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The objective of this work is to assess the feasibility of adopting artificial neural networks (ANNs) in fault detection and diagnosis for batch and semi-batch processes. Although there is a large volume of related publications available, most of them used steady-state data to train ANNs and, as such, the task of fault diagnosis can only be implemented in continuous operations. Based upon the concept of analytical redundancy, the framework of a two-stage fault monitoring system is proposed in this paper. In the first stage, a hybrid ANN is adopted to predict the long-term dynamic behaviors of the output variables under normal condition. The occurrence of fault(s) can be detected by inspecting the residuals, i.e. the differences between the measured and the predicted values of outputs. A second feedforward neural network is then used for the purpose of differentiating the residual patterns caused by various faults. In addition to the fact the results of pilot tests are quite satisfactory, it is also demonstrated in our experimental studies that the proposed fault-monitoring system is capable of detecting and diagnosing faults that cannot be described by traditional mathematical models.

KEYWORDS Fault Detection and Diagnosis Batch and Semi-Batch process Neural Network

INTRODUCTION

In order to achieve economical production scale, the capacities of chemical processes today tend to be much larger than before. Also, for the purpose of optimizing plant performance, the introduction of more complex integration schemes and the demand for more sophisticated control strategies are becoming popular trends in current design practice. As a result, the chance for accidents in the chemical industries has increased significantly during the recent years and, thus, in operating a modern plant, an efficient fault detection and diagnosis method is very critical for preventing the incipient faults from developing into serious consequences.

Most recent studies in this area are concerned with the development of computer-aided systems to assist the operator to detect abnormal conditions and to locate fault origins. Numerous approaches have been adopted in the past. For example,

- The qualitative cause-and-effect analysis using sign-directed graphs (SDGs) (Iri *et al.*, 1979; Tsunge *et al.*, 1985; Shiozaki *et al.*, 1985a,b; Kramer and Palowitch, 1987b; Chang and Yu, 1990; Yu and Lee, 1991),

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- The quantitative diagnostic methods using filtering and estimation techniques (Stanley and Mah, 1977; Himmelblau, 1978; Park and Himmeblau, 1983; Watanabe and Himmelblau, 1983a,b; Isermann, 1984; Watanabe and Himmeblau, 1987; Li and Olson, 1991; Chang *et al.*, 1993), and
- The rule-base expert systems (Kumamoto *et al.*, 1984; Chester *et al.*, 1984; Davis *et al.*, 1985; Ungar, 1990; Kramer, 1987a; Rich and Venkatasubramanian, 1987; Shum *et al.*, 1988; Petti *et al.*, 1990).

Notice that the success of these approaches hinges essentially upon the construction of representative models or rules about all possible faults. However, it is sometimes impossible to formulate mathematical models of equipment failures or malfunctions and, in some cases, expert's knowledge may simply be unavailable. Further, even if all faults can be described precisely, the tasks of building a system model or rule base can still be quite time-consuming and expensive.

Artificial neural networks (ANNs) may provide a viable alternative to the above problems. This is because of the fact that accurate prior knowledge of the faults is not necessary for its implementation. It can be "trained" to perform a given task successfully, e.g. see Quantrille and Liu (1991). The usage of ANN in fault detection and diagnosis for continuous chemical processes was first suggested by Himmeblau and his coworkers (Hoskin and Himmeblau, 1988). Using steady-state data, they demonstrated the effectiveness of multi-layer feedforward networks (FFNs). Later, further improvements have been introduced. For example, Kramer and Leonard (1990) and Leonard and Kramer (1991) adopted the distance-based classifiers and radial basis functions in diagnostic neural networks. The validity of the above approaches to solve the problem of fault identification from steady-state data was also confirmed in a number of application studies concerning a fluidized catalytic cracking unit (Venkatasubramanian and Chan, 1989), a heat exchanger (Himmeblau, 1992), a distillation column (Lee and Park, 1992), sensor failure in a control system (Naidu *et al.*, 1990) and the Syschem plant (Hoskin *et al.*, 1991). On the other hand, the feasibility of FFN in diagnosing incipient faults from transient data was assessed by Watanabe *et al.* (1989), Venkatasubramanian *et al.* (1990) and Vaidyanathan *et al.* (1990). In these studies, the basic theme was that process trends often offer better clues for diagnosis. Two types of network inputs were thus used, i.e. (i) the raw time-series data from the plant sensors and (ii) the moving average values of the same time-series data. However, in those studies, the process was assumed to be at steady state initially and the system transients were caused by the occurrence of faults. Thus, their techniques are still applicable only to the continuous processes.

From the above discussions, it is clear that the previous studies are mainly concerned with the continuous operations. However, other than the petroleum and petrochemical industries, the batch or semi-batch operation is still a common, if not dominant, mode of operation in process plants. Thus, the main objective of this study is to explore the possibility of developing neural-network-based techniques for fault detection and diagnosis in these processes.

A two-stage approach was adopted in this work. Basically, two neural networks were applied in series in the fault detection and diagnosis process. The first one was used to predict the normal behavior of the system, while the second one was used for fault diagnosis. The network structure used for diagnosis is the same as those implemented for the continuous processes, i.e. the feed forward networks (FFNs). The first network, however, has not been included in any of the publications concerning fault detection and diagnosis and thus, the reason for its adoption is further explained in the sequel.

For continuous operation, the system is usually assumed to be at steady state if it functions normally. In such case, the detection of a fault is relatively straightforward. Basically, one simply has to compare the measured output variables with their reference (steady-state) values. On the other hand, the normal behavior of a batch or semi-batch system is dynamic in nature, i.e. the measured output values are in general functions of time. This is mainly due to the facts that the inputs are varied from one step to another during batch operation and, consequently, a steady state can never be reached. In other words, the batch and semi-batch processes are always operated at *unsteady state*. Thus, an additional neural network must be introduced to generate the reference (normal) values of the output variables for these processes. This network is, of course, not needed for detecting faults in a continuous operation.

There are a large volume of literature concerning the identification of dynamic models using neural networks, e.g. Bhat and McAvoy (1990), Thibault (1991), Su *et al.* (1991) amd Koshijima and Niida (1992). Multilayer FFNs were widely used in model-predictive control (Ungar *et al.*, 1990; Lee and Park, 1992; Psichogios and Ungar, 1991; Cooper *et al.*, 1992). However, the FFNs are suitable only for short-term predictions (Su *et al.*, 1992). The effects of an incipient fault may not be detectable in this situation. This is due to the fact that, in essence, the state of the system gets "calibrated" each time a measurement is taken. The output values predicted from the present measurements may still be very close to the measurement values at the next time step. On the other hand, the recurrent neural network was believed to be capable of predicting long-term dynamic system behavior (Su *et al.*, 1992; Qin *et al.*, 1992; Schenker and Agarwal, 1992; You and Nikolaou, 1993). However, to adequately describe the variations in the output variables, a pure recurrent network configuration may not be enough. This can be attributed to the fact that, in a realistic batch or semi-batch system, the response rates of different outputs corresponding to the same set of input changes can vary widely. Thus, in the corresponding recurrent network, it is inappropriate to recycle the outputs that respond quickly to the inputs. As a result, none the available network configurations can be directly applied and they must be tailored to suit our need for long-term prediction in these processes.

Finally, it should be noted that, in the previous studies related to fault diagnosis using neural network, the training data were generated by numerical simulation almost exclusively. The majority of the computer programs used for such simulation studies were inevitably coded on the basis of mathematical models. However, as mentioned before, it is sometimes extremely difficult to construct accurate mathematical models for realistic systems, especially after faults occur. Therefore, experimental training data were obtained in all example cases studied in this work to demonstrate the practical value of the neural-network-based approach.

