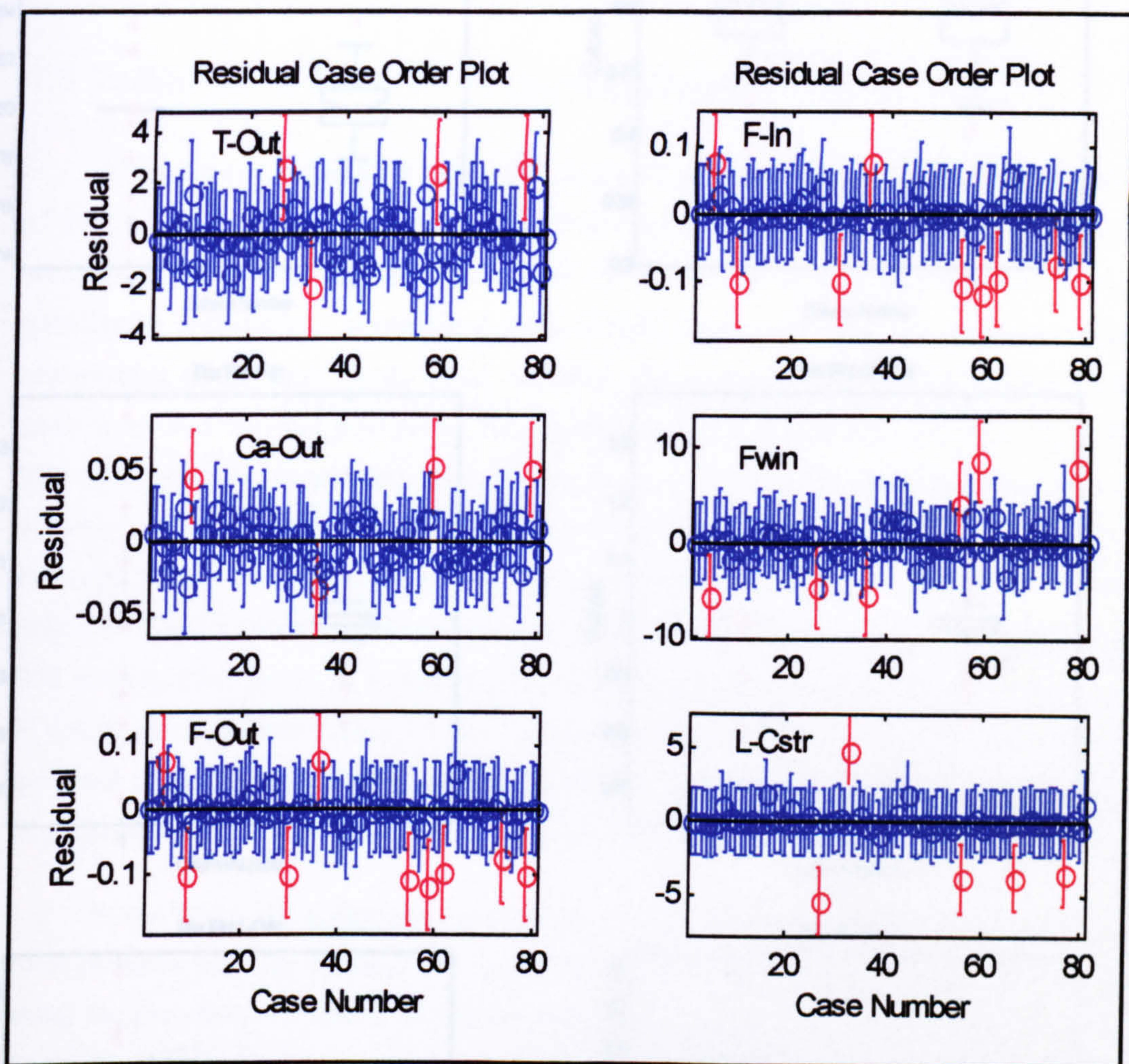


Fig. 7.3. A plot of the residuals with error bars represented 81 cases of the final process steady state conditions identified by the qualitative rules.

Fig. 7.4. The box plot for the actual variables values for the data spread from the mean.

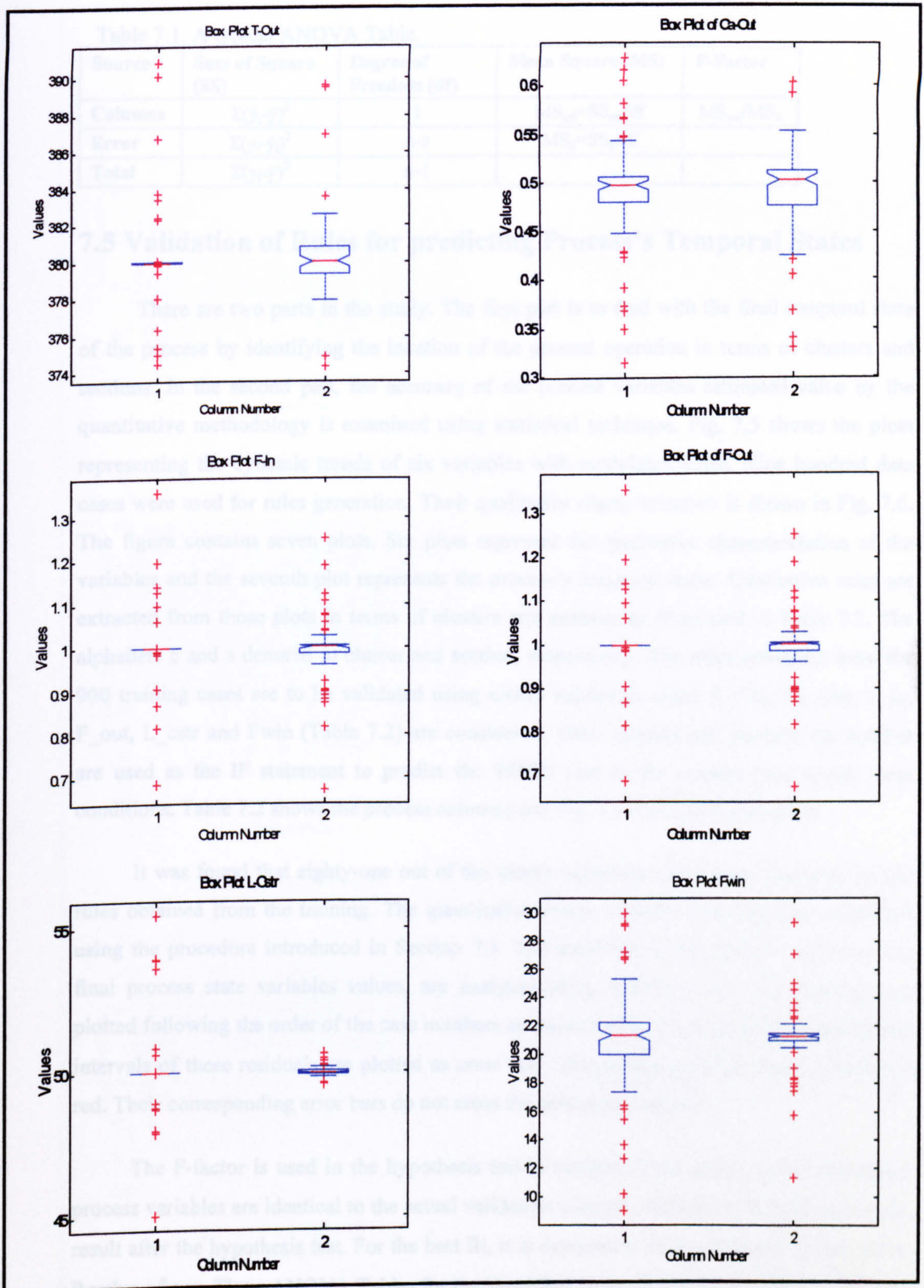


Fig. 7.4. The box plot for the actual validation values and the model calculated values showing the data spread from the mean.

Table 7.1. A typical ANOVA Table.

Source	Sum of Square (SS)	Degree of Freedom (df)	Mean Square (MS)	F-Factor
Columns	$\Sigma(\hat{y}_i - \bar{y})^2$	1	$MS_{col} = SS_{col}/df$	MS_{col}/MS_E
Error	$\Sigma(y_i - \hat{y}_i)^2$	n-2	$MS_E = SS_E/df$	
Total	$\Sigma(y_i - \bar{y})^2$	n-1		

7.5 Validation of Rules for predicting Process's Temporal States

There are two parts in the study. The first part is to deal with the final temporal state of the process by identifying the location of the process operation in terms of clusters and sections. In the second part, the accuracy of the process variables estimated value by the quantitative methodology is examined using statistical technique. Fig. 7.5 shows the plots representing the dynamic trends of six variables with modulated noise. Nine hundred data cases were used for rules generation. Their qualitative characterisation is shown in Fig. 7.6. The figure contains seven plots. Six plots represent the qualitative characterisation of the variables and the seventh plot represents the process's temporal states. Qualitative rules are extracted from those plots in terms of clusters and sections as illustrated in Table 7.2. The alphabets c and s denoted to cluster and section, respectively. The rules generated from the 900 training cases are to be validated using ninety validation cases. T_Out, Ca_Out, F_in, F_out, L_cstr and Fwin (Table 7.2) are considered. Their clusters and sections tag number are used as the IF statement to predict the THEN part of the process final steady state conditions. Table 7.2 shows the process columns and Fig. 7.6 displays the final plot.

It was found that eighty-one out of the ninety validation cases were identified by the rules obtained from the training. The quantitative values of these cases are also calculated using the procedure introduced in Section 7.3. The quantitative data, which represents the final process state variables values, are analysed using ANOVA test. The residuals are plotted following the order of the case numbers as shown in Fig. 7.3 and the 95% confidence intervals of these residuals are plotted as error bars. The outlier cases are clearly shown in red. Their corresponding error bars do not cross the zero reference line.

The F-factor is used in the hypothesis test to confirm if the values of the calculated process variables are identical to the actual validation process variables. A P-value shows the result after the hypothesis test. For the best fit, it is expected to have a F-factor of zero and a P-value of one. Three ANOVA Tables for the identified cases are shown in Tables 7.3 to 7.5.

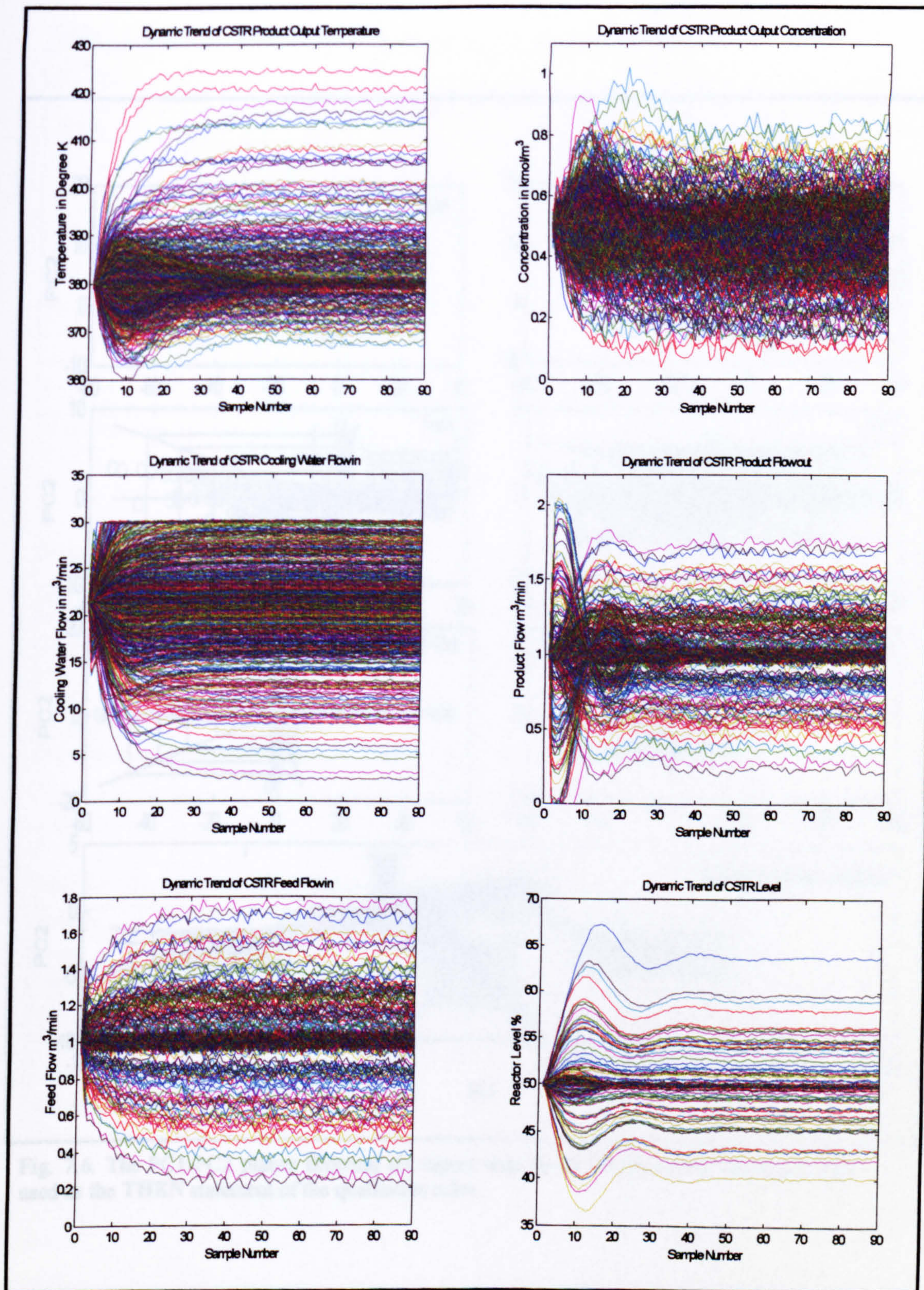


Fig. 7.5. The CSTR operation trends for all variables, each plot contains 900 trends and each trend represents 90 samples.

