Mixed Qualitative/Quantitative Dynamic Simulation of Processing Systems

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ABSTRACT: *In this article the methodology proposed by Li and Wang for mixed qualitative and quantitative modeling and simulation of temporal behavior of processing unit is reexamined and extended to more complex case. The main issue of their approach considers the multivariate statistics of principal component analysis (PCA), along with clustered fuzzy digraphs and reasoning. The PCA and fuzzy clustering provide tools to categorize the quantitative dynamic trends, describing the temporal behavior of joint human-process interactions qualitatively, and through the proposed neuro-fuzzy reasoning the system responses can be obtained when the system is exposed to uncertain disturbances. First, the method is applied to a continuous stirred tank reactor – CSTR and then to a distillation column to demonstrate the accuracy level and capability of the approach to handle more complex processes.*

KEY WORDS: *Qualitative/Quantitative simulation, Digraphs, Principal Component Analysis - PCA, Fuzzy c-means clustering.*

INTRODUCTION

Process modeling and computer simulation have proved to be extremely successful engineering tools for the design and optimization of physicochemical, and biological processes. The use of simulation has expanded rapidly during the past three decades because of the availability of high-speed computers. In the chemical process industry, large, realistic nonlinear problems are now routinely being solved via computer simulation. The tremendous impact of simulation on the chemical process industry is due to the following benefits derived; 1) Economic desirability, simulation rather than pilot construction and operation. 2) Investigating the effects of system parameters and disturbances upon operation. 3) A reasonable way of extrapolating performance and process scale-up 4) Understanding the significant process behavior and mechanisms.

There have been two main approaches of implementation to simulation; qualitative and quantitative. In qualitative simulation, the system variables are related in terms of differential algebraic equations - DAEs. In qualitative simulation, the relationships among various quantities are expressed in terms of qualitative connections, by use of graph as such. But, such a description doesn't contain as much information as a quantitative

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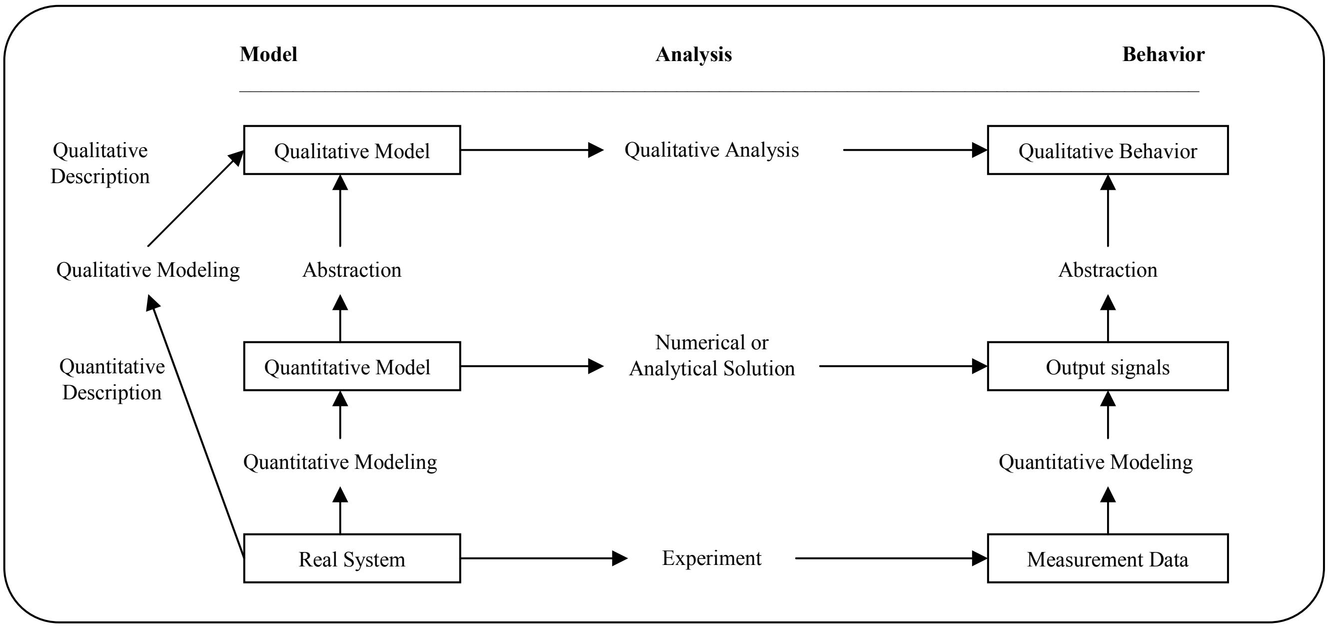

Fig. 1: Quantitative and qualitative modeling of dynamical systems.

analysis. Therefore it would be a challenge to combine qualitative and quantitative simulation to benefit the advantages of both methods simultaneously.

Iri et al. [1] first introduced the use of a graph theory based on Signed Directed Graph (SDG), the so-called digraph method to carry out failure diagnosis of chemical processes. Umeda et al. [2] extended it to handle qualitative dynamic simulation. Oyeleye and Kramer [3] extended the SDG to include certain non-physical feed forward paths that explain inverse and compensatory responses. Gujima et al. [4] improved the accuracy in diagnosis and Mohindra and Clark [5] developed a distributed fault diagnosis system. Based on these extensions, Li and Wang [6] and also Yu and Lee [7] introduced the fuzzy membership function into the branches so that qualitative and quantitative reasoning can be combined. Han et al. [8] used the fuzzy concept to quantify the input data of SDG but the reasoning is still similar to SDG. The method has been considerably improved but still suffers of the following problems: (a) the value space (-, 0, +) is still insufficiently precise for many reasoning tasks in process engineering; (b) tasks need to be classified into several categories: such as *fault diagnosis, operational supervision and simulation of behavior.* The above studies have been concerned with fault diagnosis but complications arise in the last two cases because ambiguous solution results.

The main approach of this article is based on the paper series presented by Wang and Li [6, 14, 15], especially the reference [6], by which the first case study (CSTR) has been adopted as a functional prototype and motivating example.

The article concerned with the approach of dynamical system modeling, including both quantitatively and qualitatively simulation along with appropriate tools. The reasoning mechanism using quantitative information has been further explained. The last two sections followed by a discussion argument examine two case studies to demonstrate the applicability of hybrid simulation approach.

DYNAMICAL SYSTEM MODELING

The modeling problem can be rather generally formulated as follows; for a given dynamical system S and a given set of questions about the behavior B of S, find a representation M that helps to answer the given questions. Then, M is called the model of S. This general formulation shows that the model used to solve a given problem has to be adapted to the questions to be answered. Therefore, there is no unique model but there are many different models M_i of a given system S. In a broad classification, quantitative and qualitative models have to be distinguished (Fig. 1) [9].

Quantitative modeling

In many engineering fields the modeling of a dynamical system means to find a set of differential or difference equations that precisely describe the system output y(k) for given input u(k) and initial state $\underline{x}_0$. Such difference models have the form

$$\underline{x}(k) = f(\underline{x}(k-1), \underline{u}(k-1)),\ \underline{x}(0) = \underline{x}_0 \qquad (1)$$

$$\underline{y}(k) = g(\underline{x}(k), \underline{u}(k)) \qquad (2)$$

Where $\underline{x} \in \Re^n$ denotes the system states, $\underline{u} \in \Re^m$ the inputs and $\underline{y} \in \Re^r$ the outputs. This model is the so-called quantitative model of the system. All pairs $(\underline{x}(k), \underline{u}(k))$ that satisfy equations (1) and (2) for given $\underline{x}_0$ can describe the behavior B.