THE FRAMEWORK OF A TWO-STAGE FAULT-MONITORING SYSTEM

Generally speaking, an on-line fault monitoring system should consist of two major functions, i.e. fault detection and fault diagnosis. The framework of such a system developed in this work can be found in Figure 1. A brief description of all its components is presented in the sequel.

First, the plant here refers to a general chemical process operated in batch or semi-batch mode. The outputs $\mathbf{x}(t)$ from the plant are obviously corresponding to the sensor measurements of the process conditions and the inputs $U(t)$ should be equivalent to the signals sent to the actuators. In a batch or semi-batch operation, the actuator

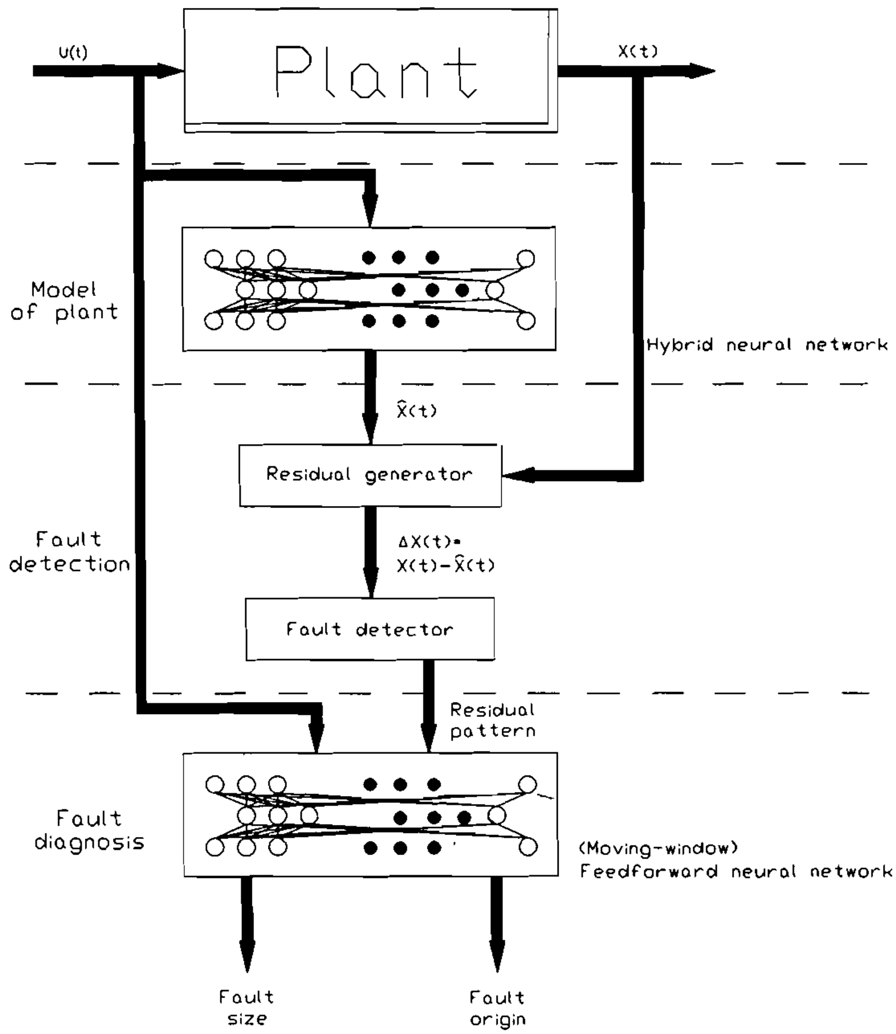

FIGURE 1 The framework of two-stage fault-monitoring system for noncontinuous processes.

inputs are usually manipulated periodically according to a recipe. Further, these inputs may vary from step to step during each batch cycle.

In this study, the residual-based approach (Kramer and Mah, 1993) is adopted for fault detection. Thus, the *residual generator* is a critical component in this fault monitoring system. The residuals, $\Delta \mathbf{x} = \mathbf{x} - \hat{\mathbf{x}}$, are measures of the discrepancy between the observed system behavior and that should result under normal condition. Significant departure from their nominal values, i.e. 0, signifies the occurrence of a fault or faults. This approach is essentially derived from the concept of *analytical redundancy* (Chow and Willsky, 1984). In other words, the inherent redundancy contained in the static and dynamic relationships among the system inputs and measured outputs are exploited in fault detection. Traditionally, the predicted outputs $\hat{\mathbf{x}}$ are computed from the input values according to a mathematical model (Isermann, 1984; Wünnenberg and Frank, 1990; Gertler and Singer, 1990). However, since it is often difficult to derive such model in realistic applications, a neural network has been used to take its place.

To detect faults(s), various statistical tests should be performed on the residuals. This implies that a statistical description of the residual under normal operation should be acquired before implementing the proposed fault-monitoring system on-line. The most general approach to obtaining probability density function (PDF) of these residual variables is to build a calibration set of residual values during normal operation, and then model the PDF using an appropriate estimator (Kramer and Mah, 1993). In this discussion, we were not concerned with the detailed decision process involving elaborate statistical analysis. Instead, a simple threshold test was used as the basis for fault detection.

The last step is fault diagnosis. Normally, this task can be further divided into the subtasks of feature (signature) extraction and classification (Chow and Willsky, 1984; Wünnenberg and Frank, 1990; Gertler and Singer, 1990; Clark *et al.*, 1991; Kramer, 1993). In our study, these subtasks are carried out with a second neural network which maps the patterns of residuals to fault origins.

MODELING THE BATCH AND SEMI-BATCH PROCESSES WITH A HYBRID NETWORK

Theoretically, the long-term dynamic behavior of a process system can be successfully predicted with an external recurrent network (ERN) if enough data are given and, also, the convergence criteria in training are satisfied (Su and McAvoy, 1992; Qin *et al.*, 1992). However, this approach is questionable if applied blindly. First of all, the weight estimates may be extremely difficult to converge in the iterative training process. Secondly, even if convergence is achieved, poor prediction may still be possible in the generalization stage. This is caused by mistakenly identifying an unsuitable local minimum.

In the present work, physical insights of the system were used as an aid for conjecturing the configurations of the neural network. It has to be realized that; in chemical engineering applications, a qualitative description of the system is almost always available. In addition to the cause-and-effect relations amongst input and output variables, some knowledge about the dynamic characteristics of the system can also be obtained. Thus, it is often possible to establish at least the *functional form* of mathematical model. In many practical batch and semi-batch process, the response rates of different output variables with respect to an input change can vary widely. The corresponding model should therefore be expressed as:

$$\mathbf{f}_1(\mathbf{x}_1^{(n)},\ldots,\mathbf{x}_1^{(1)},\mathbf{x}_1;\mathbf{x}_2^{(m)},\ldots,\mathbf{x}_2^{(1)},\mathbf{x}_2;\mathbf{u}^{(l)},\ldots,\mathbf{u}^{(1)},\mathbf{u};\mathbf{p})=0 \tag{1a}$$

$$\mathbf{f}_2(\mathbf{x}_1,\mathbf{x}_2,\mathbf{u},\mathbf{p})=0 \tag{1b}$$

where $\mathbf{x}_1$ and $\mathbf{x}_2$ are vectors of measurements output variables, $\mathbf{u}$ a vector of known inputs and $\mathbf{p}$ a vector of unknown and unmeasured parameters. Notice also that the orders of derivatives, i.e. n, m and l, dictate the dynamic characteristics of the system. A neural-network-based approach to model such batch and semi-batch process is appropriate if, in the above equations, either the orders n, m and l or the explicit formulation of $\mathbf{f}_1$ and $\mathbf{f}_2$ are unknown, or the values of parameters $\mathbf{p}$ cannot be determined with sufficient accuracy. However, from Equation (1a) and (1b), it is also clear that an ERN was not designed to handle the coupled relations implied in these equations. Difficult training process and inadequate prediction capability are its obvious drawbacks for our applications. Consequently, it is necessary to introduce modifications in the network structure.