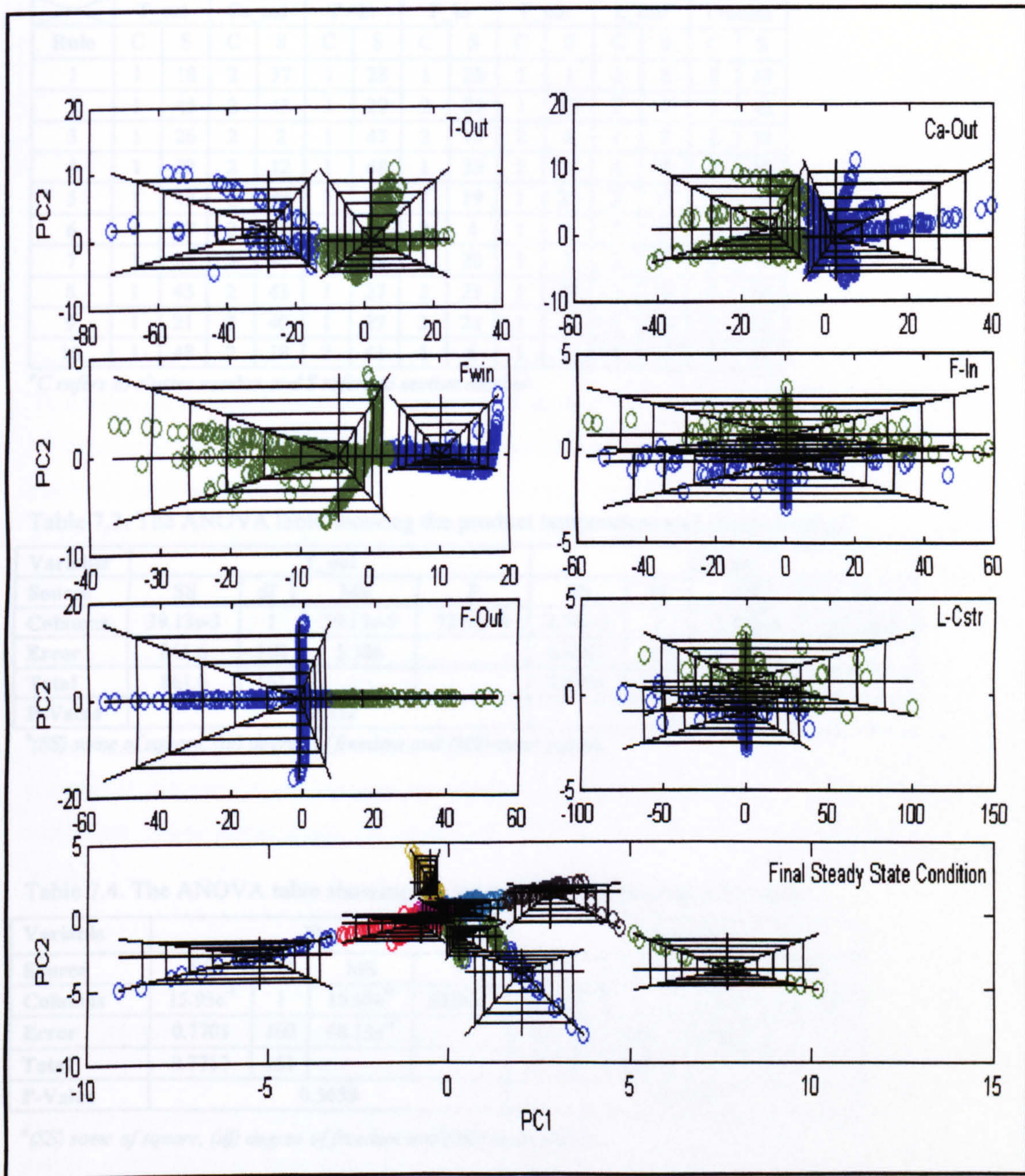


Fig. 7.6. The PC1-PC2 planes showing six inputs used as the **IF** conditions and one output used as the **THEN** statement of the qualitative rules.

Table 7.2. The first 10 qualitative rules represented by clusters and sections.^a

Rule	IF												THEN	
	T_out		Ca_out		Fwin		F_In		F_out		L_cstr		Process	
	C	S	C	S	C	S	C	S	C	S	C	S	C	S
1	1	18	2	37	1	28	1	28	1	1	2	8	8	19
2	1	45	2	43	1	29	2	21	1	22	2	7	9	48
3	1	26	2	2	1	47	2	15	2	2	1	7	2	33
4	1	32	2	12	1	48	1	35	2	25	1	7	2	10
5	1	42	2	42	1	30	1	19	1	22	2	17	8	20
6	1	37	2	38	1	6	2	4	1	1	2	17	8	43
7	1	21	2	40	1	27	1	20	1	1	2	16	8	8
8	1	43	2	43	1	27	2	21	1	22	1	9	9	48
9	1	21	2	40	1	27	2	21	1	1	2	16	8	33
10	1	48	2	18	2	41	1	6	1	1	1	17	9	43

^aC refers to cluster number and S refers to section number.

Table 7.3. The ANOVA table showing the product temperature and concentration.^a

Variable	T_out				Ca_out			
	SS	df	MS	F	SS	df	MS	F
Columns	39.13e-3	1	39.13e-3	72.66e-4	2.74e-5	1	2.74e-5	10.74e-3
Error	861.6	160	5.386		0.4084	160	25.52e-4	
Total	861.6	161			0.4084	161		
P-Value	0.9322				0.9176			

^a(SS) some of square, (df) degree of freedom and (MS) mean square.

Table 7.4. The ANOVA table showing the reactor feed and product flow rates.^a

Variable	F_in				F_out			
	SS	df	MS	F	SS	df	MS	F
Columns	15.93e-4	1	15.93e-4	33.09e-2	15.05e-4	1	15.05e-4	31.17e-2
Error	0.7701	160	48.13e-4		0.7724	160	48.28e-4	
Total	0.7717	161			0.7739	161		
P-Value	0.5659				0.5774			

^a(SS) some of square, (df) degree of freedom and (MS) mean square.

Table 7.5 The ANOVA Table showing the reactor level and cooling water flow rate.^a

Variable	L_cstr				Fwin			
	SS	df	MS	F	SS	df	MS	F
Columns	24.34e ⁻²	1	24.34e ⁻²	34.53e ⁻²	15.28e ⁻¹	1	15.28e ⁻¹	18.11e ⁻²
Error	112.8	160	70.49e ⁻²		1350	160	84.39e ⁻¹	
Total	113	161			1352	161		
P-Value	0.5576				0.6710			

^a(SS) some of square, (df) degree of freedom and (MS) mean square.

Table 7.3 shows that the T_{out} and Ca_{out} estimations are very good since the F-factors for both variables are very small and the P-values are over 0.9, which is close to one. This indicates that the F statistic is as extreme as the observed F, which would have a chance of occurrence about nine out of ten if both the actual and predicted values were equal. This has been confirmed by the top two box plots in Fig. 7.4, which show that the variables of T_{out} and Ca_{out} of the validation data have almost the same number of data spread as that determined by the model. The other ANOVA Tables for F_{in}, F_{out}, L_{cstr} and Fwin variables also show good results, but comparatively lower than that of T_{out} and Ca_{out} variables data, since the P-values indicate that F statistic that is as extreme as the observed F would occur by chance about six out of ten if both the actual and predicted values were truly equal. The box plots of the four variables is shown in Fig. 7.4 and they look less promising than the T_{out} and Ca_{out} box plot specially L-Cstr variable, which shows that the actual validation values spread along the value axis while the prediction focus around its mean value.

The next case study is to increase the number of IF condition statement (refer to Table 7.2) of the qualitative rules from six to ten elements. The number of cases identified by the qualitative rules reduced from eighty-one to twenty-one. This indicates that the model is over-fitted. For example, by fitting the system too close to the training data, it will lose its ability to improve the fitting of the system to the validation or checking data. This situation usually occurs in fuzzy logic when the model has been trained for a long time (the number of epoch is very large). Hence, the error from the training data will be the least while that from the checking data will be large, and it is higher than that when a shorter model training time is applied. The over-fit situation also occurs in neural network methodology. When the number of neurons in the hidden layers increases, the neural network model is forced to represent the training data only but not the model. The P-values of ANOVA in Tables 7.6 to 7.8 of this case study become lower than the previous one, which confirms the over-fitting.

The residual plots with 95% confidence for the twenty-one predicted cases are shown in Fig. 7.7 (for the final process steady state variables). The outlier cases are less than the previous case study because the number of cases identified by the qualitative rules is only one third of the previous case study. The ANOVA Tables 7.6 to 7.8 and the box plots in Fig. 7.8 indicate that the results are less promising than the previous case study because of the over-fit phenomena. It proves that the current proposed method is different from the normal rule-base situation, where when the number of IF statement elements increase (more description in the rule statement) the prediction of the conditions will be more accurate. For the purpose of illustration, an example of rules to predict if an animal is an elephant is given below,

IF animal huge four-footed,
And animal thick-skinned,
And animal ivory tusks,
And animal long trunk,
Then animal is elephant.

The above rule can only predict the type of the animal but will not distinguish if the elephant is from Africa or Asia. Therefore an extra statement to enhance the rule is required.

Fig. 7.8 shows the box plots for all the final process variable's states. F_{out} and F_{in} have the lowest values of the P-value and the highest values of the F-factor, which indicate that the estimated data are not identical to the validation data. The box plots of the F_{out} and F_{in} confirm this finding since the estimated data spread along the value axis while the actual values (column one) focus around the mean.

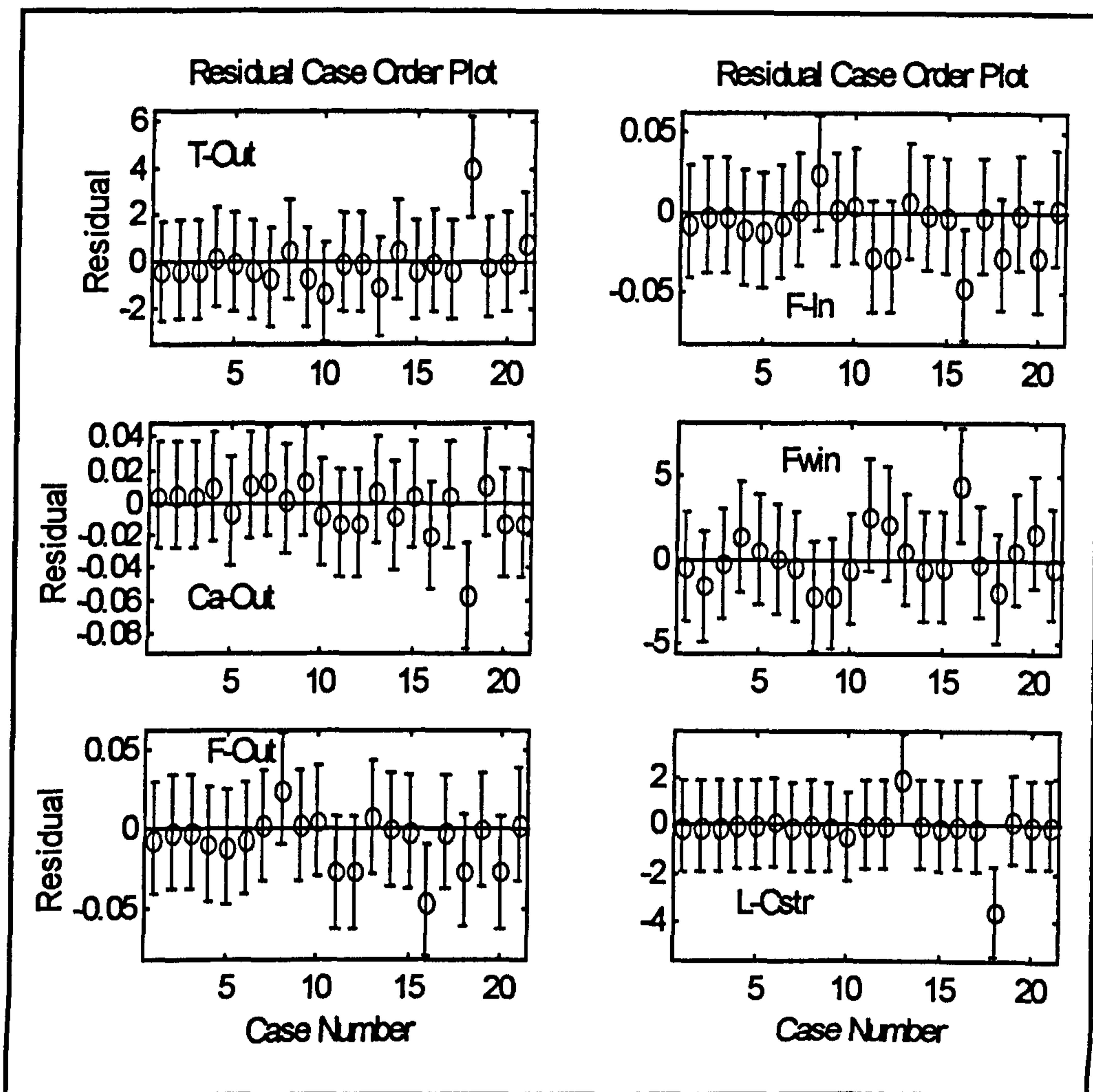


Fig. 7.7. Plots of the residuals with error bars representing 21 cases of the final process steady state condition identified by the qualitative rules.

Table 7.6. ANOVA tables for product temperature and concentration.

Variable	T _{out}				Ca _{out}			
	SS	df	MS	F	SS	df	MS	F
Columns	17.31e ⁻³	1	17.31e ⁻³	51.45e ⁻⁴	47.09e ⁻⁶	1	47.09e ⁻⁶	33.28e ⁻³
Error	134.6	40	3.364		0.05661	40	14.15e ⁻⁴	
Total	134.6	41			0.05666	41		
P-Value	0.9432				0.8562			

Table 7.7. ANOVA tables for reactor feed flow and product flow.

Variable	F_in				F_out			
	SS	df	MS	F	SS	df	MS	F
Columns	57.32e ⁻⁵	1	57.32e ⁻⁵	4.655	54.78e ⁻⁵	1	54.78e ⁻⁵	4.42
Error	49.26e ⁻⁴	40	12.31e ⁻⁵		49.58e ⁻⁴	40	12.4e ⁻⁵	
Total	0.7717	41			55.06e ⁻⁴	41		
P-Value	0.037				0.0419			

Table 7.8. ANOVA tables for reactor level and cooling water flow.