The reasons why such models dominate in engineering problems, are manifold:

- Quantitative models make it possible to precisely predict the future behavior of the system.

- Quantitative models are compact representations where a single differential or difference equation may describe the performance of the system for a large set of input functions $\underline{u}$ and initial states $\underline{x}_0$.

- Quantitative models are parameterized, i.e., they can be adjusted to different systems of a given class by simply changing the parameter values.

However, the application of such models for solving a given problem presupposes that the model together with the parameter values, the quantitative initial state $\underline{x}_0$ and input $\underline{u}(k)$ are known, and that it is really a part of the problem to precisely predict the behavior of the system.

Qualitative modeling

There is many reasons why precise quantitative models are not a suitable representation of a given system:

- If the system is incompletely known, no precise quantitative model can be set up.

- If the inputs to the system or the initial states can be measured only roughly, the quantitative model cannot be used for prediction or simulation.

- If the system behavior should not be precisely predicted but a qualitative assessment of the behavior subject to a given set of input functions or initial states has to be found, the quantitative model is not the most suitable representation of the system.

On the other hand qualitative simulation is attractive because:

- It can express incomplete knowledge, and hence handle systems that are not completely known.

- It provides general solutions for classes of system, rather than the numerical solutions of a particular case.

- One particular qualitative model can be used to describe a large range of operating conditions.

Qualitative models contain important structural information about the process static's and which can be utilized in the early stages of modeling. At the same time qualitative models can be refined by accumulating data and operational experience to obtain conventional mathematical models in the limit. Similar to other types of models, qualitative models can serve as a basis for qualitative simulation, prediction and model-based control. In addition qualitative models can be interpreted as a time dependent set of logical functions (i.e rules) which is always consistent, complete and can be a subject of different reasoning process. These general properties make qualitative models a promising tool for representing process knowledge in expert systems. There are commonly used ways to describe incomplete knowledge about values, such as probability theory, fuzzy sets, etc, but in qualitative modeling, intervals are almost exclusively used for this purpose.

A typical situation where qualitative modeling has to be applied is shown in Fig. 2. The system under consideration can be controlled merely through a block called injection. The input to the system is given by a sequence of discrete events (U, T), where U is the name of the event and T the time instant, or by the quantitative value [$\underline{u}(k)$]. The injection block maps this event series to some input function $\underline{u}(k)$.The output $\underline{y}(k)$ is not precisely known, but merely a quantized information is available, which may be a sequence of events (Y, T) or a sequence of quantized outputs [$\underline{y}(k)$]. The qualitative behaviour [B] is described by pairs of input and output sequences [(U, T), (Y, T)] or ([$\underline{u}(k)$], [$\underline{y}(k)$]).

There are many engineering problems that refer to a qualitative assessment of the behavior rather than to the quantitatively precise behavior, as illustrated by the following problems taken from process control:

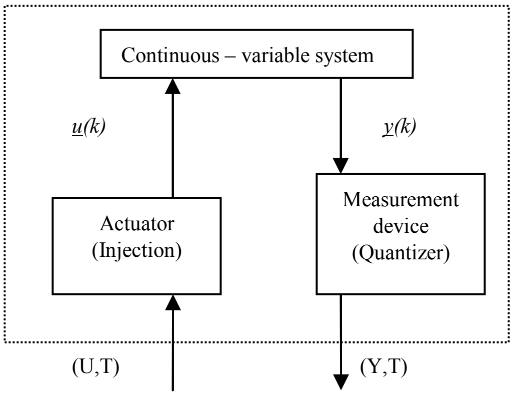

Fig. 2: Motivation for qualitative modeling.

- Process supervision: The task is to decide whether the system performance is within prescribed tolerance bands or not.

- Process diagnosis: It has to be decided whether some faults occur within the system.

- Supervisory control: Discrete control actions have to be found by using a qualitative assessment of the current operating conditions in order to avoid safety-critical operation points and to satisfy given control aims.

Mixed qualitative and quantitative modeling

In this article, the methodology proposed by Li and Wang [6], for simulating the dynamic behavior of process, both qualitatively and quantitatively in a hybrid or mixed manner has been used. There are two critical issues in the proposed method. The first is how to categorically capture the feature of a dynamic transient. The second issue is concerned with devising a rigorous rather than ad hoc reasoning mechanism in such a digraph, particularly when there are interacting and recycle nodes. Then it will be extended to include qualitative information. This is achieved through the introduction of the method of fuzzy c-means clustering for grouping node values.

Researches in various fields have modeled cause and effect relationship among process variables using directed graphs (digraphs). Digraph models are particularly appealing because they provide a pictorial representation of the interactions among the important process variables. The nodes in the digraph correspond to the process variables and the arcs show the causal relationship between them. In the signed directed graph or SDG, each arc is marked by a sign indicating the direction of change of the target variable relative to the source variable. More complex digraphs add other information to the arcs, such as the gain and response time for the changes in the target variables. Causal models based on digraphs are easy to understand, can be developed from empirical relationships or fundamental principles, and can be analyzed using the rich store of computational methods and theoretical results available from graph theory.

Li and Wang have used the SDG to demonstrate the causal and temporal behavior of system qualitatively [6]. The inclusion of interacting and recycle relationships for more complex systems through SDG nodes provides the designer to formulate deeper knowledge embedded in process more deliberately. The interacting and recycle relationships can be the result of closed control loops, process recycles and inherently related interacting causal relationship such as the temperatures of the hot and cold streams of a heat exchanger.

In the following two mathematical issues that will be used later are reviewed briefly.

Principal Component Analysis - PCA

Principal components analysis is a quantitatively rigorous method for achieving the simplification of visualizing multi-dimensionality. The central idea is to reduce 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 set. The method generates a new set of variables, called principal components. Each principal component is a linear combination of the original variables. All the principal components are orthogonal to each other so there is no redundant information. The principal components as a whole form an orthogonal basis for the space of the data. This multivariate statistics concept can be handled easily by MATLAB software package.

Fuzzy Clustering

Clustering of numerical data forms the basis of many classification/recognition and system modeling algorithms. The purpose of clustering is to identify natural groupings of data from a large data set to produce a concise representation of a system's behavior. Fuzzy c-means *(FCM)* is a data clustering technique wherein each data point belongs to a cluster to some degree that is specified by a membership grade. This technique was originally introduced by Bezdek [10] as an improvement on earlier clustering methods. It provides a method of how to group data points that populate some multidimensional space into a specific number of different clusters. It starts with an initial guess for the cluster centers, which are intended to mark the mean location of each cluster. The initial guess for these cluster centers is most likely incorrect. Additionally, *FCM* assigns every data point a membership grade for each cluster. By iteratively updating the cluster centers and the membership grades for each data point, *FCM* iteratively moves the cluster centers to the "right" location within a data set. This iteration is based on minimizing an objective function that represents the distance from any given data point to a cluster center weighted by that data point's membership grade. The output of *FCM* command line function is a list of cluster centers and several membership grades for each data point. The Fuzzy Toolbox of MATLAB has several m_function and visual utilities to handle the FCM approach deliberately.