In our study, a generalized hybrid network (Fig. 2) has been developed to facilitate the construction of proper models for the batch and semi-batch processes. Essentially, this network is built with two interconnected feed forward networks. The first one (FFN_1) maps the estimated output values and the input values at current and previous steps, i.e. $\hat{\mathbf{x}}_1(\tau)(\tau=t-1,t-2,\ldots)$, $\hat{\mathbf{x}}_2(\tau)$ and $\mathbf{u}(\tau)(\tau=t,t-1,t-2,\ldots)$, to the estimates of $\mathbf{x}_1$ at the present time, i.e.

$$\hat{\mathbf{x}}_1(t)=\mathscr{F}_1[\hat{\mathbf{x}}_1(t-1),\hat{\mathbf{x}}_1(t-2),\ldots,;\hat{\mathbf{x}}_2(t),\hat{\mathbf{x}}_2(t-1),\ldots,;\mathbf{u}(t),\mathbf{u}(t-1),\ldots] \tag{2a}$$

In other words, it is a FFN with external feedbacks, i.e. an ERN. The second network FFN_2 is used to describe the relation represented by Equation (1b). The outputs of

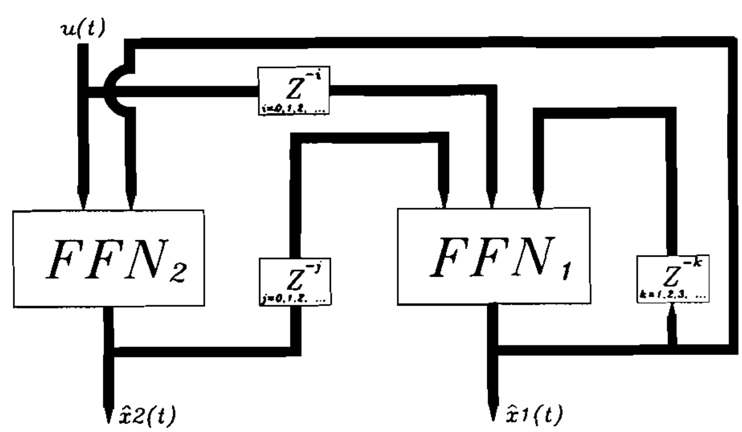

FIGURE 2 The Configuration of a generalized hybrid network.

FFN_2 are the variables in $\hat{\mathbf{x}}_2(t)$. The inputs to FFN_2 are limited to $\mathbf{u}$ asnd $\hat{\mathbf{x}}_1$at current time t, i.e.

$$\hat{\mathbf{x}}_2(t) = \mathscr{F}_2[\hat{\mathbf{x}}_1(t), \mathbf{u}(t)] \tag{2a}$$

The following simple example is provided to further clarify the general concept described in Figure 2.

Example 1

Let us consider the system behavior of an intermediate storage tank (Fig. 3) located between the batch and continuous sections in a chemical plant. This system will be referred to as System I throughout this paper. The openings of valves BV7 and NV5 on the inlet and outlet pipelines are assumed to remain constant during routine operation. There are only two process variables that can be measured on-line, i.e. the height of liquid level H and the discharge pressure of pump P. Thus, the output vector of this system is

$$\mathbf{x}^T = [H, P] \tag{3}$$

To transfer material from an upstream batch process to the storage tank, the pump on the inlet pipeline is turned on and then off periodically according to a recipe. The on/off status of pump, U, can thus be regarded as the input.

It is obvious that the rate of change of $H(t)$ is affected by the inlet and outlet flow rates. The inlet flow rate should be a function of the discharge pressure $P(t)$ and the liquid-level height $H(t)$. The outlet flow rate, on the other hand, should be a function of the height $H(t)$ only. Notice that the discharge pressure $P(t)$ should respond

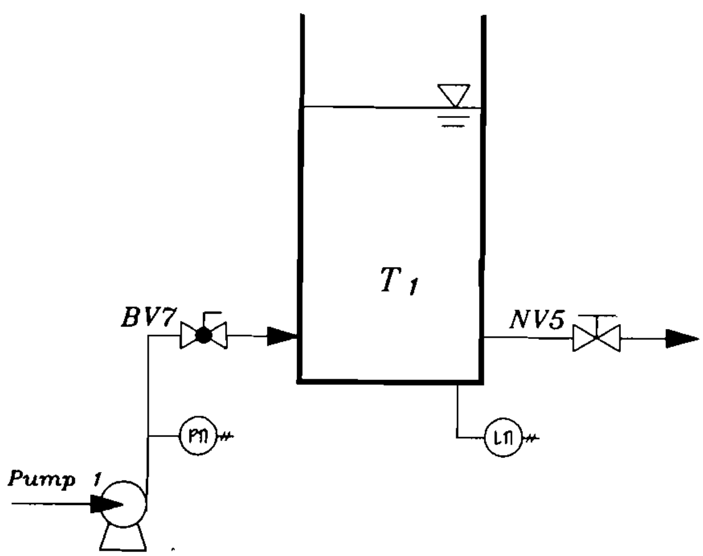

FIGURE 3 The single-tank intermediate storage system (System I).

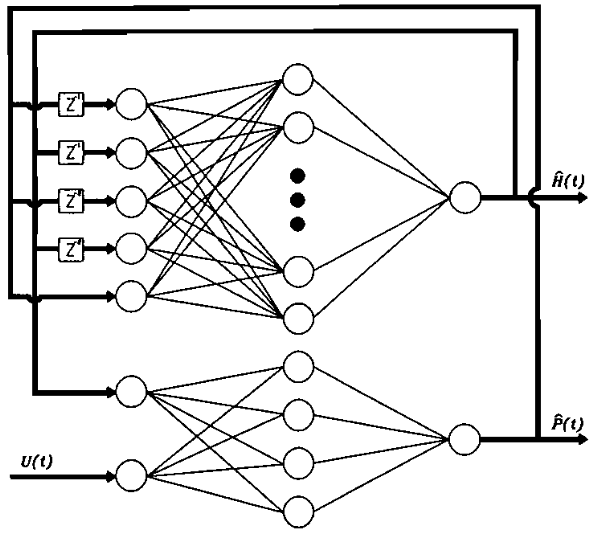

FIGURE 4 The hybrid network used for modeling the storage system I.

instantaneously to the pump status $U(t)$ and also, this pressure is affected by the local static pressure, i.e. $H(t)$. By taking into account, the above physical insights, a hybrid network (Fig. 4) can be constructed to simulate the dynamic behavior of System I under normal operating conditions.

The residuals in this case can be computed by subtracting the outputs predicted with the hybrid network from the on-line measurement values of the outputs, i.e.

$$\Delta P(t) = P(t) - \hat{P}(t) \tag{4a}$$

$$\Delta H(t) = H(t) - \hat{H}(t) \tag{4b}$$

To use these residuals in fault detection, a statistical description of their variation under normal operation should be required. Thus, it is necessary to first collect a calibration set of residual values and model the probability distribution accordingly. Then, the upper and lower threshold limits for each residual can be set to be two or three times the sample standard deviation above and below zero respectively. The occurrence of a fault is identified whenever a residual value exceeds such limits.