Variable	L_cstr				Fwin			
	SS	df	MS	F	SS	df	MS	F
Columns	11.12e ⁻²	1	11.12e ⁻²	23.04e ⁻²	53.75e ⁻²	1	53.75e ⁻²	25.93e ⁻²
Error	19.31	40	48.28e ⁻²		82.91	40	2.073	
Total	113	41			83.44	41		
P-Value	0.6339				0.6134			

However, by reducing the number of sections from forty-eight to twenty four during the development of the qualitative model will improve the number of predicted cases and also the model estimation of the final process steady state variables. Fig. 7.9 shows the PC1-PC2 plane, the clusters and the sections of all process variables employed in the case study. Each process variable has two clusters and twenty four sections, while the final steady state condition has nine clusters and twenty four sections. The region of each sections increased (in term of area) so that each region will hold more data points. The residual plots are shown in Fig. 7.10 with 95% confidence intervals. These plots show fifty five cases identified from the ninety cases of the validation data. The ANOVA Tables are shown in Tables 7.9 to 7.11 and the box plots are shown in Fig. 7.11. Both the ANOVA Tables and the box plots indicate that the qualitative model has been improved and the estimation of quantitative values of the final process variable becomes more accurate. However, it is not more accurate than the first case study where if statement elements are the three variables of T_{out}, C_{out} and Fwin as shown in Table 7.2.

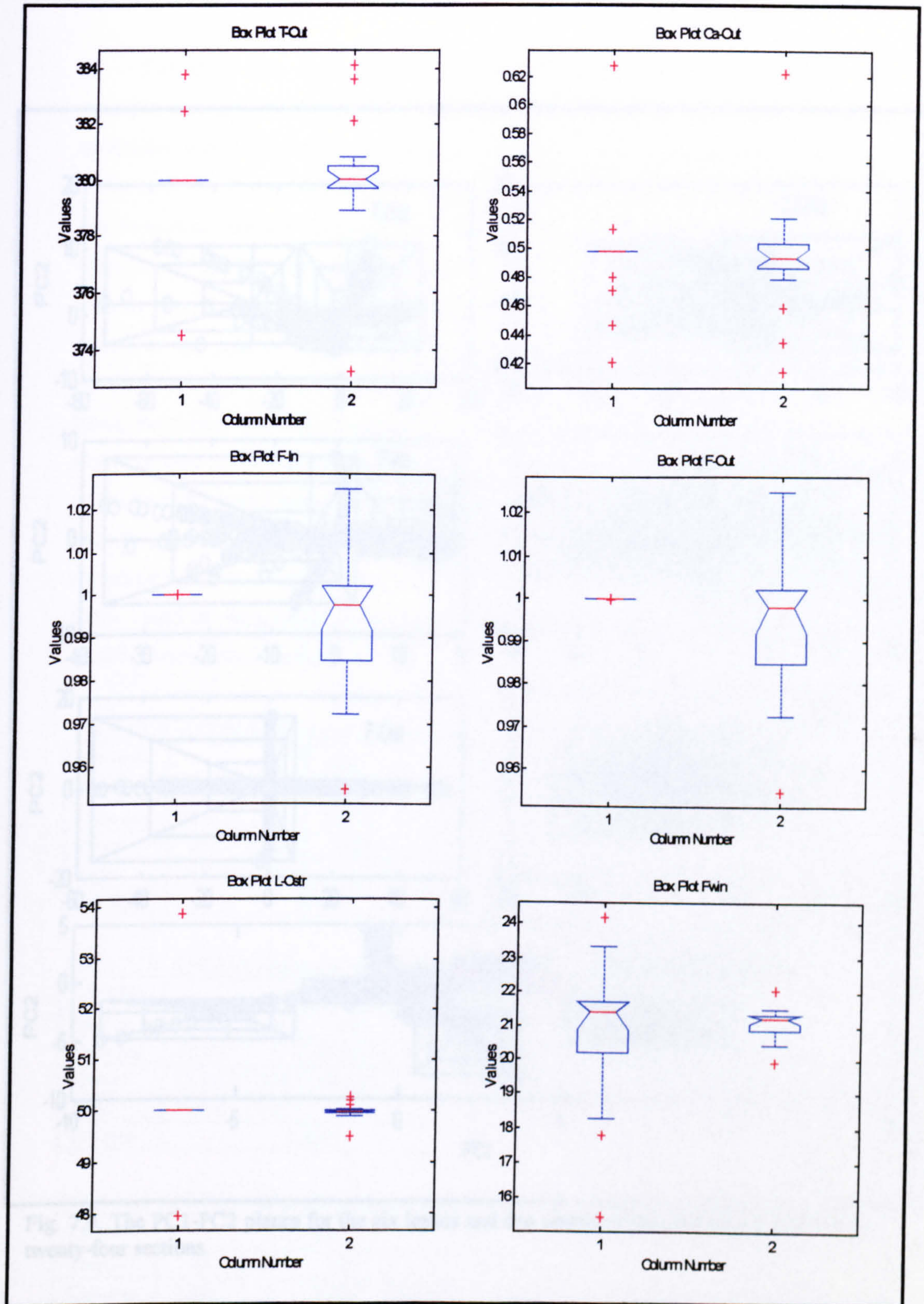


Fig. 7.8. Box plots for the actual validation values (column 1) and the model calculated values (column2) showing data spread from the mean.

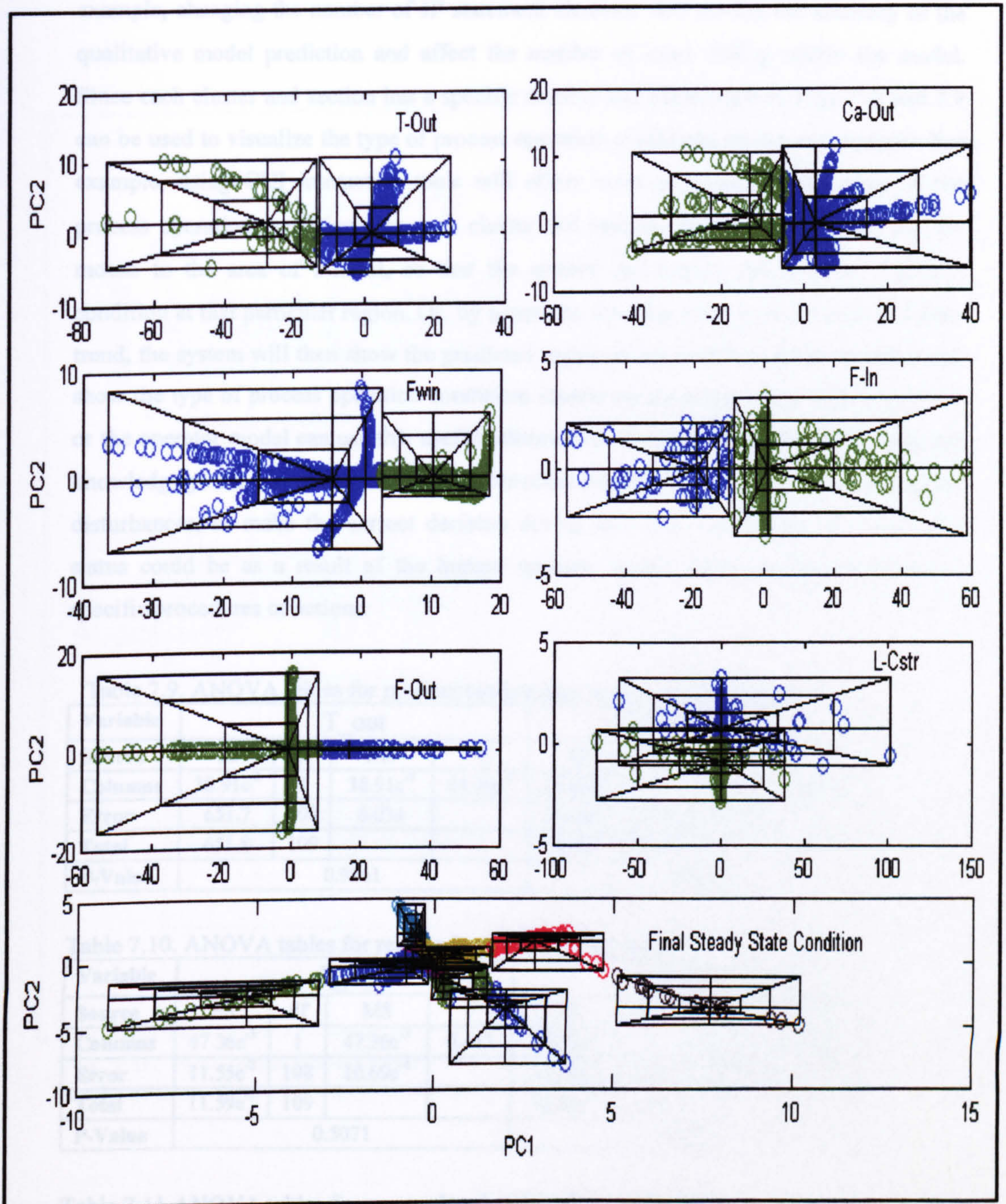


Fig. 7.9. The PC1-PC2 planes for the six inputs and one output of the qualitative model using twenty-four sections.

Columns	9.27e	1	9.27e	9.27e
Error	122.6	108	11.36e	
Total	122.6	108		
P-Value			0.353	

The above case studies indicate that the proposed methodology is flexible. For example, changing the number of IF statement elements will modify the accuracy of the qualitative model prediction and affect the number of cases falling within the model. Since each cluster and section has a specific number and identification, Figs. 7.6 and 7.9 can be used to visualize the type of process operation conditions during any analysis. For example, using GUI interactive tools will allow users to investigate the type of the process operation conditions for each cluster and section. This is done by moving the mouse to the area of interest, so that the system can display the process operation condition at that particular region. Or, by supplying the data, such as the process variables trend, the system will then show the predicted region of the overall process variables and show the type of process operation conditions clearly on the screen. The human operator or the operator model can use this useful information, in conjunction with other data and knowledge yielded by the human operator/process interaction model, such as the type of disturbances, to make the correct decision during abnormal conditions. The operation status could be as a result of the human operator model action during execution of specific procedures or actions.

Table 7.9. ANOVA tables for product temperature and concentration.

Variable	T _{out}				Ca _{out}			
	SS	df	MS	F	SS	df	MS	F
Columns	38.91e ⁻³	1	38.91e ⁻³	64.48e ⁻⁴	14.63e ⁻⁵	1	14.63e ⁻⁵	51.65e ⁻³
Error	651.7	108	6.034		30.58e ⁻²	108	28.32e ⁻⁴	
Total	651.8	109			0.306	109		
P-Value	0.9361				0.8206			

Table 7.10. ANOVA tables for reactor feed and product flow.

Variable	F _{in}				F _{out}			
	SS	df	MS	F	SS	df	MS	F
Columns	47.36e ⁻⁵	1	47.36e ⁻⁵	0.443	43.49e ⁻⁵	1	43.49e ⁻⁵	0.4054
Error	11.55e ⁻²	108	10.69e ⁻⁴		11.59e ⁻²	108	10.73e ⁻⁴	
Total	11.59e ⁻²	109			11.63e ⁻²	109		
P-Value	0.5071				0.5257			

Table 7.11 ANOVA tables for reactor level and cooling water flow.

Variable	L _{cstr}				F _{win}			
	SS	df	MS	F	SS	df	MS	F
Columns	9.87e ⁻¹	1	9.87e ⁻¹	86.92e ⁻²	25.99e ⁻¹	1	25.99e ⁻¹	61.28e ⁻²
Error	122.6	108	11.36e ⁻¹		458	108	4.241	
Total	123.6	109			460.6	109		
P-Value	0.3533				0.4354			

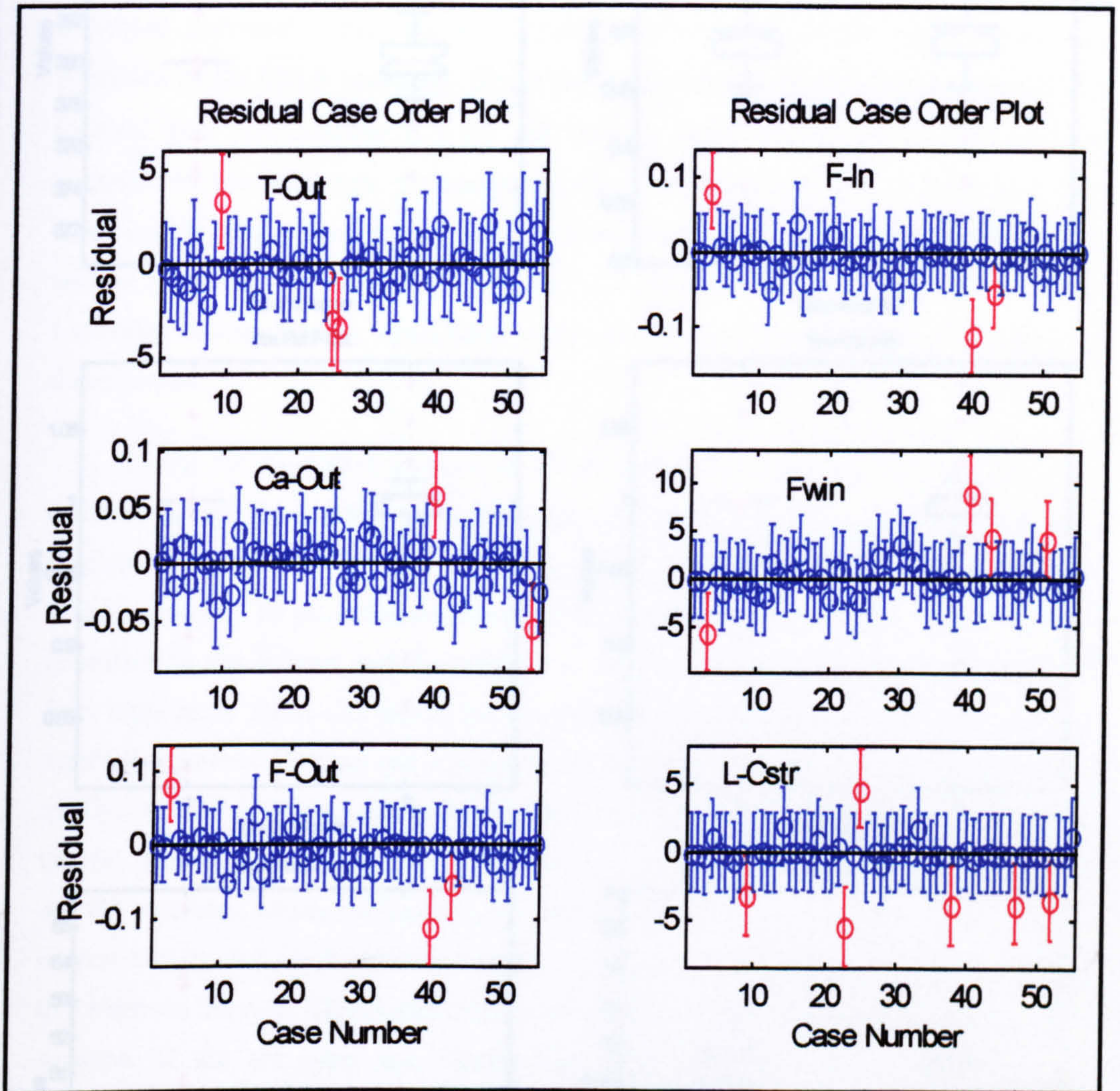


Fig. 7.10. Plots of the residuals with error bars representing 21 cases of the final process steady state conditions identified by the qualitative rules.