Reasoning mechanisms

Having described the method for the categorical characterization of the temporal trends of variables in a windowed time scale, using PCA and fuzzy clustering, it is now appropriate to develop the reasoning mechanism. The central idea is based on if-then rules, describing causal effect and consequences of variables on each other qualitatively.

For digraph containing no interacting nodes, there are three basic connections, that is, serial, convergent, and divergent. Now, assume that the three variables X_1, X_2 and X_3 of a simple process have established a serial connection or relationship, as $X_1 \rightarrow X_2$ and $X_2 \rightarrow X_3$, meaning that the change in value of X_1 has a direct effect on X_2 values and changes X_3 indirectly through the correlation of X_2 and X_3. Further, suppose that we have an experimental data case set which says (after fuzzy clustering) when X_1 varies in its domain of variation, nominated as cluster or case A_{X1} , the variables X_2 and X_3 vary in their domains, clustered by C_{X2} and A_{X3}. Note that the domains or clusters of C_{X2} and A_{X3} have been presumably recognized from other experimental data sets. The qualitative reasoning rules that we learn from these two serial relationships may be declared as following:

If $X_1 = A_{X1}$ Then $X_2 = C_{X2}$

If $X_2 = C_{X2}$ Then $X_3 = A_{X3}$

For convergent and divergent connections, we act similarly.

If the value of a node, namely due to operator's intervention or a fault, is fixed externally, it became an independent node. An independent node will not be affected by its precedent nodes, but will still influence its succeeding nodes.

The difficulty with dealing with interacting nodes was first encountered in the work of Iri et al [2] when a control loop had to be considered when applying SDG to fault diagnosis. Like Iri et al [2], later developments adopted ad hoc methods for dealing with interacting nodes, which are often based on some assumptions. They are specifically designed for fault diagnosis and adopt a hypothesis – test strategy. The difficulty with the previous works in dealing with interacting nodes was also the result of their inability to describe node values more accurately than simply +, -, and 0. An interesting and also more reasonable approach was developed by Mo et al [11] and Lee et al [12], who treat all the nodes related to a single control loop as a cluster. The Li and Wang's method of dealing with interacting as well as recycle node is similar to the approach of these authors, though their approach [6] is not restricted, and node values are not in the form of +, - and 0. However, when a node (or nodes) is a dependent node, they consider all its interacting and recycle nodes as a single, but when considering the effect of a cluster of interacting nodes on other nodes, they do not treat the interacting nodes as a single node.

It is clear that, unlike earlier works on SDG, the causal relationship between two nodes or two node clusters is not simply positive or negative. It is a mapping of two spaces of the categorical values of the two variables. Therefore, the method works independently of the complex relationship between the two nodes or variables (or node clusters) linked by a branch. There is no compromise on the complexity of the relationship in devising the reasoning mechanism. In contrast, in all versions of SDG, the relationships between two nodes were simply + (increase), - (decrease) or 0 (no change); representing positive, negative, or no influential relationship. Consequently, the reasoning rules are derived based on the signs of the connections. This is clearly an over-simplified treatment. Such a simplified treatment of causal variables not only is not accurate but also may lead to difficulties in reasoning. For example, suppose a variable X_3 has two and only two incoming connections from X_1 and X_2, both with + signs. When X_1 is increasing while X_2 is decreasing, it will not be possible to predict whether X_3 will increase, decrease, or remain unchanged. Although there have been several efforts at combating such ambiguity, the methods are far from rigorous.

In the next section, we treat the sequel and steps of proposed method through two case studies.

Case Study I- Non-isothermal continuous stirred tank chemical reactor (CSTR)

To illustrate the approach more clearly, we reintroduce the case study of CSTR examined by Li and Wang [6]. It should be noted that the results we obtained have some discrepancies with their results. It may be due to the different noise level introduced and unrecorded data, different assumptions and even the simulator, which has been used.

A non-isothermal continuous stirred- tank chemical reactor (CSTR) is shown in Fig. 3.

A single reaction A $\rightarrow$ B takes place in the reactor. Detailed description and parameter values can be found in the book by Marlin and therefore are not described here [13]. The method is applied to the case study in the following procedures:

Step 1

A dynamic simulator was developed for the CSTR, which has included three controllers as show in Fig 3. To generate a data set or data case, run the simulator at steady state and introduce a disturbance or fault and at the same time start to record the dynamic responses. Fifty-five data sets were generated, using the simulation runs summarized in Table 1.

For each data set, the nine variables shown in Table 1 were recorded, including F_i , C_i , T_{ci} , F_c , T_R , C_o , and L. In each data set, each variable was recorded as a dynamic trend consisting of 80 sampling points. Therefore, for each variable the data size is a matrix 55 (the number of data sets) $\times$ 80 (the number of data points representing a dynamic trend).

Step 2

PCA is applied to such a matrix of each variable. Table 2 gives the Eigen values of the first two PCs for each variable and shows that the first two PCs can capture most at the information. As stated earlier, there are some differences in PCs values in comparison with the results obtained by Li and Wang [6]. However, we can use only two principal components to replace the dynamic trends.

Consider F_i, plotting the first two principal components gives three clusters, that is, A, B, and C. Similarly, for the variable L, the dynamic trends are also grouped into three clusters, D, E, F, in the PC1 – PC2 plane.

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

In cases where the first two PCs are not able to capture most of the variance, more PCs need to be included in clustering the trends. For this purpose, fuzzy c-means clustering can be also used, as will be described in the next case study. Even in such cases, the two – dimensional PC1 – PC2 plot can still be used as a display tool because of its visual effect. The current use of PCA is clearly different from previous works. In previous works, PCA was almost inevitably used to process data involving a number of variables, and the purpose was to eliminate dependencies between variables. But in this study, it is used as a tool to categorically characterizing dynamic trends of individual variables [6].

Step 3

Then we use the fuzzy c-means clustering approach for automatic fuzzy grouping of the data points in the PC1 – PC2 plane. Given the number of clusters and an estimation of the cluster centers, that is, the pairs of values on the PC1 and PC2 axes, the fuzzy c-means approach will automatically find the true cluster centers, and for each cluster, calculate the distance of each data case to the center. All the PC1 – PC2 clusters have been processed using the fuzzy c-means algorithm. It is found that the method is very tolerant of the initial center approximations and can generally find the center in 3 to 10 steps.

A key issue in developing a PCA model is to choose

Table 1: The data sets used in CSTR reactor.

Data sets	data detail
1-10	All control loops at AUTO and S.P of T_R = 400ºK Change F_i (m^3/min)
11-15	All control loops at AUTO and S.P of T_R = 400ºK Change T_i (ºK)
16-20	All control loops at AUTO and S.P of T_R = 400ºK Change C_i (Kmol/m^3)
21-30	All control loops at AUTO and S.P of T_R = 400ºK Change $T_{c,i}$ (ºK)
31-35	All control loops at AUTO and S.P of T_R = 390ºK Change F_i (m^3/min)
36-40	All control loops at AUTO and S.P of T_R = 370ºK Change T_i (ºK)
41-50	All control loops at AUTO and S.P of T_R = 370ºK Change F_i (m^3/min)
51-60	All control loops at AUTO and S.P of T_R = 370ºK Change the output of the CSTR level controller (%)
61-70	All control loops at AUTO and S.P of T_R = 370ºK Change the output of T_R controller (%)
71-85	Disturbance occurred in F_i , C_i , $T_{c.i}$

Variables	PC-1	Variance captured PC-1 + PC-2
F_i	95.5	97.0
T_i	97.3	98.7
C_i	96.8	98.6
$T_{c,i}$	97.5	98.9
F_c	92.1	94.2
T_R	92.6	94.4
F_o	92.2	95.5
L	95.6	99.2
C_o	90.2	95.2

Table 2: Variance captured by the first two PCs.