DIAGNOSING FAULT ORIGINS WITH A MOVING-WINDOW FFN

After the occurrence of a fault is confirmed, the feedforward network is used in this study to map the corresponding residual pattern to its origin. Since the behavior of a batch or semi-batch process is dynamic in nature, the residuals associated with abnormal operating conditions may also vary with time. Thus, it is important to include, as the inputs to FFN, informations concerning both the current and the past states of the system. Intuitively, this task can be accomplished with a moving-window FFN similar to the ones reported in several previous publications, e.g. Vaidyanathan and Venkatasubramanian (1990).

A number of different approaches in processing the input data have been investigated in this work. The simplest one, i.e. to use the raw data directly, is reported here. Specifically, the inputs to the network at time t are $\Delta \mathbf{x}_1(t - i\Delta t)(i = 1,2,\dots,I)$, $\Delta \mathbf{x}_2(t - j\Delta t)(j = 1,2,\dots,J)$, and $u(t - k\Delta t)(k = 1,2,\dots,K)$. Let us use an example to illustrate this approach.

Example 2

Let us again consider System I presented in Figure 3. Assume that there are four different fault origins, i.e. (i) a leak in the inlet pipeline, (ii) partial blockage in the inlet pipeline, (iii) partial blockage in the outlet pipeline and (iv) a leak in the tank. Thus, if a feed forward network (see Fig. 5) is to be used for fault diagnosis, the number of the outputs should be 4. Each signifies the intensity of one of the faults with a value between zero and one. The number of nodes in the input layer is the sum of the window sizes, I, J, and K, corresponds with ΔH, ΔP and U respectively. These window sizes can be adjusted to improve the diagnostic performance of moving-window FFN. The most appropriate number of nodes in the hidden layer is dependent upon the number of input nodes. It can also be determined on a trial-and-error basis in the training process.

EXPERIMENTAL SETUP

One of the most celebrated advantages of artificial neural network is its ability to capture the complex input/output relations of a variety of physical systems directly from realistic data without the need to derive mathematical models from fundamental principles of chemical engineering. To verify the feasibility and effectiveness of this

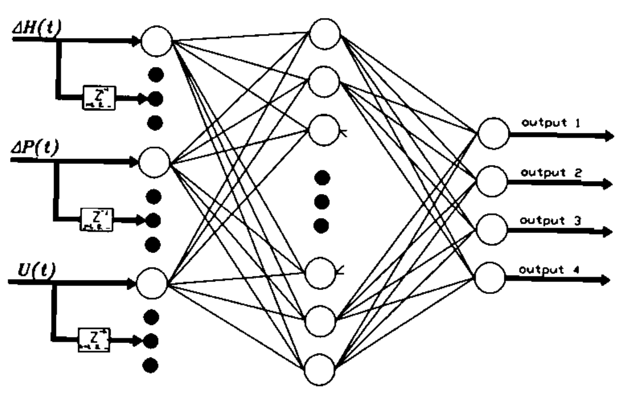

FIGURE 5 The moving-window feedforward network used for fault diagnosis in system I.

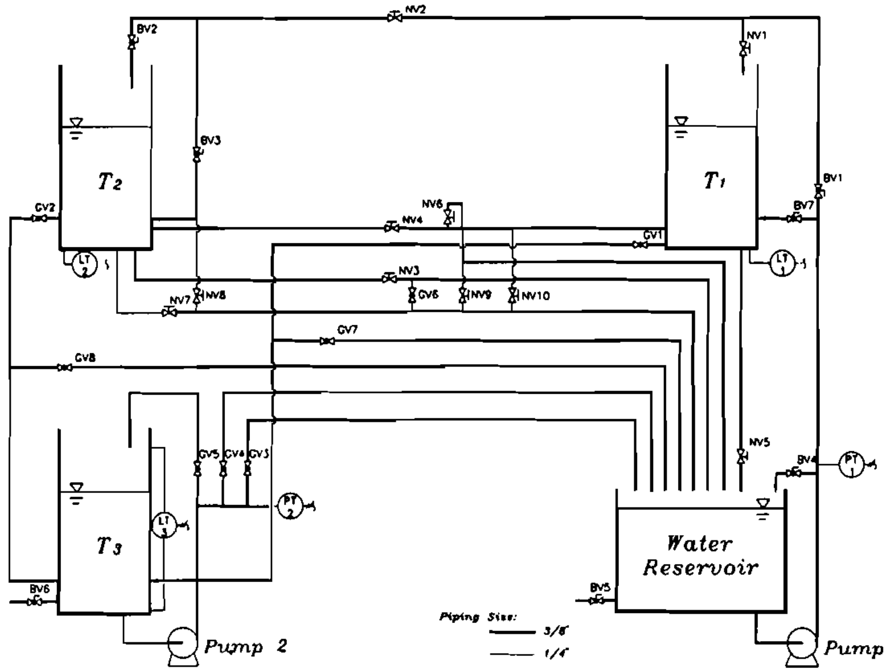

FIGURE 6 The simplified P & ID of experimental setup.

approach, a pilot plant (shown in Fig. 6) has been built in this study for producing the training and testing data.

It can be seen from Figure 6 that this experimental setup consists of a water reservoir, three open tanks (T_1, T_2 and T_3) and the connecting pipelines. The reservoir is made from 304 stainless steel. Its height is 70 cm and the diameter of its cross-sectional area is 75 cm. The three tanks are also made with 304 stainless steel and they are identical in dimensions. The height and bottom diameter of each equal 123 cm and 50 cm respectively. The water reservoir and tank T_3 are on the ground. The other two tanks, i.e. T_1 and T_2, are placed on a bench with a height of 77 centimeters.

The connecting pipelines are mainly made of $\frac{3}{8}''$ copper tubes. They are marked in Figure 6 with thick solid lines. In order to regulate the interconnecting flows and to alter system configuration, needle valves, i.e. NV1, NV2, ..., NV7, ball valves, i.e. BV1, BV2, ..., BV7, and globe valve, i.e. GV1, GV2, ..., GV8, are installed on these pipelines. In addition, branch pipelines which are made of $\frac{1}{4}''$ copper tubes are attached to the 3/8" pipelines. By opening the normally-closed needle valves, e.g. NV8, NV9 and NV10, on these branches, small leaks in the pipelines can be simulated. These $\frac{1}{4}''$ pipelines are indicated by thinner solid lines.

Two pumps are installed in our experimental setup to drive the water flows in the connecting pipelines. Water is delivered from the reservoir into T_1 and/or T_2 with a 0.5 hp centrifugal pump. Another pump of the same type and capacity is used for transferring water from tank T_3 to the reservoir. The flows in other pipelines are induced by gravity.

In our experimental setup, a number of process variables can be measured on-line. The discharge heads of the above two pumps are monitored with two identical pressure transmitters $PT1$ and $PT2$. The corresponding measurement range is from 0 to 15 psig. The levels in T_1 and T_2 are measured via differential-pressure type level transmitters, i.e. $LT1$ and $LT2$. Their ranges are from 0 to 2.5 psig. The level in the third tank T_3 is detected with an external-displacer type level transmitter $LT3$ (Smith and Corripio, 1985). The signals from the above transmitters are collected in a PC-486 via an ADDA card with 32-channel port and 12 bit resolution.

EXPERIMENTAL PROCEDURES

To generate the data needed for training and testing the proposed hybrid and moving-window feedforward network, it is necessary to operate the experimental equipments in two different modes, i.e. normal and abnormal. Their respective experimental procedures are outlined below:

Normal Mode

The first step in all experiments is to establish the system configuration. A large number of different systems have been studied in this work with the same experimental setup described in Figure 6. For example, System I in Figure 3 and the systems presented in Figure 7a to Figure 7d can be realized by setting the valve positions according to Table I. Each value given in the table represents the opening of the corresponding valve, i.e. the number of counterclockwise turns from the fully-closed position. Notice that valves BV1 and BV2 remain fully opened in all five cases, and the valve openings of BV4 and GV5 on the recycle lines were adjusted once in each case to produce proper flow rates for all related experiments. Also, in each case, the other unlisted valves and those corresponding to the blanks in Table I were kept closed.