Fig. 7.11. Box plots for the actual validation dataset, showing the data spread from the mean.

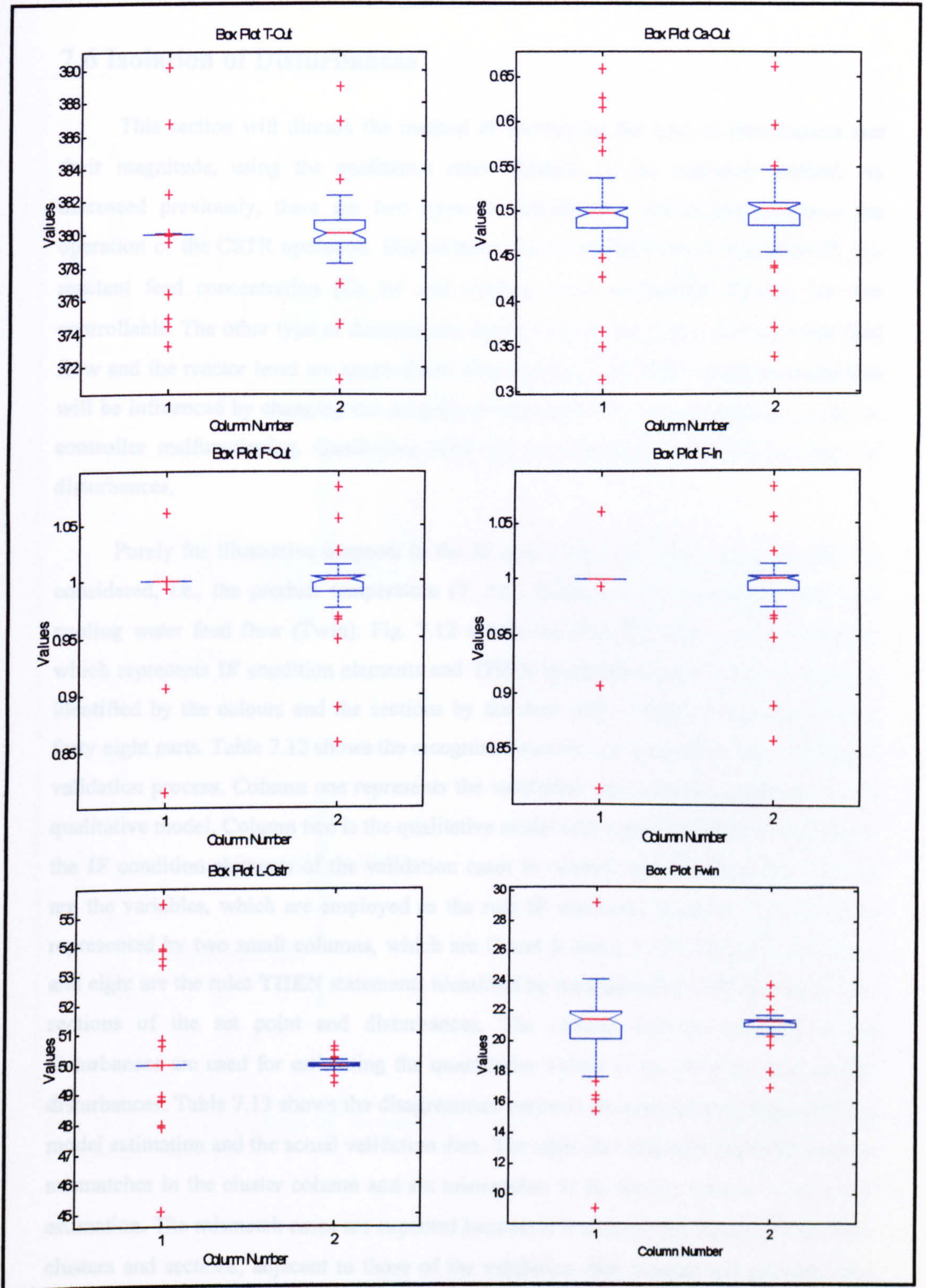


Fig. 7.11. Box plots for the actual validation (column 1) and the model estimation (column 2) values, showing the data spread from the mean

7.6 Isolation of Disturbances

This section will discuss the method of identifying the type of disturbances and their magnitude, using the qualitative rules obtained by the proposed method. As discussed previously, there are two types of disturbances, which can influence the operation of the CSTR operation. Disturbances due to reactant feed temperature (T_{in}), reactant feed concentration (Ca_{in}) and cooling water temperature (T_{win}) are non controllable. The other type of disturbances due to reactant feed flow, cooling water feed flow and the reactor level are controllable disturbances. The CSTR operation conditions will be influenced by changing the set point of the controller, e.g. by operators or due to controller malfunctioning. Qualitative rules can be developed to predict the type of disturbances.

Purely for illustrative purpose, in the **IF** part of the rule, only three variables are considered, i.e., the product temperature (T_{out}), product concentration (Ca_{out}), and cooling water feed flow (T_{win}). Fig. 7.12 shows the PC1-PC2 plane of the variables, which represents **IF** condition elements and **THEN** statements of the rules. The clusters identified by the colours and the sections by the dark lines, which cut the clusters into forty eight parts. Table 7.12 shows the recognised cases by the qualitative rules during the validation process. Column one represents the validation case numbers identified by the qualitative model. Column two is the qualitative model rule numbers, which are similar to the **IF** condition elements of the validation cases in column one. Columns three to five are the variables, which are employed as the rule **IF** statement elements. Each variable represented by two small columns, which are C and S (table 7.12). Columns six, seven and eight are the rules **THEN** statements identified by the qualitative rules as clusters and sections of the set point and disturbances. The clusters and the sections of the disturbances are used for estimating the quantitative values of the set point and process disturbances. Table 7.13 shows the disagreement between the clusters and sections of the model estimation and the actual validation data. The table also indicates that there are two mismatches in the cluster column and six mismatches in the section column in set point estimation. The mismatch cases are expected because it is possible for the model to reveal clusters and sections, adjacent to those of the validation data clusters and sections. The last two columns of the table give the types of influences causing the process operation to shift from one state to another. Number two indicates that the human operator intervenes in the process operation, which causes the existing situation due to altering the controller set points.

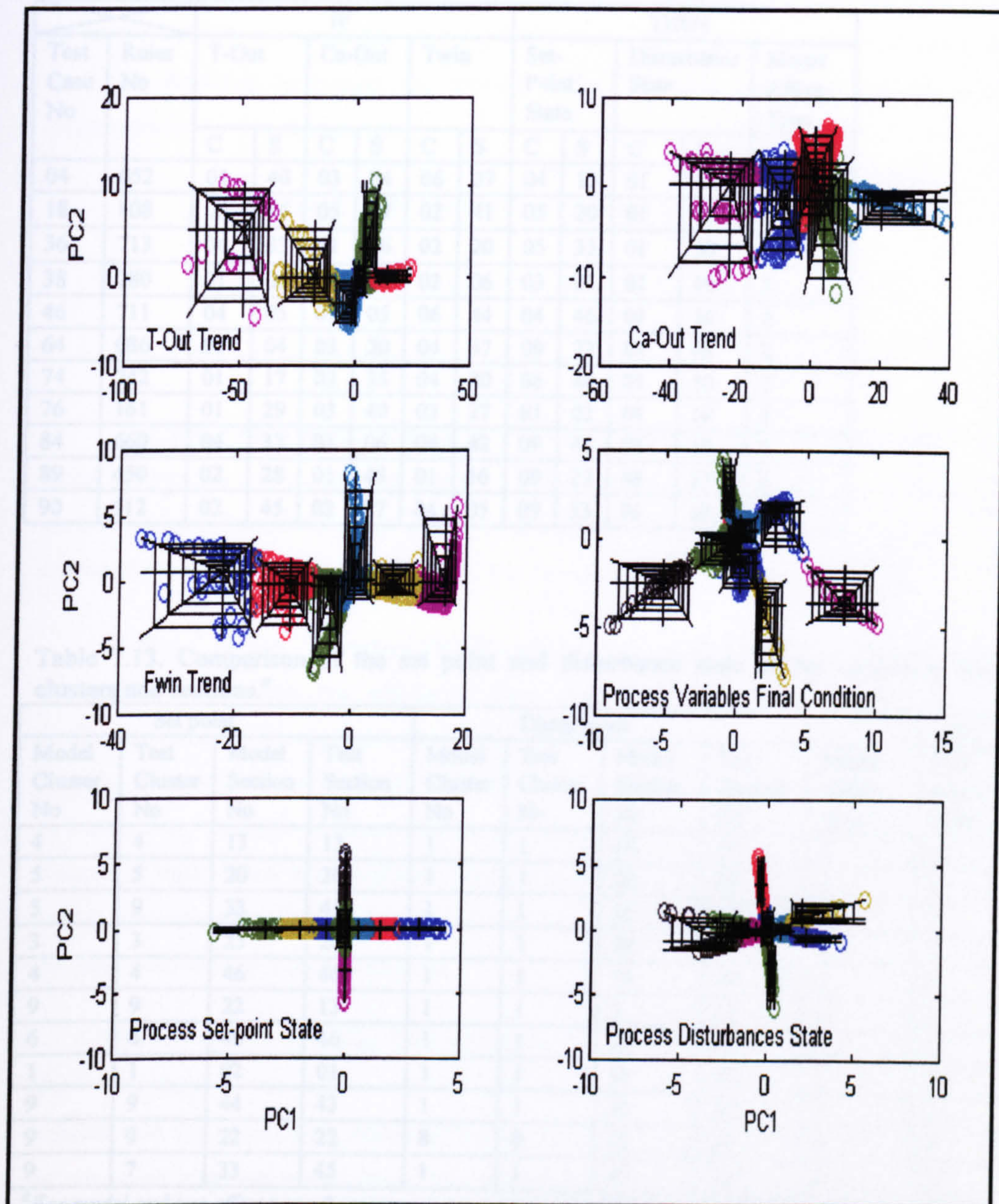


Fig. 7.12. PC1-PC2 planes of the process variables used as the qualitative model for disturbance isolation.

Number three indicates that the process variables are not independent. This is because the process variables are not independent. There were two missed for the effect. Theoretically, it is impossible to predict the effect of the process variables on the process variables, since both disturbances are independent. This is demonstrated by the following example. If y_1, y_2, y_3 are the process variables and x_1 and x_2 are the process variables, but x_1 and x_2 cannot be estimated just by increasing the process variables.

Table 7.12. Qualitative model clusters and sections outcome.

Test Case No		Rules No		IF						THEN				
				T-Out		Ca-Out		Twin		Set-Point State		Disturbance State		Model Affect Type
				C	S	C	S	C	S	C	S	C	S	
04	052	01	40	03	04	06	37	04	13	01	10	2		
18	808	06	46	05	27	02	41	05	20	01	10	2		
36	713	04	33	01	06	02	20	05	33	01	10	2		
38	280	01	06	02	24	02	06	03	25	01	10	3		
46	711	04	05	03	05	06	44	04	46	01	10	2		
64	086	01	04	03	20	04	37	09	22	01	03	2		
74	242	01	17	03	35	04	20	06	46	01	10	2		
76	161	01	29	03	40	03	27	01	02	01	10	2		
84	660	04	33	01	06	04	42	09	44	01	10	2		
89	450	02	28	01	45	01	16	09	22	08	23	2		
90	512	02	45	02	27	04	05	09	33	01	10	2		

Table 7.13. Comparison of the set point and disturbance state of the validation data clusters and sections.^a

Set point				Disturbance					
Model Cluster No	Test Cluster No	Model Section No	Test Section No	Model Cluster No	Test Cluster No	Model Section No	Test Section No	Model Affect Type	Test Affect Type
4	4	13	13	1	1	10	10	2	2
5	5	20	20	1	1	10	10	2	2
5	9	33	45	1	1	10	10	2	2
3	3	25	26	1	1	10	10	3	2
4	4	46	46	1	1	10	10	2	2
9	9	22	13	1	1	3	10	2	2
6	6	46	46	1	1	10	10	2	2
1	1	02	01	1	1	10	10	2	2
9	9	44	43	1	1	10	10	2	2
9	9	22	22	8	8	23	23	2	3
9	7	33	45	1	1	10	10	2	2

^aFor model and test affect types 2 mean operator intervene and 3 mean disturbances.

Number three indicates that the process operation conditions are caused by the process disturbances. There were two misses due to one condition sharing two types of effect. Theoretically, it is impossible to predict the type of the disturbances of the two missed cases, since both disturbances are independent variables. This can be demonstrated by the following example. If $y = x_1 + x_2$, y can be estimated by knowing x_1 and x_2 , but x_1 and x_2 cannot be estimated just by knowing y only because x_1 and x_2 can

have any value. This type of problem can be solved by analysing the historical data, such as the probability of occurrence of these faults during the operation or by examining the previous condition to predict the present faults. The last suggestion can be easily demonstrated by this simple rule.