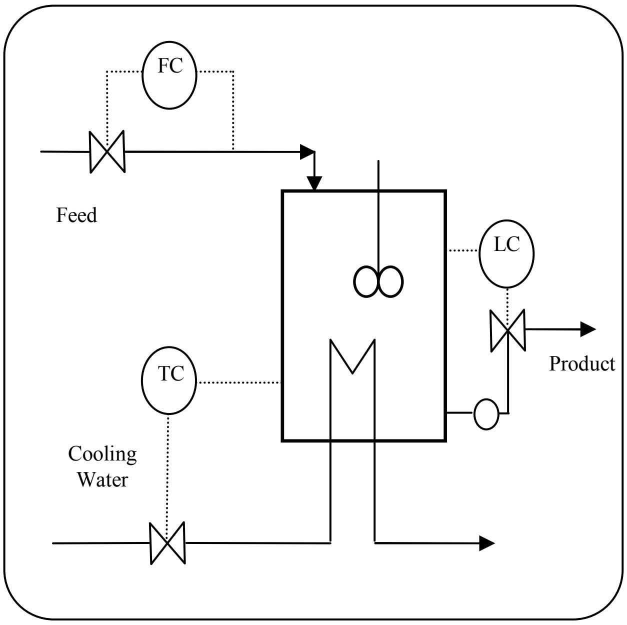

Fig. 3: Schematic representation of a controlled CSTR (case study I).

the adequate number of PCs to represent the system in an optimal way. If fewer PCs are selected than required, a poor model will be obtained and an incomplete represents action of the process results. On the contrary, if more PCs than necessary are selected, the model will be over-parameterized and will include noise. Different approaches had been proposed in the past to select the optimal number of PCs; Akaike information criterion (AIC), minimum description length (MDL), imbedded error function IEF, cumulative percent variance (CPV), screen test on residual percent variance (RPV), average Eigen value (AE), parallel analyses (PA), autocorrelation (AC) and variance of the reconstruction error (VRE) [14]. In the original study [6], a simple rule has been used, which states that the number of PCs chosen should represent more than 90% of the variance. Once PCA analysis and fuzzy c-means clustering were applied, the next step is to design the CSTR's digraph.

Step 4

The digraph for the CSTR reactor should be intuitively drawn, concerning the interacting and recycle nodes or relationships. It has four independent nodes F_i, C_i , T_i and $T_{c,i}$ and two dependent nodes clusters $L \leftrightarrow F_o$ and $C_o \leftrightarrow T_R \leftrightarrow F_c$.

Step 5

To illustrate the reasoning procedure in a fuzzy clustered diagraph, we describe a typical relationship. Nodes L and F_o interact because of the existence of the level controller. The PC1 – PC2 planes for F_i , L and F_o indicate that each variable takes three categorical values. With the fuzzy quantification of node values, a causal rule between node F_i and the node clusters of L and F_o should be in the form of:

If F_i = (A, or B, or C, μ_{F_i})

Then L = (D, or E, or F, μ_L)

And F_o = (A, or B, or C, μ_{F_o})

Thus, the digraph establishment is continued to generate the reasoning rules, which are summarized in Table 3. Separate rules are generating for the two dependent node clusters $L \leftrightarrow F_o$ and $C_o \leftrightarrow T_R \leftrightarrow F_c$.

Step 6

Neural network implementation of fuzzy systems has been proposed as possible approaches for fuzzy system designs. The resulting systems, which are sometimes, called neurofuzzy or neural network based fuzzy system will posses the advantage of both types of systems and overcome the difficulties of each type of system.

The fuzzy neural network discussed in the original study [6] is a hybrid system that functions as a fuzzy system that the processing mechanism is realized by a neural network. Thus, the capability of learning imposed upon a fuzzy system can be achieved by the learning algorithm of a neural network. In principle, a fuzzy neural network is a fuzzy system implemented within the framework of neural networks so as to achieve the capability of learning using input – output data that will lead to improvement of fuzzy rules and fuzzy system intelligence. Therefore the authors [6] have used a fuzzy neural network to learn the fuzzy membership values. The first impression of the method seems to be the way of describing the causal relationships between two nodes. In essence, this does not necessarily imply a deficiency of the current method, because in application of either SDG for fault diagnosis or the current fuzzy clustered digraph for temporal behavior modeling, we are only interested in the links and values of nodes, not in the signs of links. The signs on the links in an SDG are only used to facilitate the reasoning. This is similar to Bayesian network in which the branches only mean a link between two nodes.

The relationship is represented by the perception of Fig. 4, which is trained using the error feedback algorithm adapted from feedforward neural network. Fig. 5 shows the comparison results of rigorous quantitative simulation and qualitative / quantitative simulation mentioned above for the CSTR reactor.

***Case Study II- Multicomponent Distillation* Column**

In the above sections the fuzzy clustered digraph approach has been illustrated using a CSTR case study.

In this section we apply the approach to a more complicated case study, a ternary equilibrium column of five stages including a partial condenser and a reboiler. Detailed description and parameter values can be found in the associated reference [15] and therefore are not described here. The system is shown schematically in Fig 6. The modeling of column is accomplished by

	If					Then			
Rules Generated for the Dependent Node Cluster $L \leftrightarrow F_o$.									
	F_i	L	F_o						
Rule1	A	D	A						
Rule 2	B	E	B						
Rule 3	C	F	C						
Rules generated for the Dependent Node Cluster $C_o \leftrightarrow T_R \leftrightarrow F_w$.									
	F_i	T_i	C_i	$T_{c,i}$	F_o	L	C_o	T_R	F_c
Rule 4	A	A	B	B	A	D	A	A	A
Rule 5	B	A	B	B	B	E	B	B	B
Rule 6	C	A	A	B	C	F	A	A	A
Rule 7	C	A	C	B	C	F	C	C	B
						OR	C	D	B
Rule 8	C	A	B	A	C	F	C	A	A
Rule 9	C	A	B	B	C	F	D	E	C
Rule 10	C	B	B	B	C	F	D	E	A
Rule 11	C	B	B	B	C	F	D	E	A

Table 3. Rules generated for the CSTR reactor.

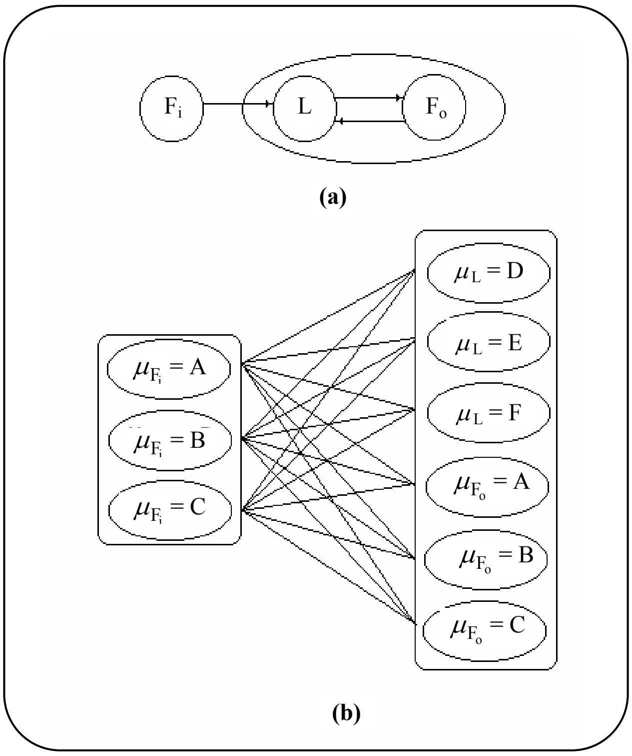

Fig. 4: The learning procedure.