The next step is to initialize the system before startup. Specifically, the tank(s) should be filled to a level within acceptable range and the pumps primed.

The final step is to carry out the actual experiment for a period of 2 to 3 hours. As mentioned before, our experiments are designed to simulate the operation of intermediate storage tanks in a batch or semi-batch process. To imitate the intermittent input to T_1 and/or T_2 from an upstream batch process, the power source of pump No. 1 is manually switched on and off at constant or arbitrary intervals. Similarly, pump No. 2 is operated in the same fashion to produce the effect of periodical withdrawal of the content from T_3. Notice that pump No. 2 is used only in System V.

Abnormal Mode

After the system has been successfully operated in normal mode, faults can be introduced by manipulating the openings of various valves at different locations. As an example, the faults that have been simulated in System III can be found in Table II. Notice that faults associated with pipeline leakage have been included in our study. In

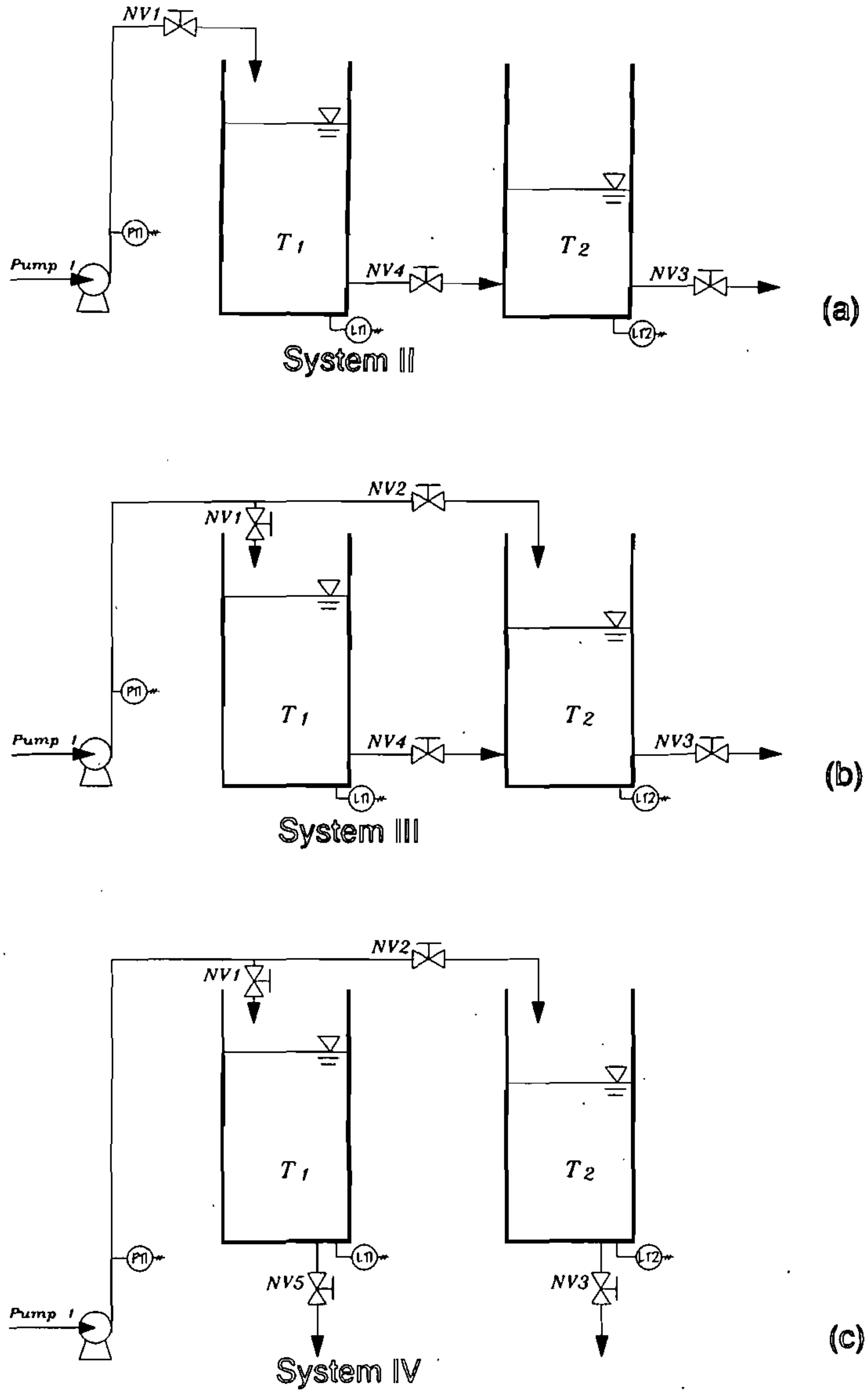

FIGURE 7 The simplified flow diagram of system II, III, IV and V.

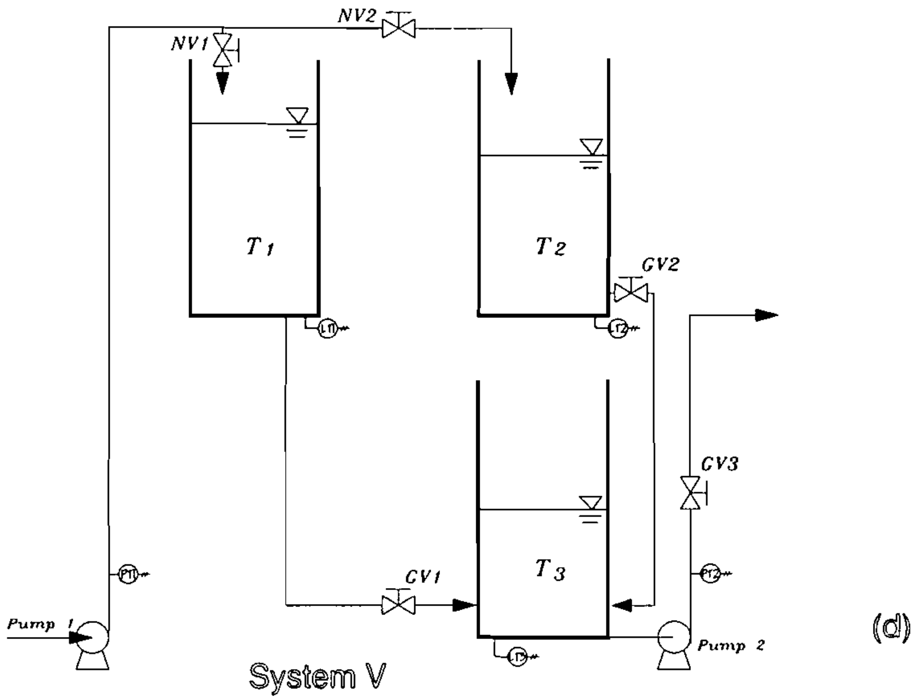

FIGURE 7 *(Continued)*

TABLE I

Valve Settings for Five System Configurations

System No.	Valve Opening NV1	NV2	NV3	NV4	NV5	GV1	GV2	GV3	BV7
I					9				$\frac{1}{2}$
II	2		3	3					
III	2	2	3	3					
IV	$2\frac{1}{2}$	$2\frac{1}{2}$	3		3				
V	3	3				4	4	4	

general, such faults are very difficult to describe mathematically and thus the model-based techniques are not suitable for their diagnosis.