IF previous=A and present=2 or present=3 **THEN** disturbance=3.

IF previous=D and present=2 or present=3 **THEN** disturbance=2.

A and D could be the cluster and section of IF statement.

The quantitative values of the set point and the process disturbances are calculated using the clusters and sections of Table 7.12. The residual plots with 95% confidence for human operator intervention are shown in Fig. 7.13. The plots show two outliers. One occurs in the cooling water feed set point and the other in the reactor feed set point.

Tables 7.14 and 7.15 reveal that the estimated set point for the identified cases is acceptable. The values are estimated from clusters and sections predicted by the qualitative rules, which represent the location of the disturbances. These tables also show that the estimated values and the validation values are identical because the P-value indicates that F statistic is as extreme as the observed F would occur by a 9 out of ten chances if both actual and predicted values are truly equal. The box plots in Fig. 7.14 shows the validation data (column one) has the same spread as the estimated values (column two) with overlapped notches.

The residual plots in Fig. 7.15 with 95% confidence for the process disturbances show that there is one outlier case in each plot. The ANOVA Tables 7.16 and 7.17 indicate that the quantitative values estimated for process disturbances is not as good as the set point value estimation cases. The box plots in Fig. 7.16 shows that the estimated values are spread along the value axis while the actual are concentrated around the mean.

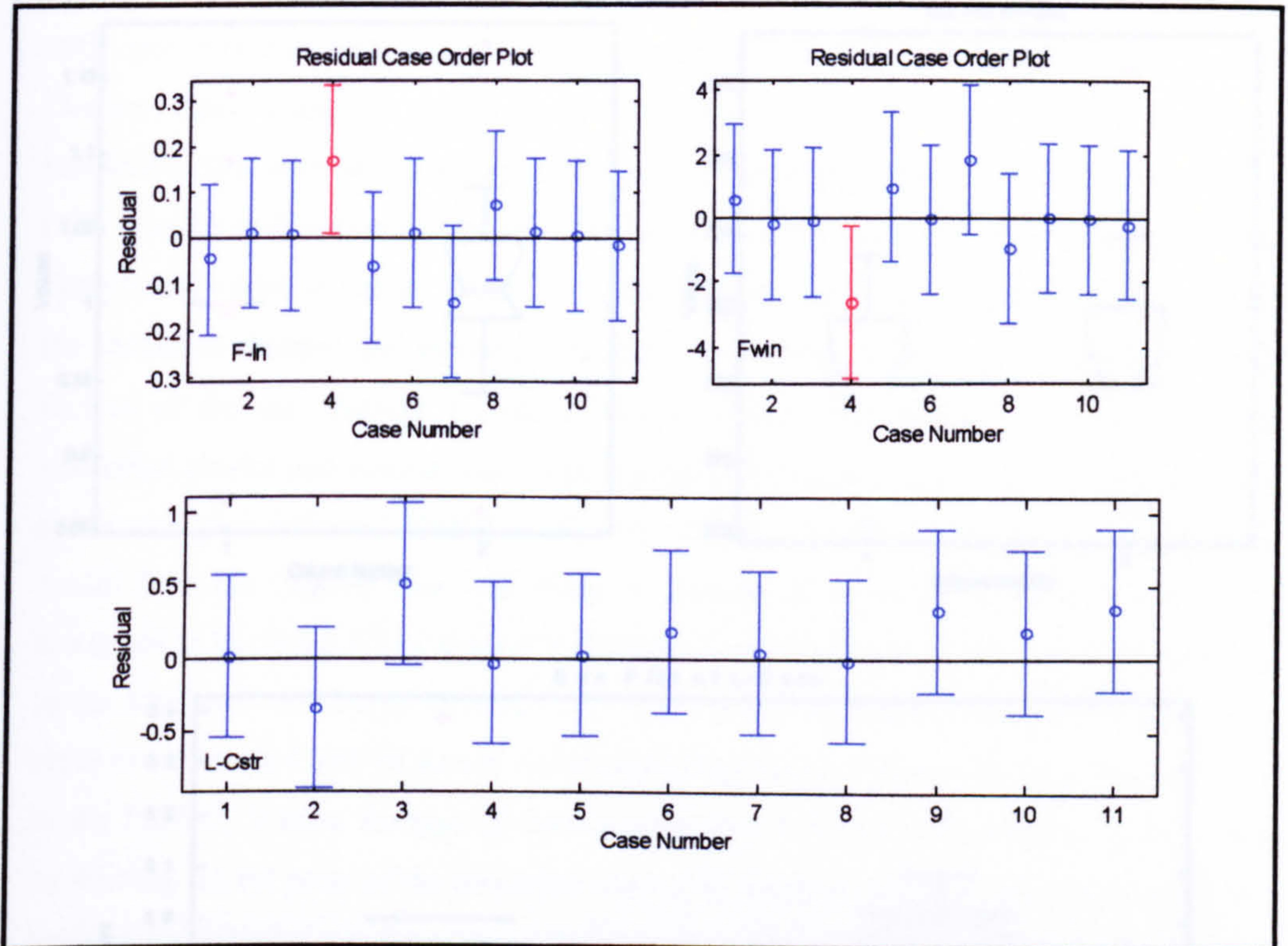


Fig. 7.13. Plots of the residuals with error bars representing 11 cases identified by the qualitative rules.

Table 7.14. ANOVA tables for feed and cooling water flow set point state.

Variable	F_in				F_out			
	SS	df	MS	F	SS	df	MS	F
Columns	62.01e ⁻⁶	1	62.01e ⁻⁶	11.89e ⁻³	78.72e ⁻³	1	78.72e ⁻³	83.86e ⁻⁴
Error	10.43e ⁻²	20	52.17e ⁻⁴		18.77e ¹	20	93.87e ¹	
Total	10.44e ⁻²	21			18.78e ¹	21		
P-Value	0.9143				0.9279			

Table 7.15. ANOVA table for reactor level set point state.

Variable	L_cstr			
Columns	19.28e ⁻³	1	19.28e ⁻³	76.05e ⁻⁴
Error	50.71	20	25.36e ⁻¹	
Total	50.73	21		
P-Value	0.9314			

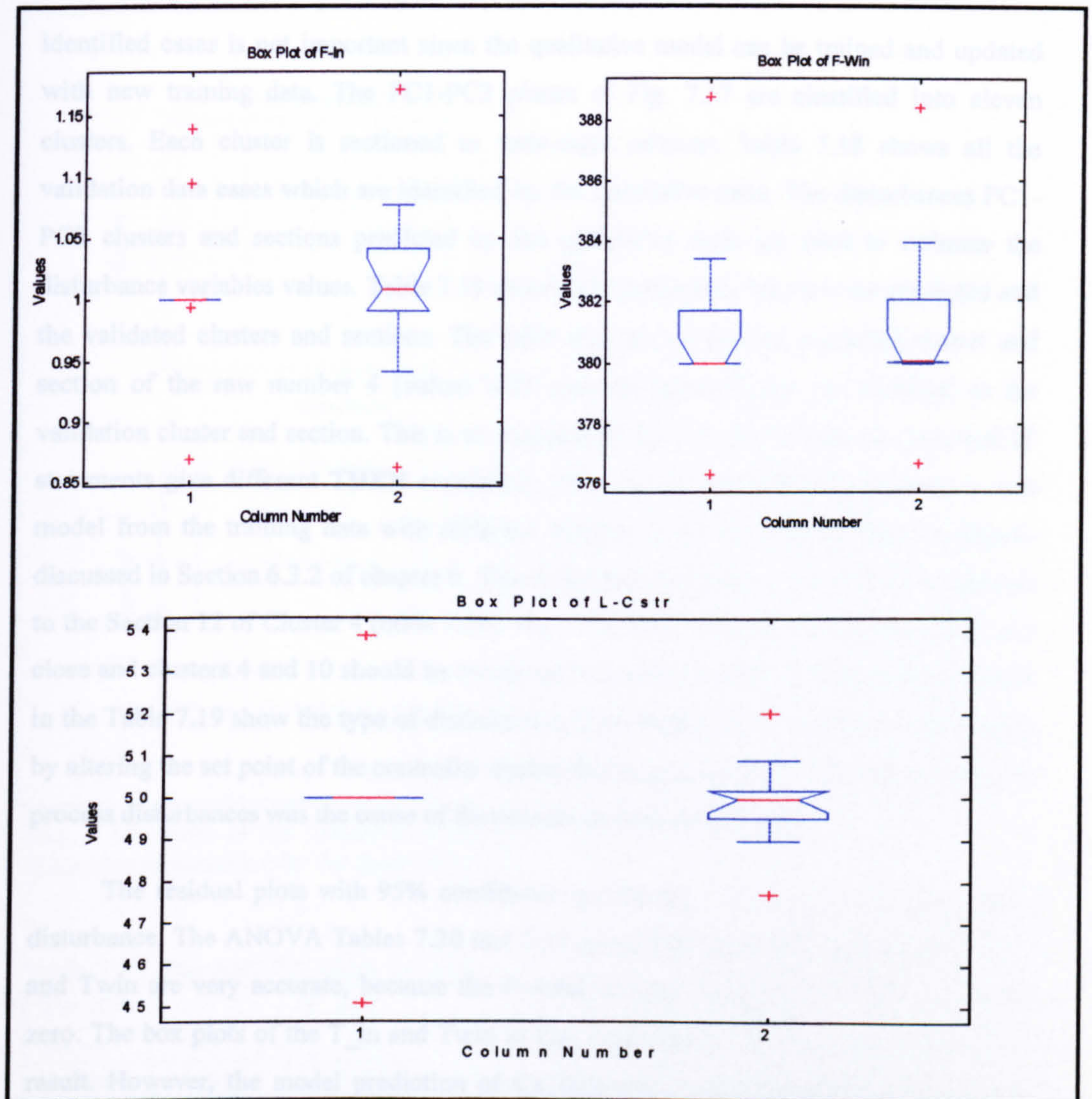


Fig. 7.14. Box plots for the validation values (column 1) and the model estimated values (column 2) showing the data spread from the mean for controller set points.

The final case study is to predict the type of disturbances and the process disturbances variable data from the first few samples of the dynamic operation trends. Fig. 7.17 shows the qualitative model, which is constructed from samples 7, 8 and 9 of the dynamic trends. A matrix was constructed, which has rows representing the case runs (number of operations) and columns representing the six process variables, which are T_{out} , C_{out} , F_{out} , F_{in} , T_{win} and $Lcstr$.

The three qualitative models developed from Samples 7, 8 and 9, as shown in Table 7.18, represent the IF statement elements. These samples are chosen because their data range has the highest variation during the operation (see Fig. 7.5). The number of the

identified cases is not important since the qualitative model can be trained and updated with new training data. The PC1-PC2 planes of Fig. 7.17 are classified into eleven clusters. Each cluster is sectioned to forty-eight sections. Table 7.18 shows all the validation data cases which are identified by the qualitative rules. The disturbances PC1-PC2 clusters and sections predicted by the qualitative rules are used to estimate the disturbance variables values. Table 7.19 shows the comparison between the predicted and the validated clusters and sections. The table also shows that the predicted cluster and section of the row number 4 (values with grey background) are not identical to the validation cluster and section. This is an example of rules conflict where two identical **IF** statements give different **THEN** conditions. This can be eliminated by creating a new model from the training data with different number of clusters and sections as already discussed in Section 6.3.2 of chapter 6. This is because Section 3 of Cluster 10 is adjacent to the Section 12 of Cluster 4 (table 7.19). Fig. 7.18 shows that the two locations are very close and clusters 4 and 10 should be combined to a single cluster. The final two columns in the Table 7.19 show the type of disturbances. Two means human operator intervention by altering the set point of the controller during the process operation and three means the process disturbances was the cause of the present operational situation.

The residual plots with 95% confidence are shown in Fig. 7.19 for each process disturbance. The ANOVA Tables 7.20 and 7.21 reveal that the model prediction of T_{in} and T_{win} are very accurate, because the P-value is close to one and F-factor is almost zero. The box plots of the T_{in} and T_{win} in Fig. 7.20 confirm the outcomes of ANOVA result. However, the model prediction of Ca_{in} is not so promising since the P-value indicates that F statistic as extreme as the observed F would occur by a chance of only 3 out of 10 if both the actual and predicted values are truly equal to each other.

Two methods are used in the isolation cases studies. The first method is developed using the trends of the independent variables of the process. The second method is developed using only the first few samples from process variables trends to estimate the disturbances. The second method can also be used online with the CSTR process for estimation of disturbances during process operation. Both methods indicate that some variables can be estimated more accurately than the others. Although the qualitative rules do not identify all the validation cases, this should not be considered as a limitation since all the qualitative rules can be trained with more data obtained from training cases covering all the regions of process operation conditions.