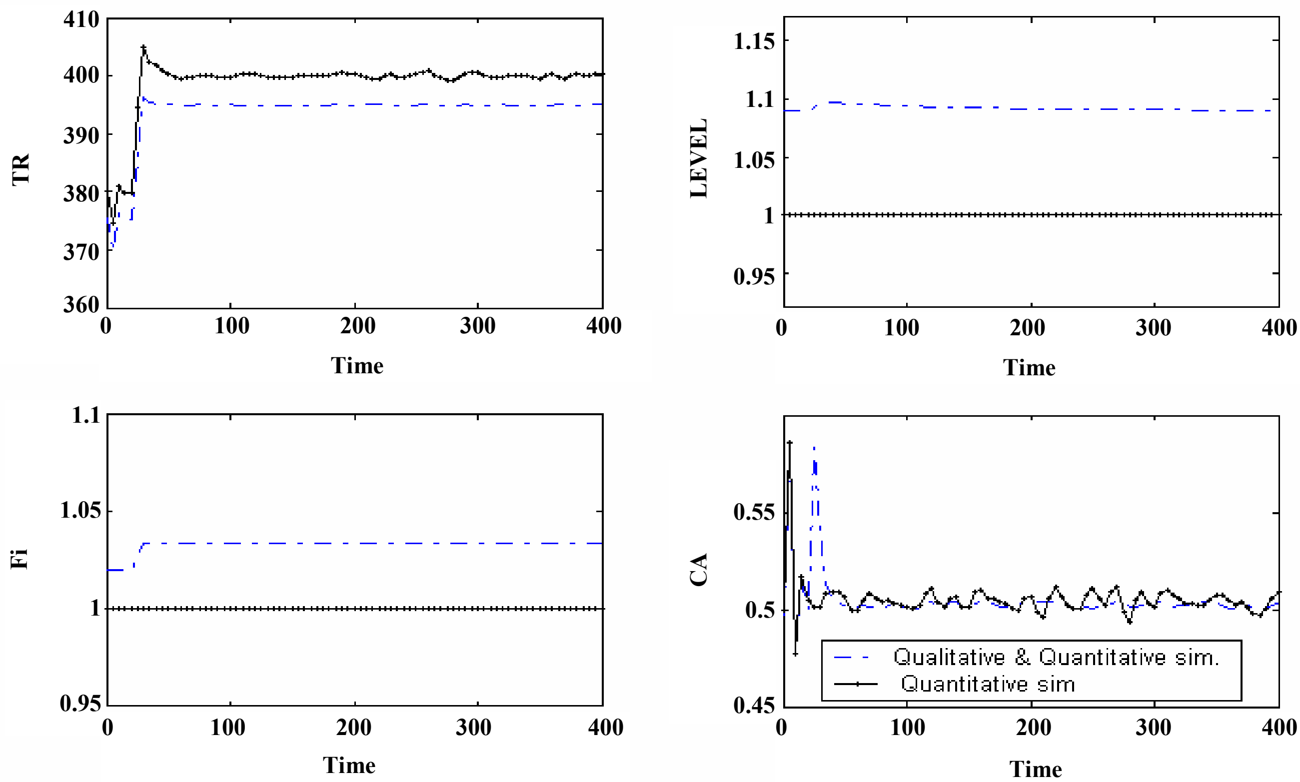

Fig. 5: The comparison of two simulation methodologies (rigorous or pure quantitative and qualitative/quantitative).

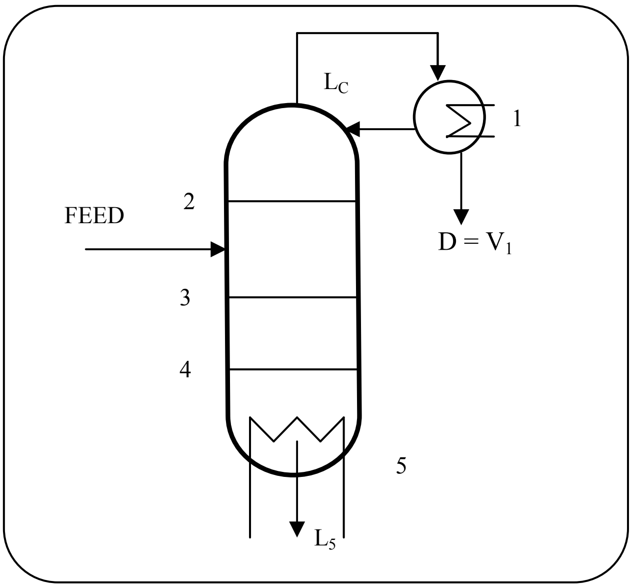

Fig. 6: Multicomponent distillation column.

individual analysis of each stage and then the lumping together of all stages for an overall and simultaneous solution. These solution equations are integrated with respect to time for the dynamic response of the system. To apply the approach on this case study a database of 70 sets was obtained by carrying out various tests on the simulator. Most of data sets correspond to various operations, which are regarded as abnormal or under significant disturbances. The rest are considered as normal operations. Each data set consists of 26 variables and each variable represent a dynamic trend consisting of 21 sampling points. Henceforth, the size of the data to be analyzed is $70 \times 26 \times 21$.

Early discussion has indicated that in same cases with two PCs it is not possible to capture most of the feature of a dynamic trend. To further demonstrate this, we apply PCA analysis to temporal trends of column's variables.

The dynamic trends of some variables are shown in Fig. 7. Only those variables that will later appear on the column's digraph are shown.

Fig. 8 shows the variance captured by principal components for some variables. In this case the first two PCs are not able to capture most of the variance, thus more PCs need to be included in clustering the trends. Fig. 9 shows the PCs plane, when three PCs are considered, fuzzy c-means clustering can automatically identify the centers of clusters.

The digraph for the multicomponent distillation column of Fig. 6 is given in Fig. 10. There are five independent nodes: R (reflux), z_{feed}, F_{feed}, T_{feed}, $Q_{reboiler}$ and three dependent clusters: $L_1 \leftrightarrow V1$, $L_2 \leftrightarrow V_2$,$L_4 \leftrightarrow V_4 \leftrightarrow L_5$.

The digraph (Fig. 10) is combined with Fig. 9 to generate the reasoning rules. Separate rules are generated for the dependent node clusters, which are summarized below.