EXPERIMENTAL RESULTS

Although a large volume of results have been generalized in this work, only the experimental data obtained from Systems I and III are included in this article. This is due to the need for keeping the paper within a reasonable length. Detailed descriptions

TABLE II

The Operating Procedure for Simulating Faults in System III

Fault No.	Fault Origins	Operating Procedure
(i)	Partial blockage in the inlet pipeline of T_2	Close NV2 slightly
(ii)	Partial blockage in the inlet pipeline of T_1	Close NV1 slightly
(iii)	Partial blockage in the pipeline between T_1 and T_2	Close NV4 slightly
(iv)	A leak in the exit pipeline of T_2	Open GV6 slightly
(v)	A leak in the storage tank T_2	Open NV7 slightly
(vi)	A leak in the pipeline between T_1 and T_2	Open NV6 slightly
	or	
	A leak in the storage tank T_1	Open NV5 slightly

of these unreported case studies have been presented elsewhere (Chen, 1993). Three examples are described in this section. In examples 3 and 4, the advantages of adopting the proposed hybrid network for fault detection are demonstrated with experimental data obtained from System I. The long-term prediction capability of a hybrid network is compared with that of a conventional ERN in the former example. In the latter example, the applicability of the proposed approach and also a short-term prediction approach for residual generation has been accessed thoroughly. Finally, in Example 5, the effectiveness of the suggested fault diagnosis scheme is verified with pilot data obtained from System III.

Example 3. Prediction of the Long-Term Dynamic Behavior

As indicated above, the batch operation described in Example 1 is considered here in the present example. To implement the residual-based fault detection methods, the outputs must be predicted on the basis of input values. Two network configurations have been tested for this purpose.

First, an external recurrent network (Fig. 8) was constructed to predict the values of the outputs, i.e. the height of the liquid level in the tank (H) and the discharge pressure

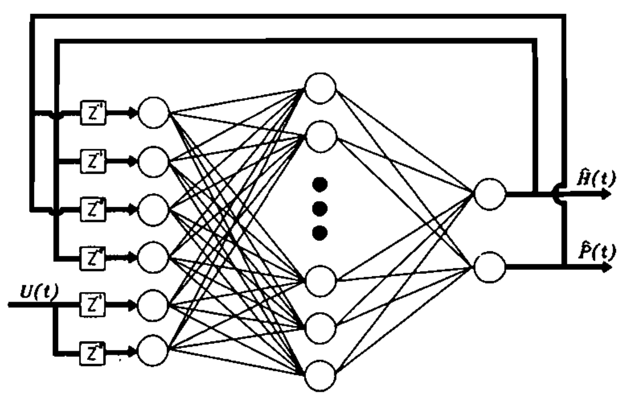

FIGURE 8 The external recurrent network used for modeling the storage system I.

of pump (P). In this work, 6, 9 and 2 nodes were selected for the input layer, the hidden layer and the output layer respectively. In our experiment, the measurement data were taken every 40 seconds and, in total, 568 data sets were obtained. The first 320 sets were used for training and the remaining data were used for generalization. The objective of the corresponding iteration process was to minimize

$$\sqrt{\frac{\sum_{i=1}^{n_d}\sum_{j=1}^{n_o}(\varepsilon_{ij})^2}{n_d \times n_o}} \tag{5}$$

where, ε_{ij} is the difference between the predicted and experimental values of the jth output variable in the ith data set; n_d is the number of the data sets; n_o is the number of the output nodes.

Twelve initial guesses were used to start the training calculation. The weights corresponding to the smallest minimum objective function (0.03) were adopted to produce the results presented in Figure 9a to Figure 9d. Notice that the pressure

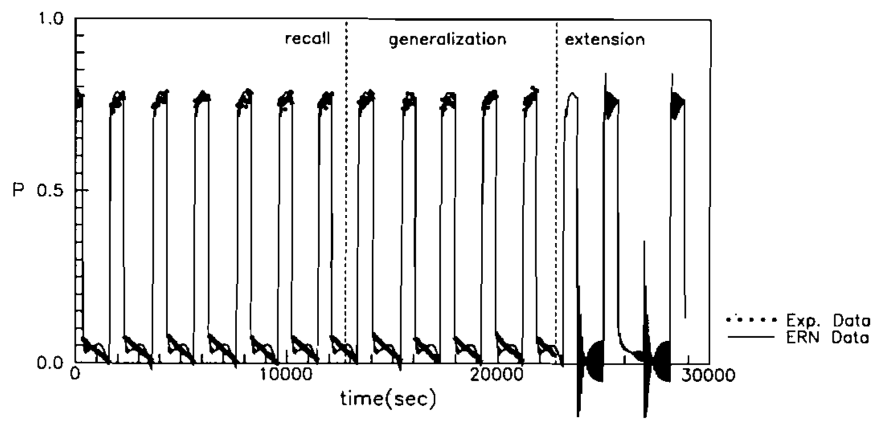

FIGURE 9a Results of applying ERN in system I: long-term prediction of the inlet pressure.

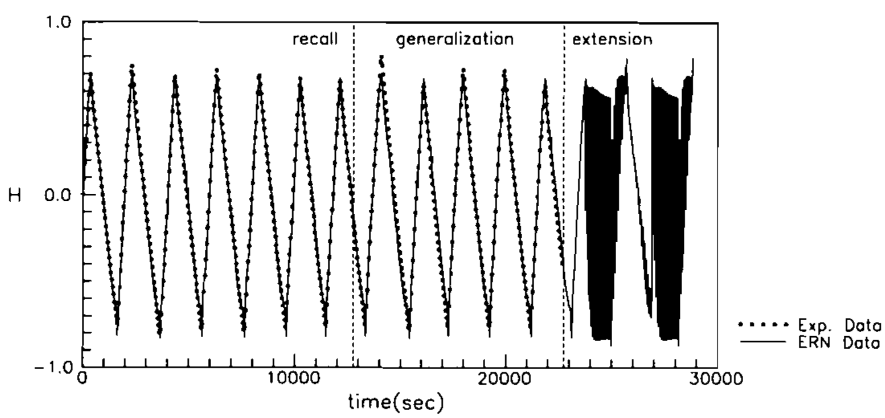

FIGURE 9b Results of applying ERN in system I: long-term prediction of the liquid level.

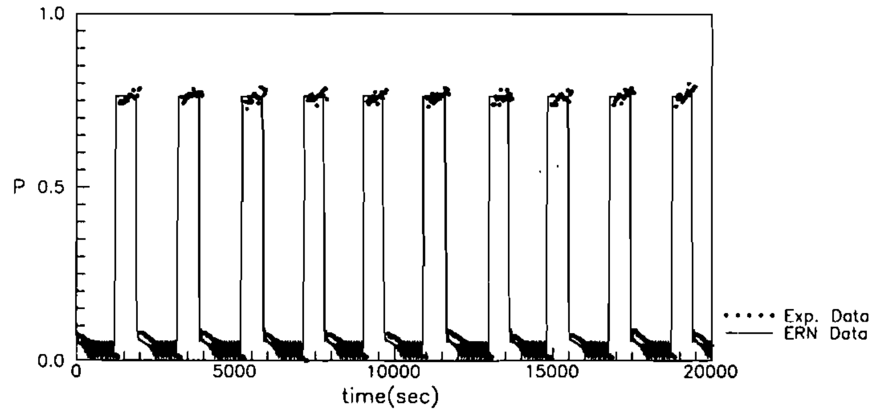

FIGURE 9c Results of applying *ERN* in system I: extended prediction of the inlet pressure with a different set of initial conditions.