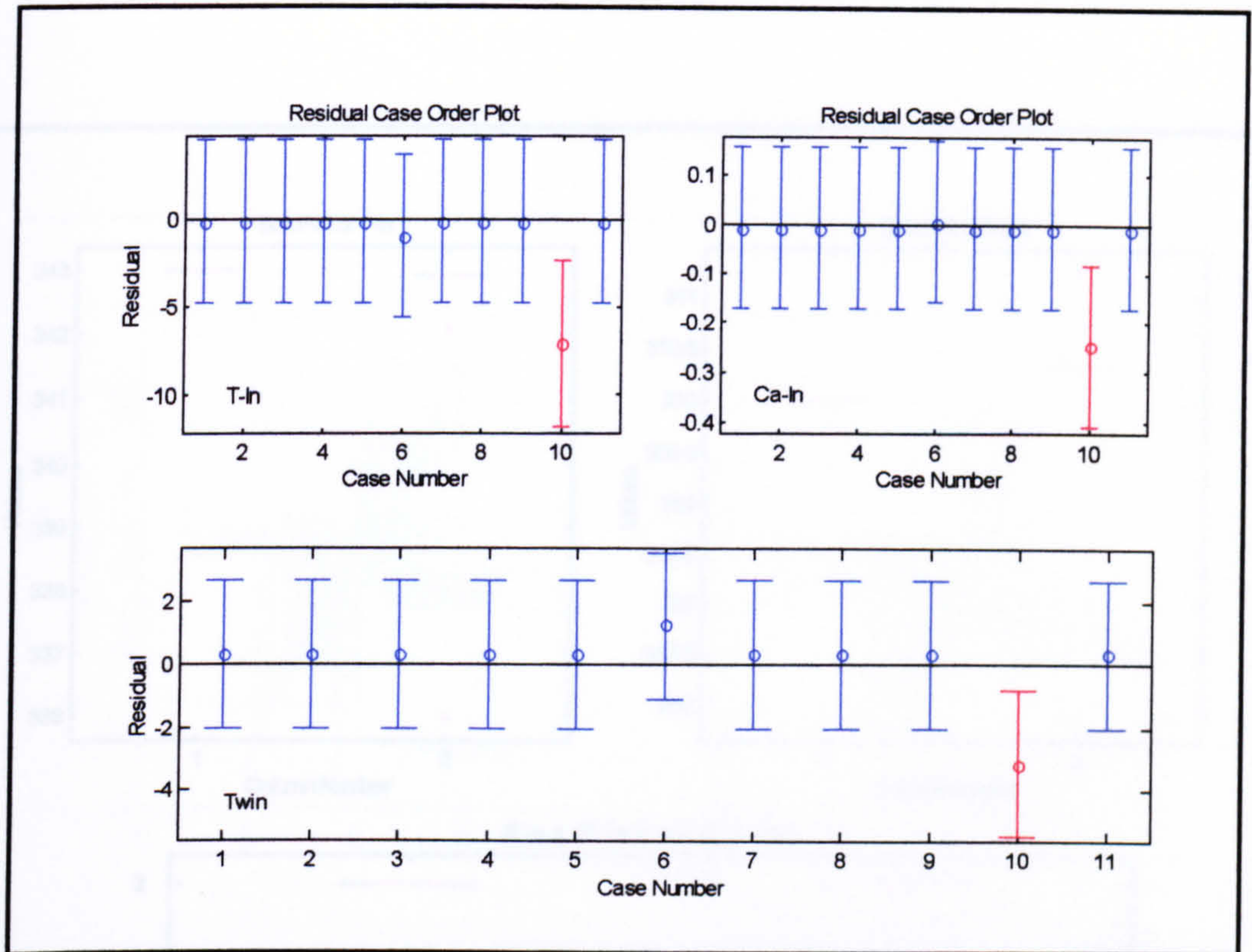


Fig. 7.15. Plots of the residuals with error bars representing 11 cases of the process disturbances identified by the qualitative rules.

Table 7.16. The ANOVA tables for inlet feed and cooling water temperature.

Variable	T_out				Ca_out			
	SS	df	MS	F	SS	df	MS	F
Columns	34.36e ⁻¹	1	34.36e ⁻¹	15.75e ⁻¹	64.08e ⁻³	1	64.08e ⁻³	10.38e ⁻²
Error	43.62	20	21.88e ⁻¹		12.34	20	61.72e ⁻²	
Total	47.05	21			12.41	21		
P-Value	0.2223				0.7506			

Fig. 7.16. Box plots for the model variables. The mean values (columns 1) and standard deviation values (column 2) of the model variables are reported.

Table 7.17. The ANOVA table for inlet feed concentration.

Variable	Ca-In			
	SS	df	MS	F
Columns	42.84e ⁻⁴	1	42.84e ⁻⁴	26.51e ⁻²
Error	32.32e ⁻²	20	16.16e ⁻³	
Total	32.75e ⁻²	21		
P-Value	0.6123			

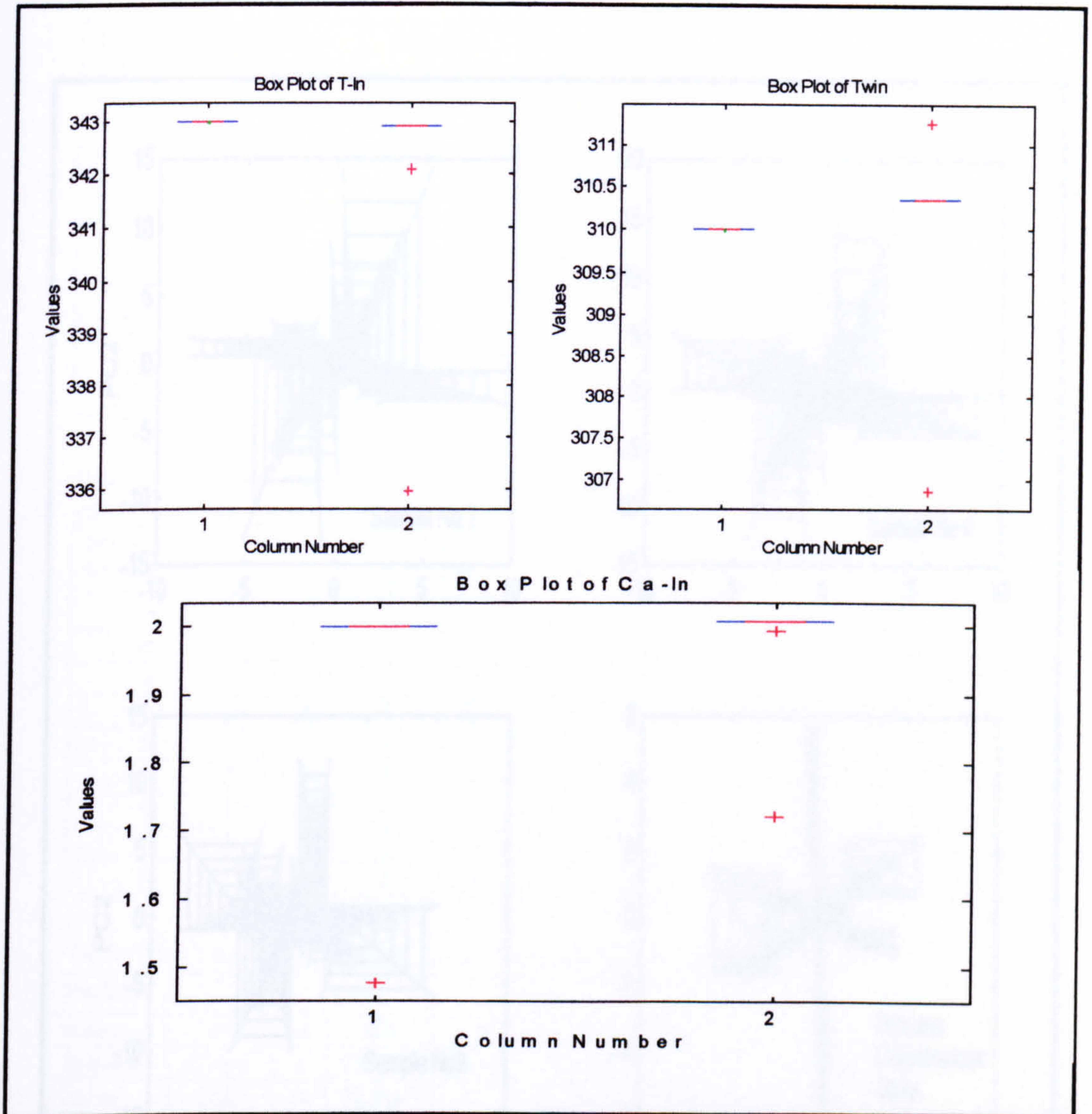


Fig. 7.16. Box plots for the actual validation values (column 1) and the model estimated values (column 2) of disturbances data spreading from the mean.

Fig. 7.17. PC1-PC2 plot for model 1. The model estimated values are compared with the qualitative model.

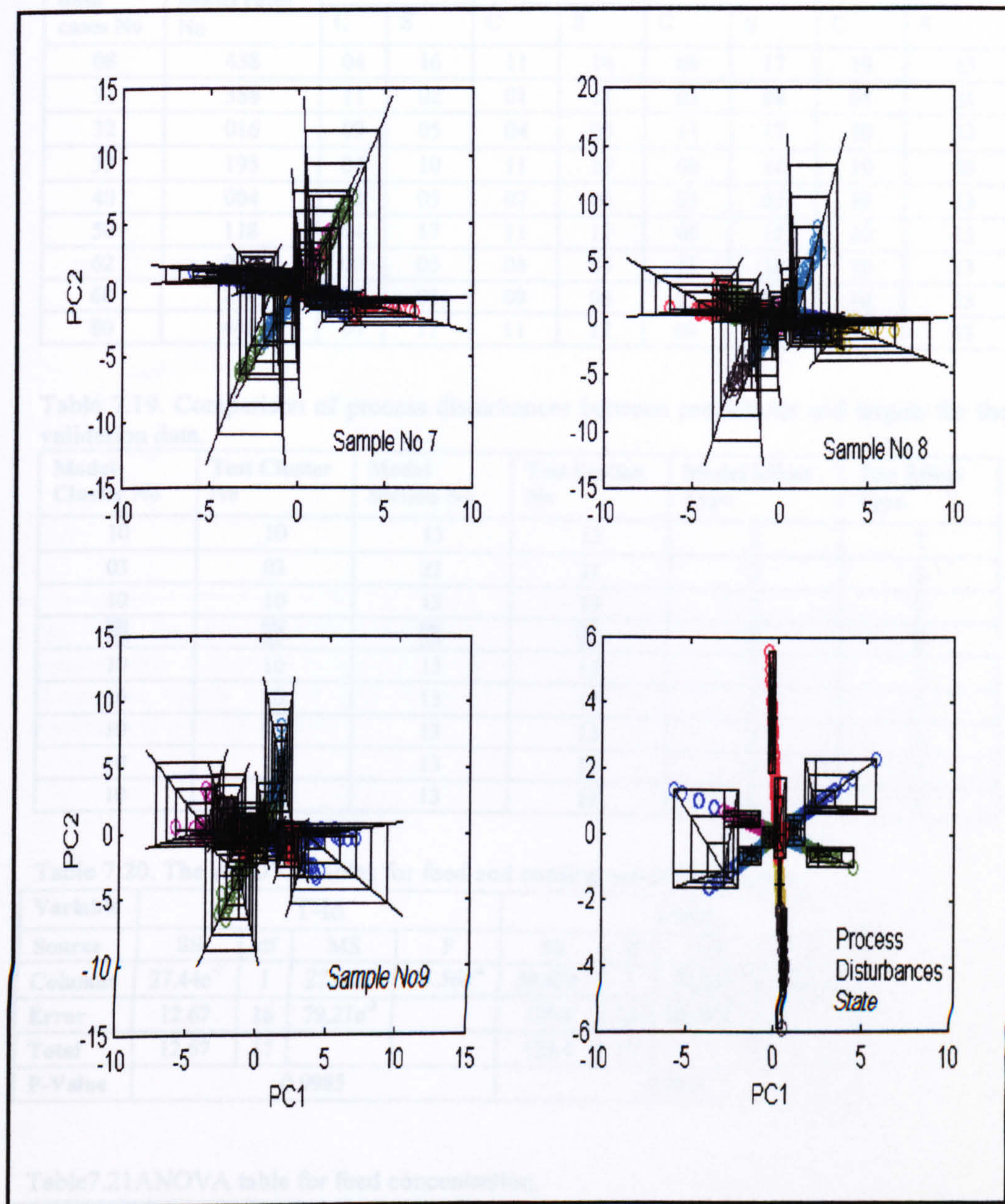


Fig. 7.17. PC1-PC2 planes for samples 7, 8, 9 and process disturbances used as qualitative models.

Table 7.18. The clusters and the sections of the training data predicted by the qualitative models.

		IF						THEN	
		Sample 7		Sample 8		Sample 9		Disturbance State	
		C	S	C	S	C	S	C	S
Training data cases No	Qualitative model rules No								
08	438	04	16	11	16	06	17	10	13
31	388	11	02	01	11	03	08	03	21
32	016	09	05	04	05	11	17	10	13
33	195	04	10	11	23	06	14	10	03
40	004	02	05	07	06	07	05	10	13
50	118	04	17	11	17	06	18	10	13
62	026	09	05	04	05	11	18	10	13
68	200	05	04	09	08	02	07	10	13
80	440	04	17	11	17	09	06	10	13

Table 7.19. Comparison of process disturbances between predictions and targets for the validation data.

Model Cluster No	Test Cluster No	Model Section No	Test Section No	Model Effect Type	Test Effect Type
10	10	13	13	2	2
03	03	21	21	2	3
10	10	13	13	2	2
10	04	03	12	3	3
10	10	13	13	2	2
10	10	13	13	2	2
10	10	13	13	2	2
10	10	13	13	2	2
10	10	13	13	2	2

Table 7.20. The ANOVA tables for feed and cooling water temperature.

Variable	T-In				Twin			
	SS	df	MS	F	SS	df	MS	F
Columns	27.44e ⁻⁷	1	27.44e ⁻⁷	53.56e ⁻⁸	50.62e ⁻⁴	1	50.62e ⁻⁴	62.6e ⁻⁵
Error	12.67	16	79.21e ⁻²		129.4	16	80.85e ⁻¹	
Total	12.67	17			129.4	17		
P-Value	0.9985				0.9985			

Table 7.21 ANOVA table for feed concentration.