Rules generated for the dependent node cluster ($L_1 \leftrightarrow V_1$):

If $R =$ (A, or B, or C, μ_R)

Then $L_1 =$ (A, or B, or C, μ_{L_1})

And $V_1 =$ (A, or B, or C, μ_{V_1})

Rules generated for the dependent node cluster ($L_2 \leftrightarrow V_2$): If F_{feed} = (A, or B, or C, $\mu_{F_{feed}}$)

And z_{feed} = (A, or B, or C, $\mu_{z_{feed}}$)

And T_{feed} = (A, or B, or C, $\mu_{T_{feed}}$)

And L_1 = (A, or B, or C, μ_{L_1})

Then L_2 = (A, or B, or C, μ_{L_2})

And V_2 = (A, or B, or C, μ_{V_2})

Rules generated for the cluster ($L_4 \leftrightarrow V_4 \leftrightarrow L_5$)

If F_{feed} = (A, or B, or C, $\mu_{F_{feed}}$)

And z_{feed} = (A, or B, or C, $\mu_{z_{feed}}$)

And T_{feed} = (A, or B, or C, $\mu_{T_{feed}}$)

And $Q_{reboiler}$ = (A, or B, or C, $\mu_{Q_{reboiler}}$)

Then L_4 = (A, or B, or C, μ_{L_4})

And V_4 = (A, or B, or C, μ_{V_4})

And L_5 = (A, or B, or C, μ_{L_5})

And other connections will be as follows:

If L_1 = (A , or B , or C , μ_{L_1})

And V_1 = (A , or B , or C , μ_{V_1})

And V_2 = (A , or B , or C , μ_{V_2})

Then $x_{b,1}$ = (A, or B, $\mu_{x_{b,1}}$)

And $x_{t,1}$ = (A, or B, $\mu_{x_{t,1}}$)

And also: If L_4 = (A, or B, or C, μ_{L_4})

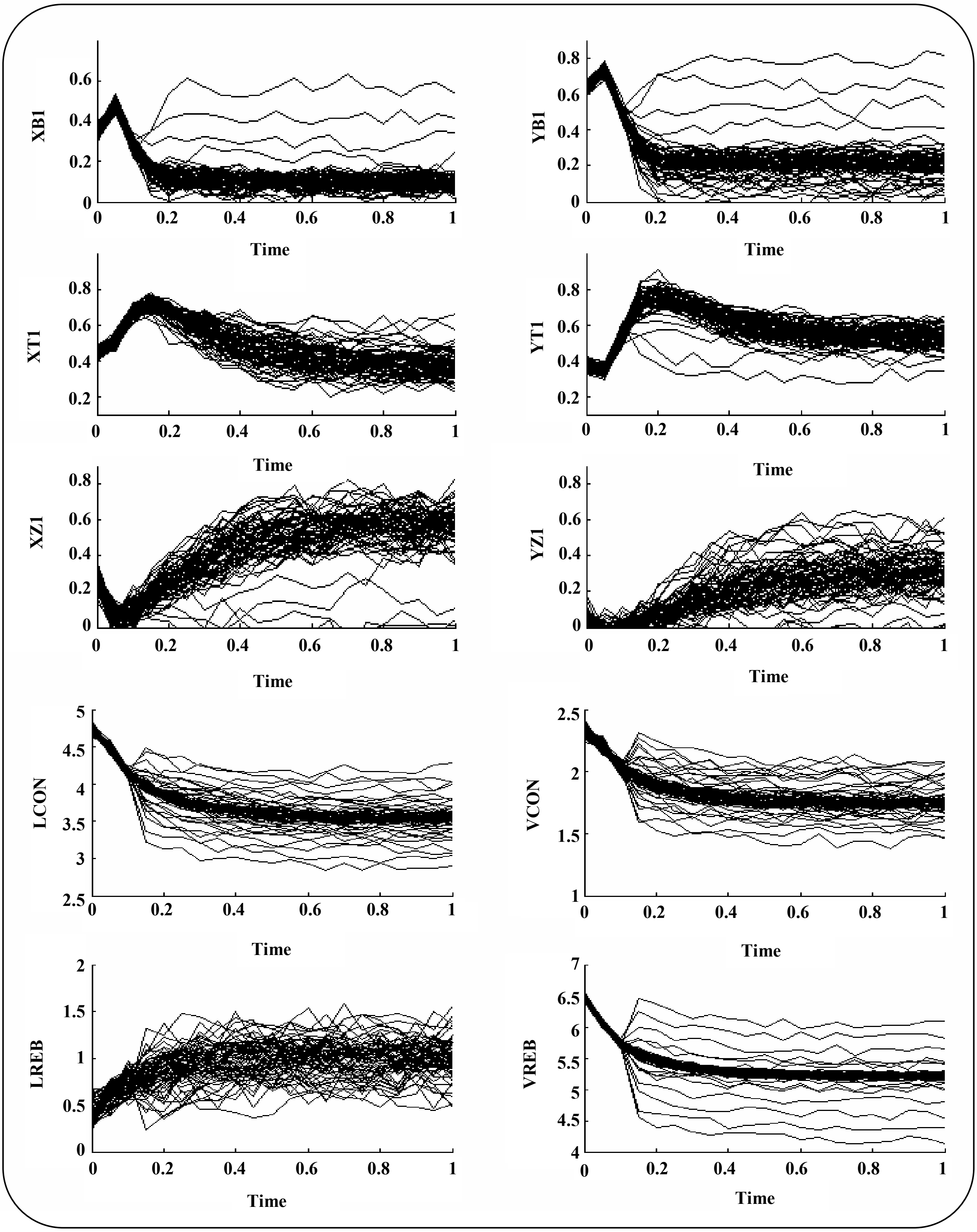

Fig. 7: Dynamic trends of distillation column.

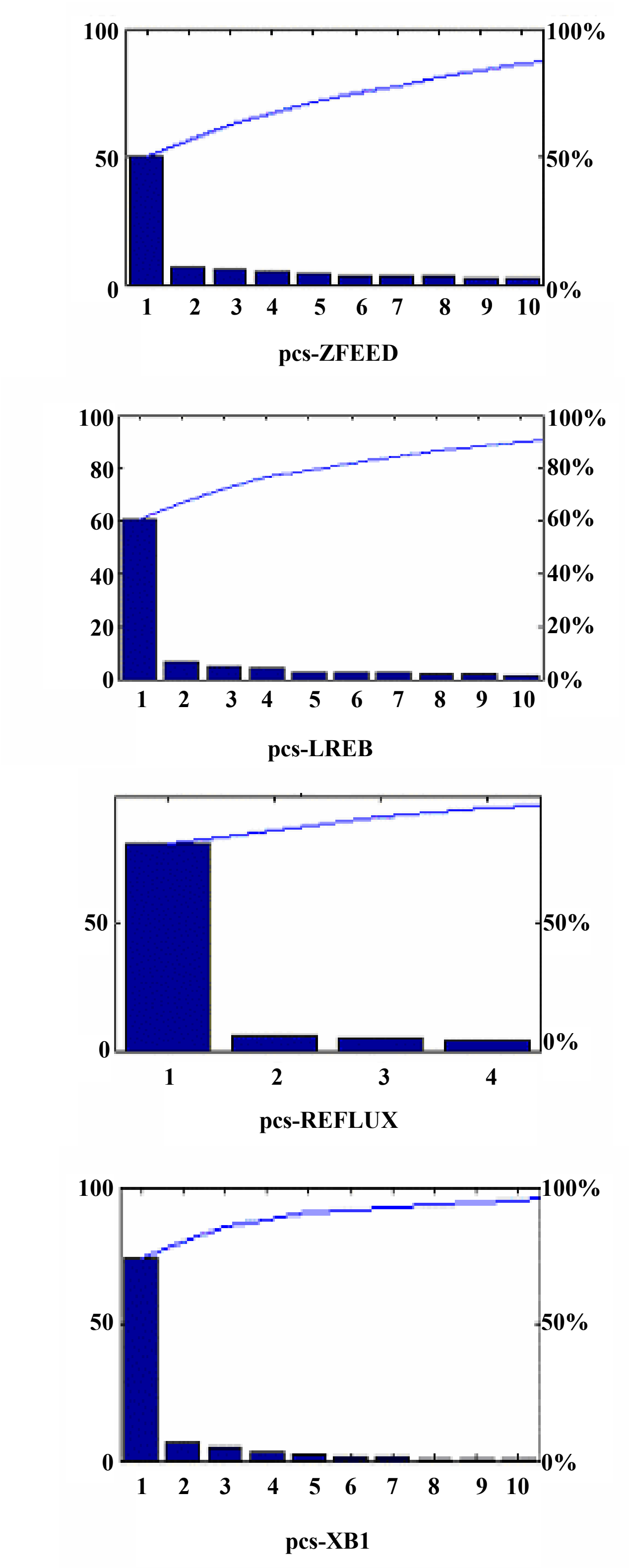

Fig. 8: Variance captured by the principal component for six variables

And V_4 = (A, or B, or C, μ_{V_4})