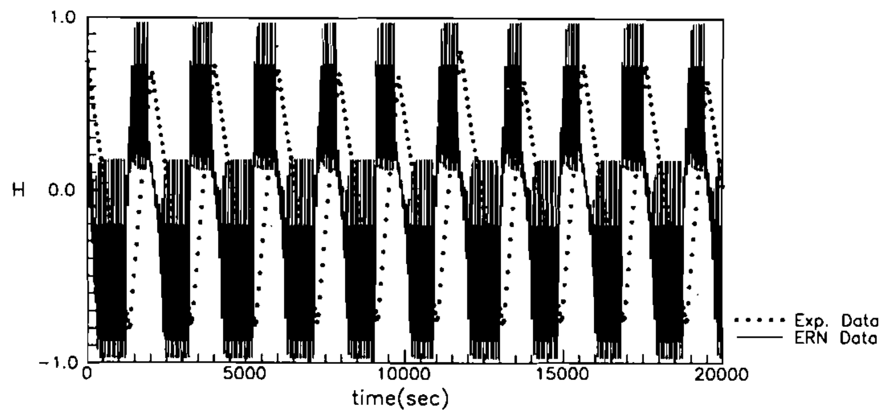

FIGURE 9d Results of applying ERN in system I: extended prediction of the liquid level with a different set of initial conditions.

measurements have been linearly normalized between 0 and 0.8 from the original range of $0 \sim 7.32$ psig and, also, the level measurements were converted from a range of 68.77 to 115.3 cm to values between -0.8 and $+0.8$.

It can be observed from Figure 9a and Figure 9b that, when compared with both the trained and untrained data, the predictions of ERN in the recall and generalization period are in general acceptable. This observation seems to suggest that an ERN can be adopted to describe the dynamic behavior of the intermediate storage tank in this example. However, if the prediction computation is extended further, then erratic results may be generated. One can also observe from Figure 9a and Figure 9b that, with the same ERN, the predicted values of pressure and height oscillate severely in the extended period. Further, if a different set of initial values for P and H are adopted, drastically oscillation and even chaos-like behavior were found throughout the entire prediction period, e.g. Figure 9c and Figure 9d. It should be emphasized that similar results were obtained with all other sets of weights determined in training. Thus, it becomes apparent that a modified version of the ERN must be implemented.

The above problems can actually be attributed to the fact that the output variables (H and P) respond to the input (U), i.e. the signal to activate or deactivate the pump, at widely different rates. The pressure P at the pump exit responds to the input almost immediately. On the other hand, the present liquid level is affected by the inlet flow rates and the liquid level at present and previous time steps. Since the network structure in Figure 8 fails to reflect this situation directly, a hybrid network (Fig. 4) has been developed. In this network, 4, 7 and 1 nodes were used in the input, hidden and output layer of FFN_1 and, in the corresponding layers of FFN_2, 2, 8 and 1 nodes were used respectively.

The above network were trained with the same experimental data. The convergence rate of the iteration process was found to be faster and smaller objective function (0.025) can be achieved easily. The results of recall and generalization are presented in Figure 10a and Figure 10b. It can be clearly observed that the performance of the

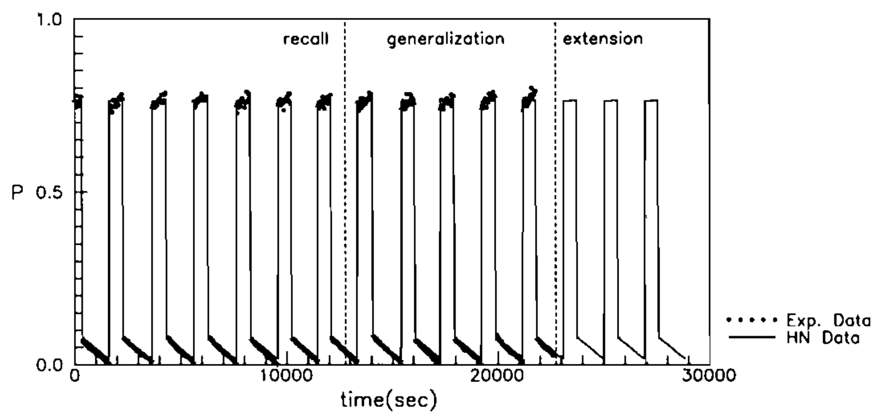

FIGURE 10a Results of applying hybrid network in system I: long-term prediction of the inlet pressure.

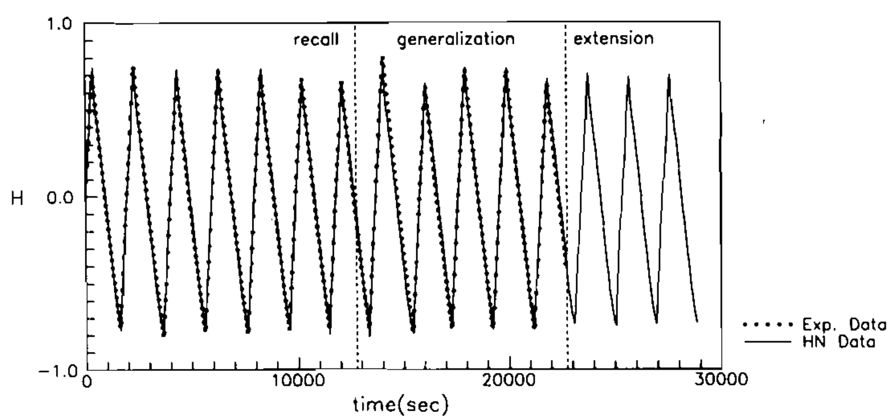

FIGURE 10b Results of applying hybrid network in system I: long-term prediction of the liquid level.

proposed network is quite satisfactory. Further, even with a different set of initial conditions, the prediction of the hybrid network is still very accurate (Fig. 10c and Fig. 10d).

Finally, although in most cases the inputs to the storage system in Figure 3 are manipulated periodically, the feasibility of the proposed approach for predicting noncyclic system behaviors has also been assessed in our study. For this purpose, experimental data were generated by arbitrarily changing the ON/OFF status of the inlet pump in System I. In this case, the normalized ranges for P and H were $[0, 0.8]$ and $[-0.8, +0.8]$ respectively. It can be observed from the results obtained in recall and generalization state (Fig. 11a and Fig. 11b) that the hybrid network is indeed capable of tracing the long-term variations of the output variables in noncyclic processes. In addition, the trained network could be applied to predict the system response caused by

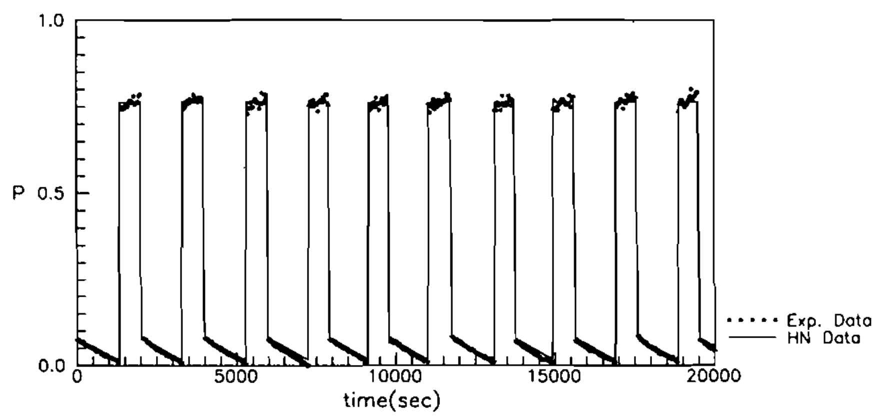

FIGURE 10c Results of applying hybrid network in system I: extended prediction of the inlet pressure with a different set of initial conditions.