Variable	Ca-In			
	SS	df	MS	F
Columns	40.9e ⁻⁵	1	40.9e ⁻⁵	1.257
Error	52.07e ⁻⁴	16	32.55e ⁻⁵	
Total	56.16e ⁻⁴	17		
P-Value	0.2788			

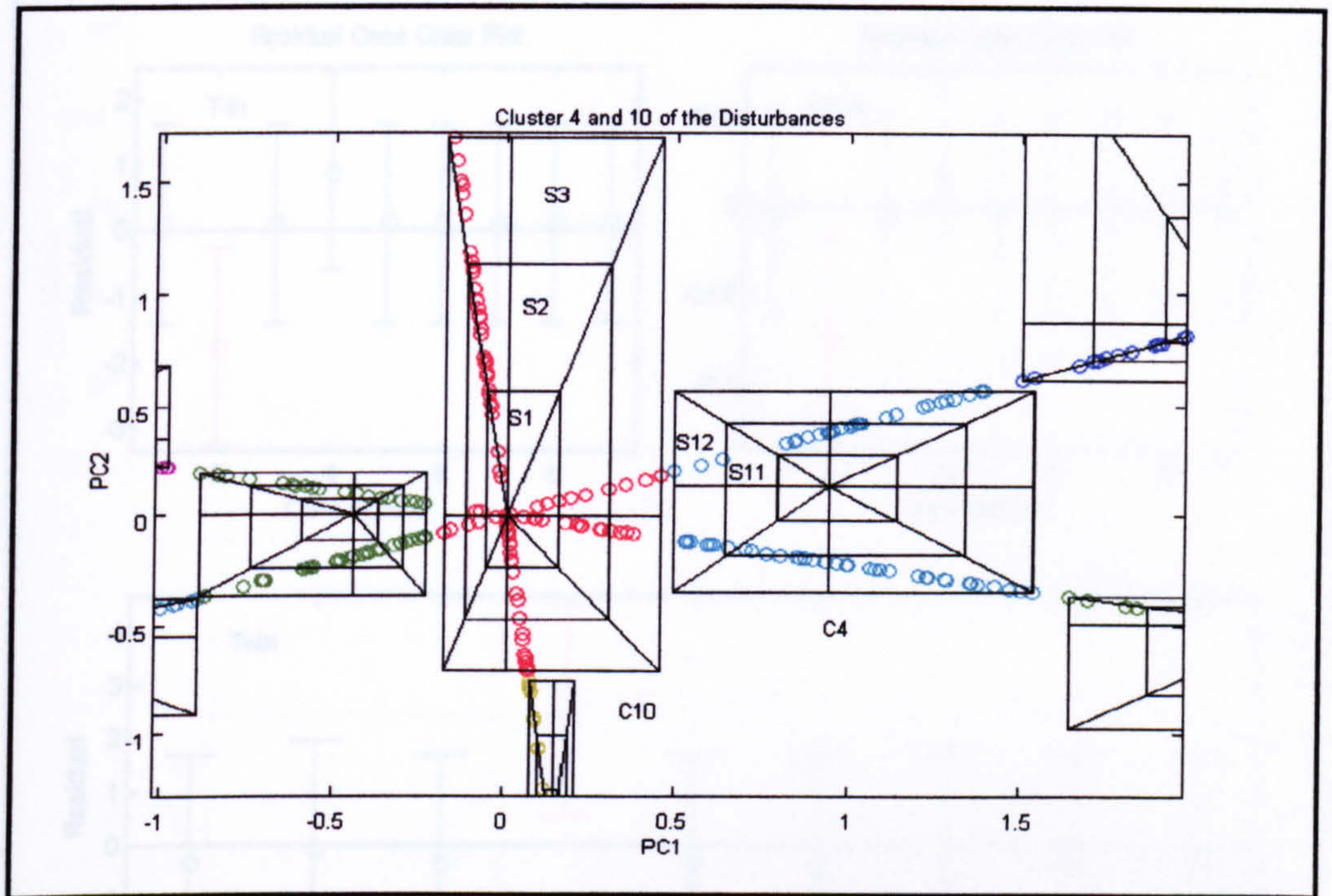


Fig. 7.18. Zoom in PC1-PC2 plane for clusters 4 and 10 of disturbances in Fig. 7.17, showing that cluster C4 is adjacent to cluster C10 (row number 4 of Table 7.19, which shows the values with a grey background), therefore these two clusters should be combined to a single cluster.

Fig. 7.19. Plots of the members with small norm differences between the two clusters identified by the optimization step.

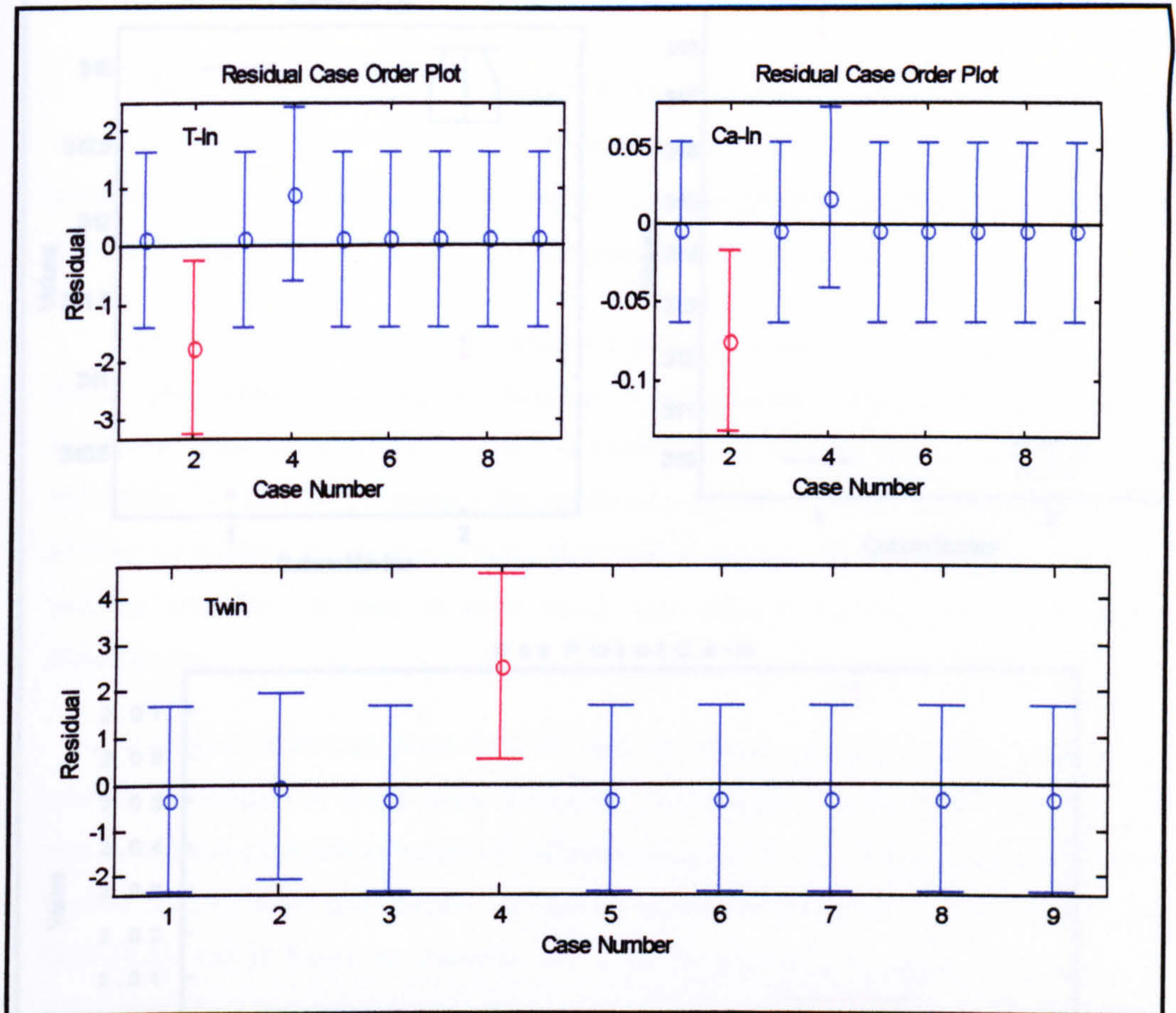


Fig. 7.19. Plots of the residuals with error bars representing 9 cases of the process disturbances identified by the qualitative rules.

Fig. 7.20. Box plots for the validation values of the training sets (shown in black) and the model estimated values (shown in red) of disturbances case spread from the cases.

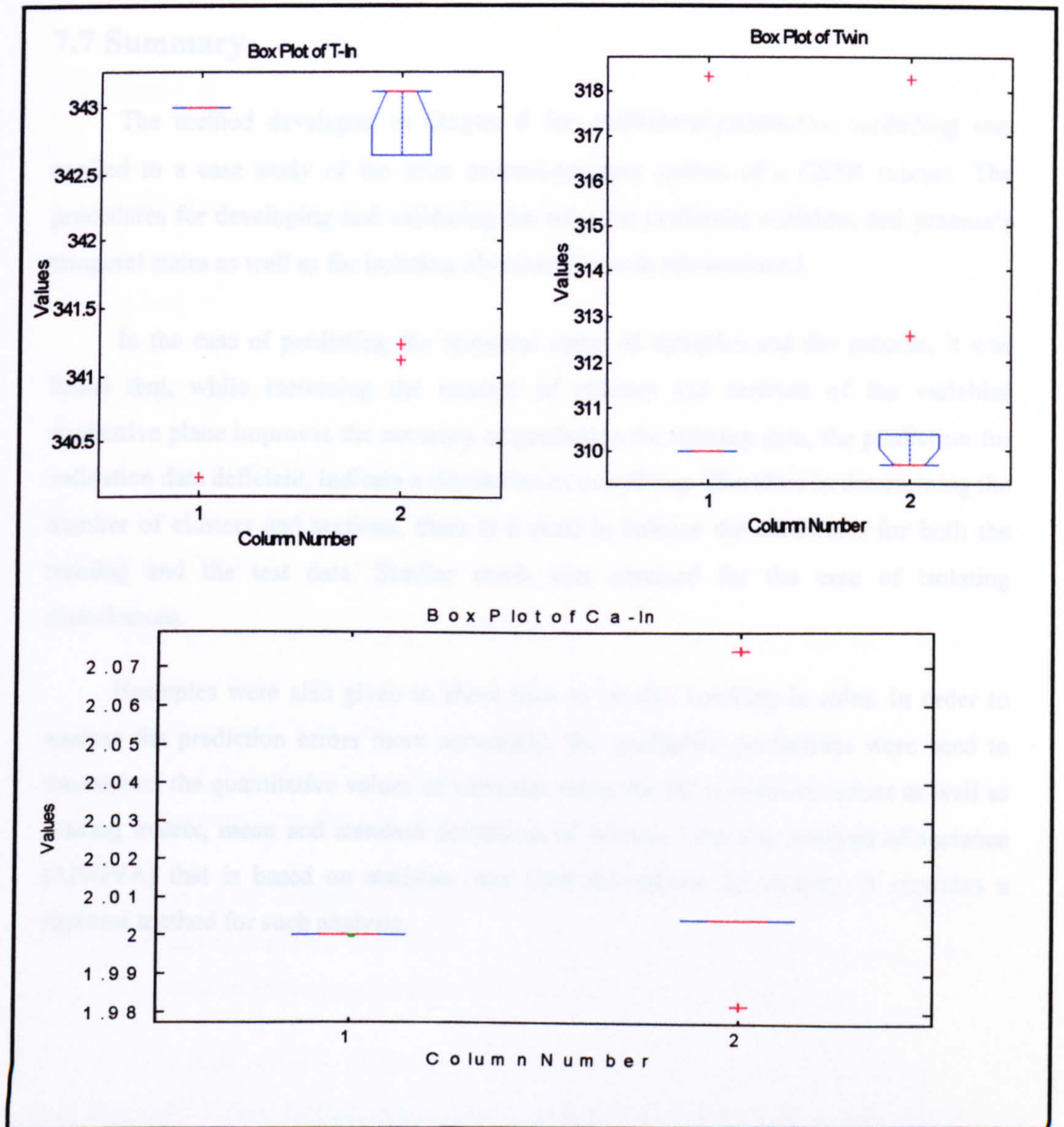


Fig. 7.20. Box plots for the validation values or the training data values (column 1) and the model estimated values (column 2) of disturbances data spread from the mean.

7.7 Summary

The method developed in chapter 6 for qualitative/quantitative modelling was applied to a case study of the joint process-operator system of a CSTR reactor. The procedures for developing and validating the rules for predicting variables and process's temporal states as well as for isolating disturbances were demonstrated.

In the case of predicting the temporal states of variables and the process, it was found that, while increasing the number of clusters and sections of the variables qualitative plane improves the accuracy of prediction for training data, the prediction for validation data deficient, indicate a simulation of *overfitting*. Therefore in determining the number of clusters and sections, there is a need to balance the accuracies for both the training and the test data. Similar result was obtained for the case of isolating disturbances.

Examples were also given to show how to resolve conflicts in rules. In order to analyse the prediction errors more accurately, the qualitative predictions were used to reconstruct the quantitative values of variables using the PC coordinate values as well as loading matrix, mean and standard deviations of models. One-way analysis of variance (ANOVA) that is based on statistics was used throughout the chapter. It provides a rigorous method for such analysis.

Chapter 8

Conclusions and Suggestions for Future Work

8.1 Conclusions

The work reported in this thesis is motivated mainly by the following observations *on previous studies on computer aided systems for automatic identification and diagnosis of abnormal operations of processes.*

- Most previous studies assumed that after a fault occurring, the process would evolve without operators intervention. For example, high fidelity dynamic simulators have been widely used in developing and testing various techniques and tools for fault detection and diagnosis. They only emulate the process behaviour without considering possible operators intervention during the dynamic transition.
- Almost all the studies on automatic fault detection and diagnosis have focused on only part of the integrated system, i.e., the process part. No effort has been made on automatic monitoring and assessing the other part, i.e., the operators.

The lack of effort in integrating operators' factors into automated fault detection and diagnostic system is disproportionate to statistics. According to a worldwide survey carried out by a Honeywell led consortium (Nimmo, 1995), 40% of faults happened in chemical history is due to human errors. A parallel study on case histories by the Health and Safety Commission (Larder and Fleming, 1996) indicated that 80% of accidents have human factors involved. Efforts to address human errors in process safety have so far limited to hazard and operability studies in the process design stage, training of operational personnel and prediction of human reliability.

The overall objectives of the research were to develop a methodology to involve the human factors into the development of systems for automatic identification and diagnosis of abnormal operations, and to investigate methods and techniques that can be used to capture, characterise and assess the performance of operators as well as that of the process.