And L_5 = (A, or B, or C, μ_{L_5})

Then $x_{b,5}$ =(A, or B , $\mu_{x_{b,5}}$) And $x_{t,5}$ =(A, or B, $\mu_{x_{t,5}}$)

Fuzzy neural networks are used to learn these fuzzy rules. And results are depicted in Fig. 11 in which pure quantitative (rigorous) method is compared with proposed hybrid method.

CONCLUSION

Many real systems may be high-order and/or time-varying and/or non-linear to the extent that conventional modeling and analysis techniques can no longer be applied. The use of qualitative reasoning can avoid complex mathematical operations, and can be employed to overcome some of the difficulties. Engineers are used to solve problems on different level of abstraction. It is, therefore, an interesting challenge to investigate ways for combining qualitative models. In this study fuzzy clustered digraph approach, proposed by Li and Wang [6] is applied to more complex case. The method is able to not only capture temporal behavior of a variable using principal component analysis, but also modeling process as a causal digraph with interacting and recycle nodes. A critical step in the approach is how to categorically capture the feature of a dynamic transient. For this purpose, an approach using principal analysis as proposed by Li and Wang [6] was used. The advantage of PCA qualitative representation of dynamic trends is that it allows one to describe a trend with only one simple categorical value. The digraph method is also more advantageous than other methods, such as decision trees, because the latter doesn't allow interacting and recycle nodes and therefore it is an oversimplified representation. The introduction of fuzzy c-means also allows qualitative and more accurate description of temporal behavior of variable and their dynamic causal relationships. The approach was examined on a CSTR reactor and applied to a distillation column. It is found that the approach is capable of giving acceptable results compared with just qualitative method, even in complex cases.

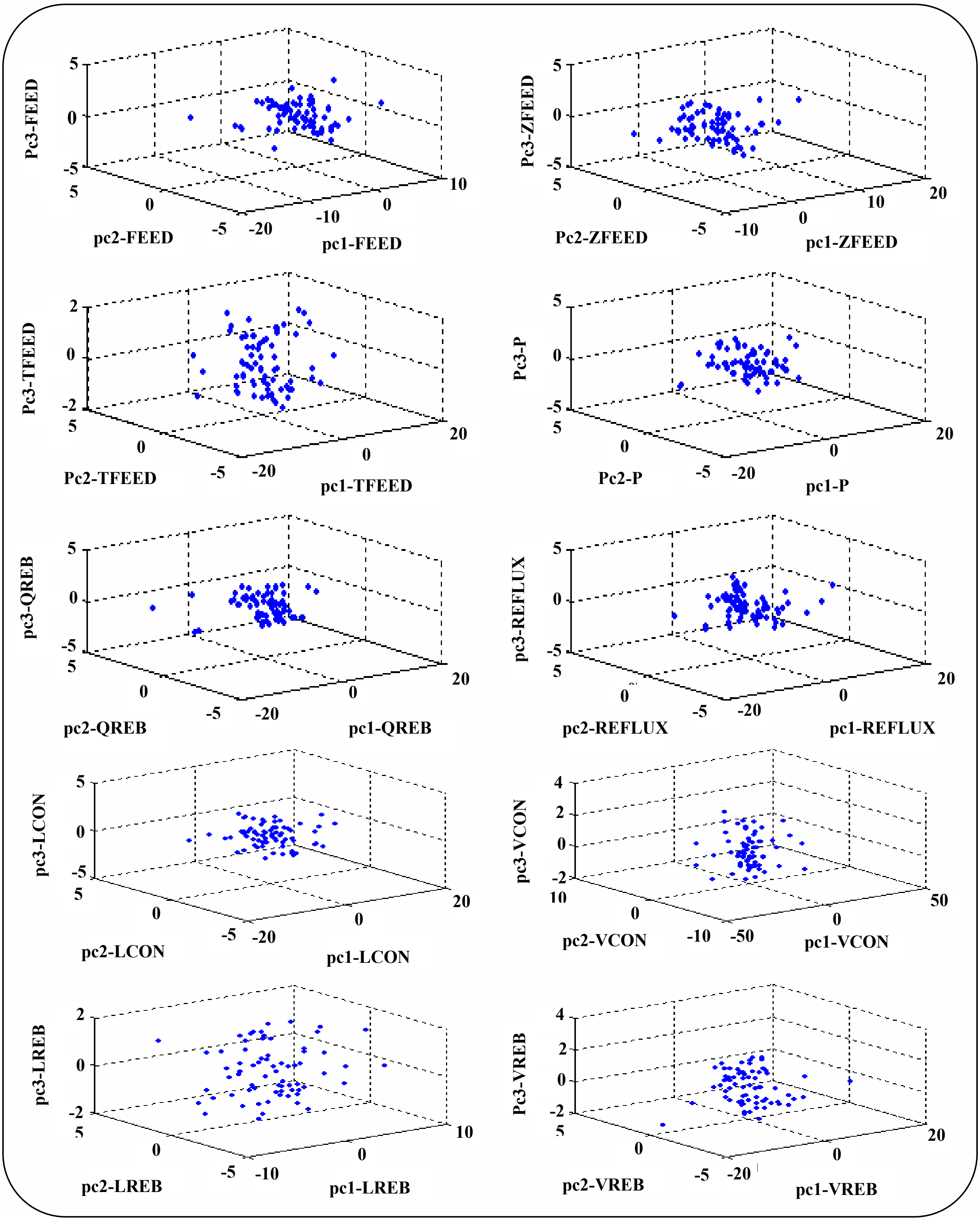

Fig. 9: PC1-PC2-PC3 plots of column variables.

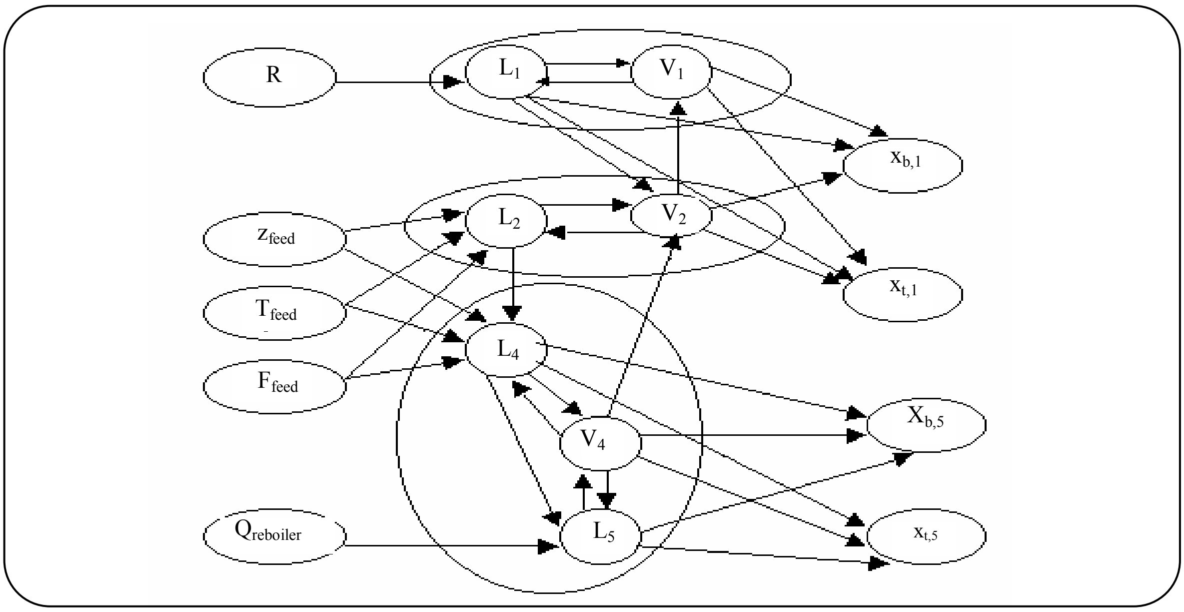

Fig. 10: Digraph of distillation column.

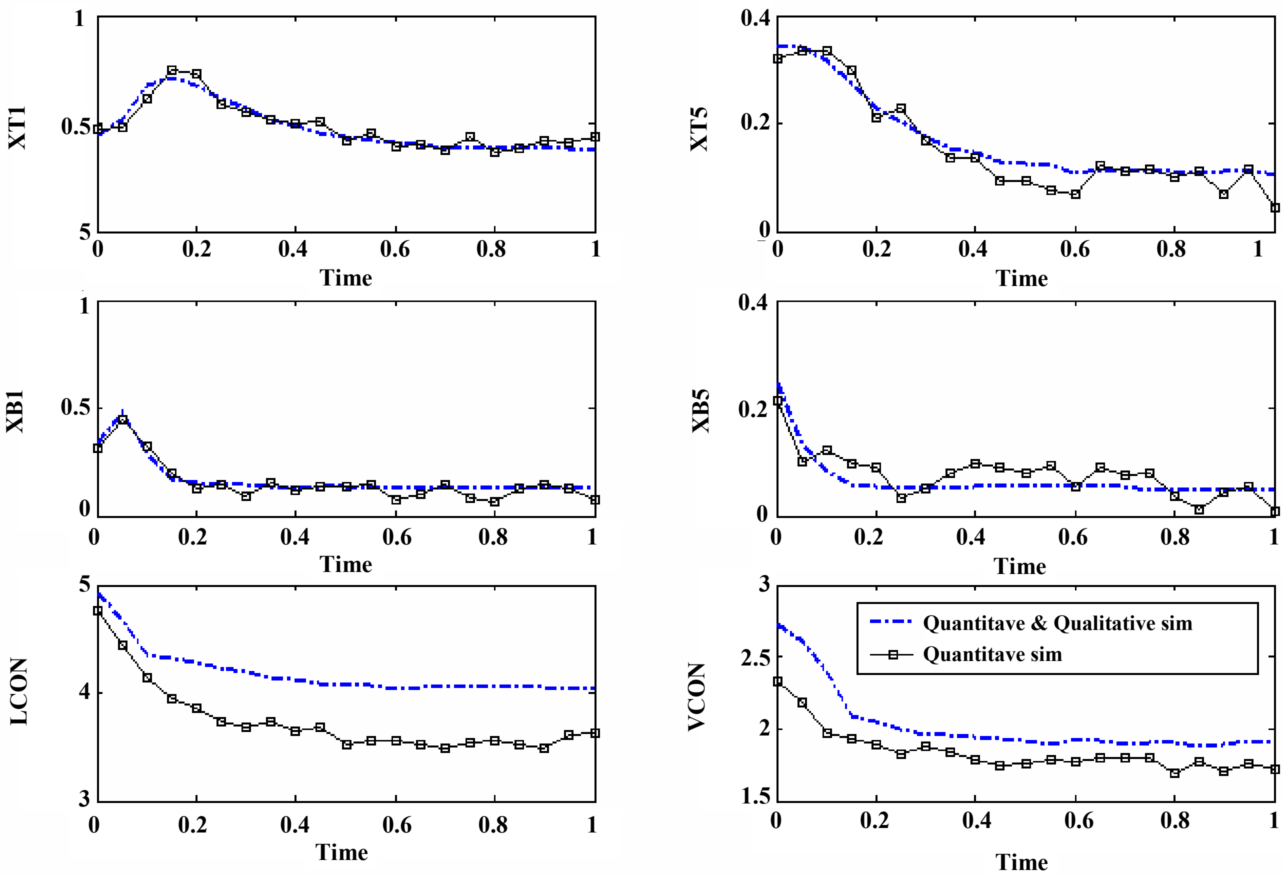

Fig. 11: Quantitative method is compared with proposed hybrid method.

Nomenclature

A	Representative fuzzy set
B	Dynamical behavior symbol, representative Fuzzyset, distillation column bottom product flow Rate (lbmol/hr)
C	Representative fuzzy set
C_i	Concentration of component A in the inlet Feed stream, (kmol/m^3)
C_o	Concentration of component A in the product stream leaving the CSTR, (kmol/m^3)
D, D	Representative fuzzy set, vapor distillate flow rate, (lbmol/hr)
E	Representative fuzzy set
F	Representative fuzzy set
F	Cooling-water flow rate of CSTR, (m^3/min)
F_{feed}	Flow rate of feed to the distillation column, (lbmol/hr)
F_i	Feed flow rate to the CSTR, (m^3/min)
F	Product stream flow rate of CSTR, (m^3/min)
f	General notation of function
g	General notation of function
L	Liquid level in the CSTR, (m)
L_i	Liquid flow rate of feed from stage i (lbmol/hr)
m	Dimension of input vector space, as superscript
Ma	Dynamical model symbol
n	Dimension of state vector space, as superscript
r	Dimension of output vector space, as superscript
S	Dynamical system symbol
T,T	Sampling time, time instance
$T_{c,i}$	Inlet temperature of cooling water
T_{feed}	Temperature of the inlet feed to the Distillation column (ºF)
T_i	Temperature of inlet feed to the CSTR (ºK), temperature of the distillation column i-th stage (ºF)
T_r	Temperature of reaction mixture in the CSTR (ºK)
U	Dynamical event symbol
U(k)	Input vector value at instance k
V_i	Vapor flow rate of feed from stage i (lbmol/hr)
X, X, x_i	General notation of states
x_o	Initial state vector
x(k)	State vector value at instance k
$x_{b,i}$	Liquid mole fraction of benzene, stage i
$x_{t,i}$	Liquid mole fraction of toluene, stage i
Y	Dynamical consequence (output) symbol
Y(k)	Output vector value at instance k
z_{feed}	Toluene concentration (mole-fraction) of feed to the distillation column
μ_i	Membership function value of variable i

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