The main achievements of the research are:

- (1) A critical review has been made in chapter 2 of the previous work on computer-based automatic detection and diagnosis of process abnormal operations. The review covered the techniques of real-time expert systems, univariate and multivariate statistic process control, supervised and unsupervised neural networks as well as data pre-processing technologies, hybrid systems and digraphs. The review also revealed the need to carry out studies on integrating human factors into the development of fault detection and diagnosis systems.
- (2) A platform is developed for carrying out the studies, which is a joint process-operator dynamic simulation environment. The process part is a dynamic process simulator, which emulates in high fidelity the dynamic behaviour of the process under the influence of various disturbances as well as operator's actions. The operator part is coded as a real time expert system emulating operators' behaviour and the interaction between the process simulator and the real time expert system was managed through an interaction model. The dedicated interaction model manages the synchronisation through dynamic data exchange (DDE), transformation of data formats, and also serves as an interface for initiating variations and performing data analysis. The effectiveness of the platform was proved in case studies presented in chapters 4, 6 and 7. The tools include principal component analysis (PCA) fuzzy c-means, fuzzy logic, neural networks and signed digraphs.
- (3) As part of the joint process-operator simulation platform, a system has also been developed for modelling and simulation of operator's behaviour. The system was developed based on the theoretical model of Cacciabue (1999) on operator's behaviour which breaks operator's activities into perception of the signal and the interpretation of received information, planning for actions and execution of the decisions. The system was implemented as a real-time expert system using visual Prolog. The advantage of the rule-based system is that the rules can be easily revised to reflect various cognitive scenarios. Numerical models were also integrated into the expert system, e.g., the stress models of operators.
- (4) As part of the effort to use the platform to develop methods and tools for characterising and assessing the dynamic behaviour of operators, processes and the joint system, a digraph method for qualitative/quantitative modelling of the dynamic behaviour of combined process-operator systems was developed. The method

involves categorical characterisation of dynamic trend signals using PCA and fuzzy *c*-means, and sectioning of the clusters. A method based on the *global* performance was derived for defining the numbers of clusters and sections. Compared with previous methods, the proposed approach is more accurate, has higher resolution, and is able to deal with joint process-operator systems.

The proposed methods and systems developed have been tested and evaluated using simulated and industrial case studies. They proved to be able to capture and characterise operator's behaviour in terms of stress, time of intervention, frequency of interventions, error handling procedure and near-miss or near-hit. The methods are also proved effective in capturing the dynamic behaviour of the joint system.

8.2 Suggestions for Future Work

While the value of the proposed methods has been demonstrated, there are even greater potential benefits to be realised through the following studies.

- (1) Developments of a multifunctional data mining system that can be fully integrated into modern computer control systems to continuously capture, characterise and assess the performance of operators skills and behaviour in fingerprint detail (Fig 8.1, 8.2). The results of this study using principal component analysis and qualitative/quantitative digraphs have proved the feasibility of the idea. Such a system can be very useful because it has the potential to capture the near-miss situation and help correct operator's inappropriate operations. It is expected that more tools need to be integrated and carefully coordinated in order to be effective for practical use. However there is information about operators that cannot be captured by the data recorded by control computers, therefore there is also a need to investigate what other information is vital and how to collect it.

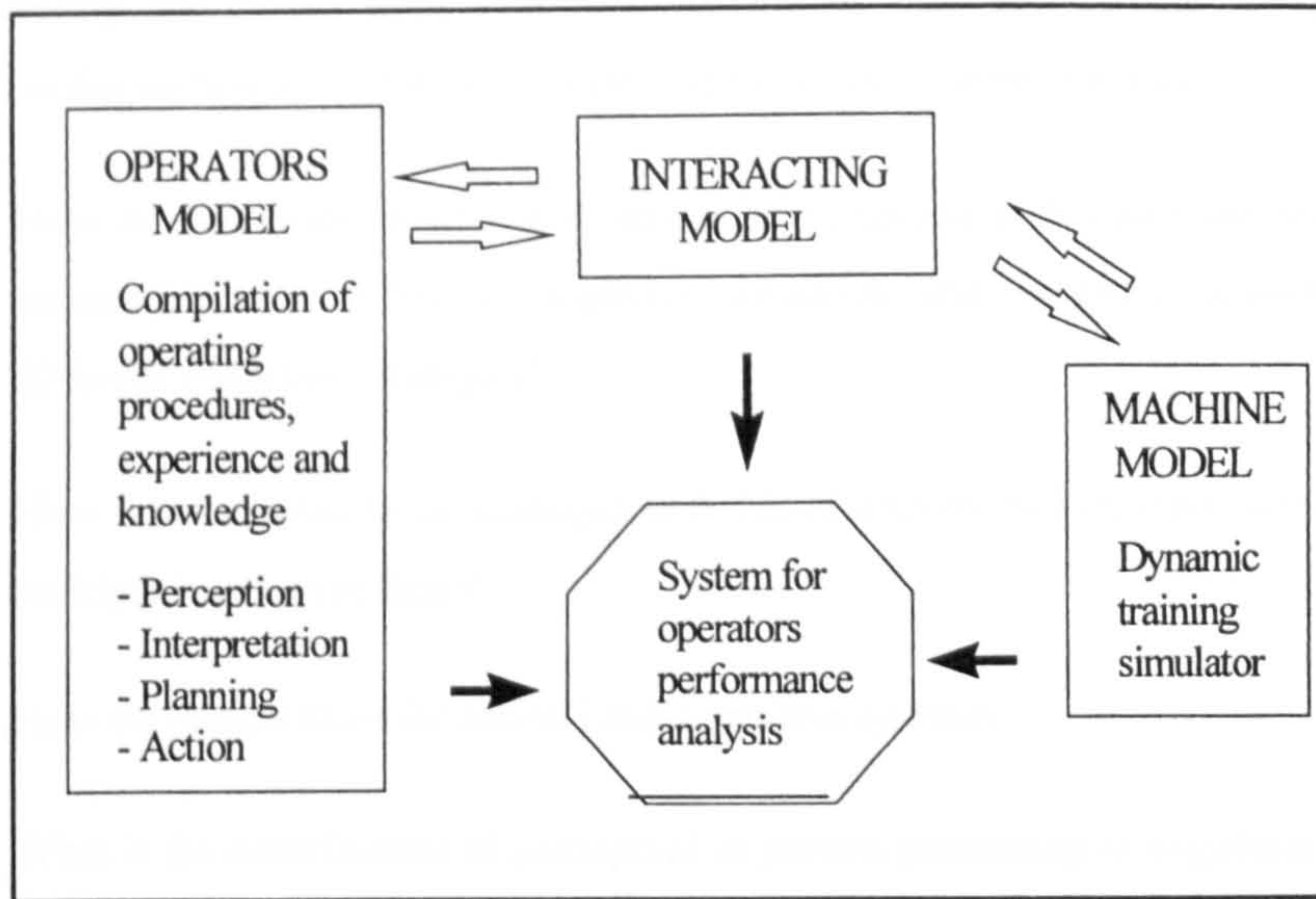


Fig 8.1. The joint operator-process simulation system.

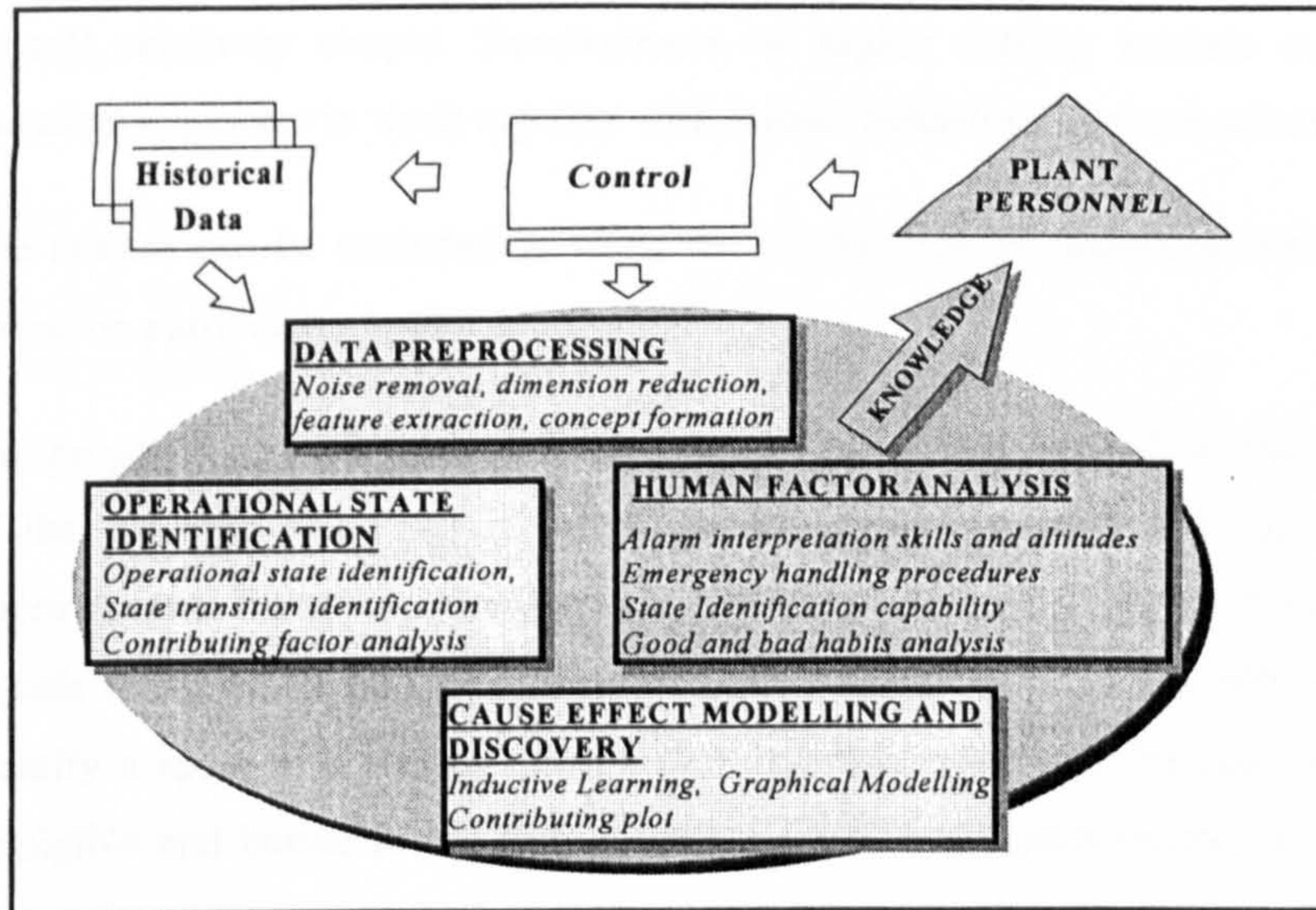


Fig 8.2. System architecture.

- (2) Making use of the joint simulation system to carry out studies on other issues concerning human factors in process operation and control, such as:
- How do temporally evolving situation, as compared with static one shot decision situation, create different cognitive demands and provides opportunities for different cognitive strategies?
 - How is intentional focus managed in fields of activity that are data rich and involve multiple interleaved tasks?
 - How do possibilities for action limit cognitive systems?
 - What is the contribution of perceptual or pattern processing to cognition?
 - How does effort or cognitive cost play a role in cognition systems given finite resources accessible to human or machine agents within a cognitive system?
- (3) To carry out the study of (2), there is the need to develop more sophisticated human models. The operator's model in this work, though is sufficient for the current study, is still relatively simple. Development of higher fidelity models may require chemical engineers to work together with human behaviour research scientists.
- (4) The system can be extended to study the cooperation of operators during process operation particularly in abnormal situations.
- (5) The proposed digraph method for qualitative/quantitative modelling and simulation of the dynamic behaviour of joint process-operator systems still has scope for improvement. First, the approach of qualitative interpretation of dynamic trend signals using PCA, fuzzy *c*-means and sectioning of clusters are still not able to identify a spike of a sudden change (*see* Figs 6.14 and 6.15) because the spike is negligible and buried in the data. In addition, efficient optimisation methods could be developed to replace the iterative method for determining the numbers of clusters and sections of individual variables and of the process.
- (6) This study has focused on continuous processes. It is expected that batch processes will pose more challenges because of the distinctive nature of batch operations that there are no steady states. The operator's factor can be even more important than in continuous processes.

Nomenclature

A - the number of the selected first few principal components (PC's)

a_1, a_2 - two scalars used to define the membership value, (e.g. $a_1=3, a_2=8$)

c - number of cluster

C_i - the i^{th} cluster number

d_{ij} - the Euclidean distance of j^{th} data case from i^{th} cluster centre

df - degree of freedom

e - effect strength in a fully signed directed diagraph

E - sum of squares of difference between the neural networks outputs and the target values

k - number of observation

L - liquid level

m - membership value, function of v and depend on a_1 & a_2

m - number of data case

M - fuzzy set

M - number of training data patterns

MS - mean square

n - total number of data point

N - number of neurons in the output layer

p_1 - first row of the PCA loading matrix

p_2 - second row of the PCA loading matrix

R_{xj} - the value range of the j^{th} node

R_{xj+1} - the value range of the $j^{\text{th}} + 1$ node

S_{ii} - estimated variance of the i^{th} principal component t_i

S_{jj+1} - sensitivity of the j^{th} node to the $j^{\text{th}} + 1$ node

SPE - squared prediction error

SS_{col} - sum of square of the columns

SS_E - sum of square of the error

t_1 - first principal component (PC1)

t_2 - second principal component (PC2)

T^2 - Hotelling T-squared statistic

t_i - the i^{th} Principal component

$t_i^{(m)}$ - target value of the i^{th} output neuron for the given m^{th} data pattern

μ - Membership function

v - vector represent the normalised value of liquid level (L)

x_j - the j^{th} data case

y_{ij} - matrix of observation

y_i - actual observation value

y_i - the i^{th} cluster centre

$y_i^{(m)}$ - the prediction for the i^{th} output neuron given the m^{th} data pattern

$y_{new,I}$ - new observation

$\hat{y}_{new,I}$ - estimated value from the reference PCA model

\hat{y}_i - model estimated values

\bar{y} - means of the observation values

Symbols

β - Degree of fuzziness parameter

ε_{ij} - matrix of random disturbances

$\alpha_{.j}$ - matrix whose columns are the group means (the 'dot j' notation means that α applies to all rows of the j^{th} column)

ϕ_{ij} - Fuzzy membership value of j^{th} data case belonging to i^{th} cluster

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