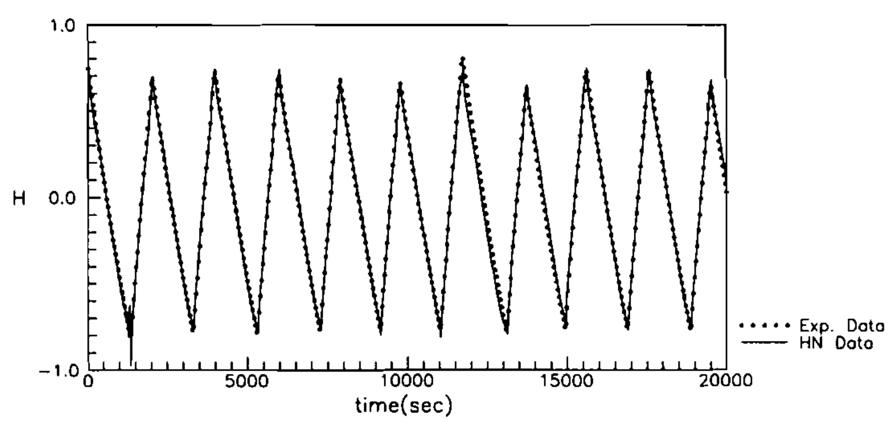

FIGURE 10d Results of applying hybrid network in system I: extended prediction of the liquid level with a different set of initial conditions.

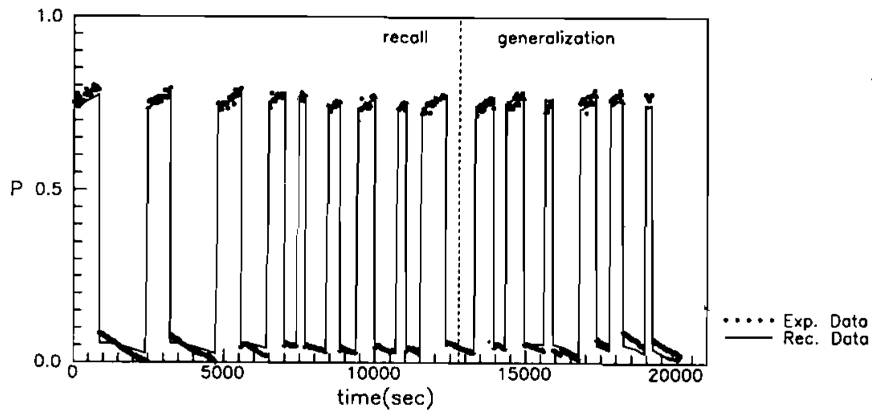

FIGURE 11a Results of applying hybrid network in system I: long-term prediction of the inlet pressure in noncyclic operation.

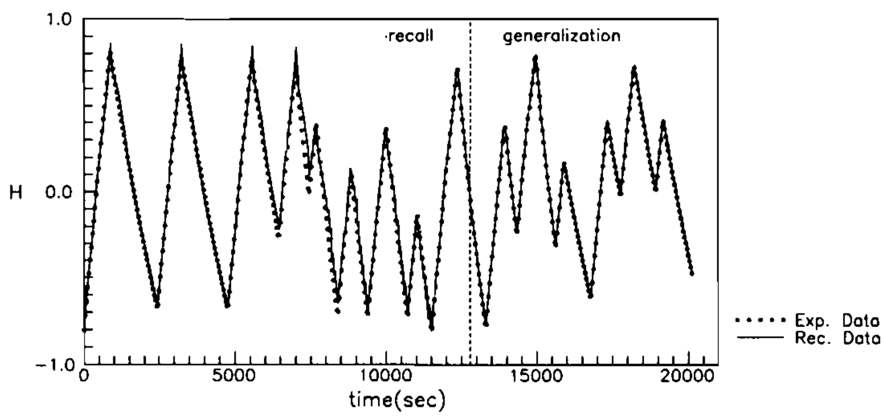

FIGURE 11b Results of applying hybrid network in system I: long-term prediction of the liquid level in noncycle operation.

an operation sequence not adopted in training. From the results presented in the generalization period, it can be concluded that the performance of the proposed network is more than acceptable.

Example 4. Residual Generation

The focus of this example is to address the practical issues in implementing the residual-based fault detection procedure. As mentioned before, the purpose of on-line prediction of the outputs is to reconstruct the normal state of dynamic system and then compute the residuals accordingly. Since the observed outputs values are always affected by the random measurement error and random disturbances to the process, it is not likely to find $\Delta x = 0$ even in systems without faults. Thus, it becomes necessary to first establish the threshold limits of the residuals from the data obtained under normal conditions. In this example, the calibration sets of residuals associated with inlet pressure and liquid level in System I were obtained from the data presented in Figure 10a and Figure 10b. The values of sample mean and standard deviation corresponding to ΔP are -0.00511 and 0.009237, and those corresponding to ΔH are 0.000294 and 0.034796 respectively. The threshold limits of ΔP and ΔH were set to be three times the estimated standard deviations, i.e. ± 0.02771 and ± 0.104388, respectively.

After the threshold limits were established, the experiments were repeated under the influence of a fault. More specifically, to simulate the phenomenon that the outlet pipeline is partially blocked, the opening of the exit valve in System I (i.e. NV5 in Fig. 3) was reduced slightly after the experiments has been carried out under "normal" operating condition for 3040 seconds. The corresponding residuals can be found in Figure 12 of this paper. We can see that abnormal operation condition is detected at 3360 second on the time axis, which is 320 seconds after the introduction of fault.

In this study, the feasibility of using residuals generated with a short-term prediction approach, i.e. the feedforward network, has also been assessed. It was found that in general a trained FFN is capable of predicting the dynamic behavior of a batch or semi-batch process under *normal* operating conditions. However, the residuals generated by this prediction approach are *not* suitable for the purpose of fault detection. This is due to the facts that the network uses the measured outputs at previous time steps as its inputs for predicting the outputs at present time, and thus the estimated outputs are always close to the measurement values even when a fault does occur during operation. This phenomenon can be clearly observed from the results produced with the feedforward network in Figure 13a. The corresponding residuals are presented in Figure 13b. Notice that the values of ΔP and ΔH stay close to zero throughout the entire period of operation. The occasional spikes in these curves are mainly due to the alternation in the operation modes (ON/OFF) associated with the inlet pump.

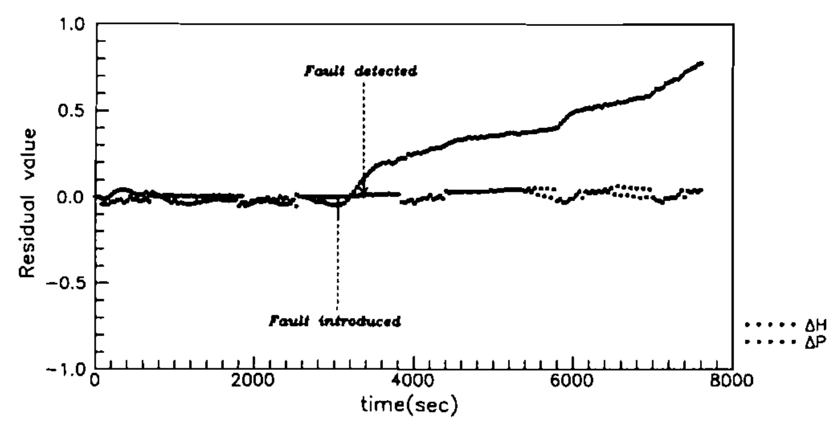

FIGURE 12 The residuals obtained with the long-term prediction approach under the influence of exit pipeline plugging in system I.

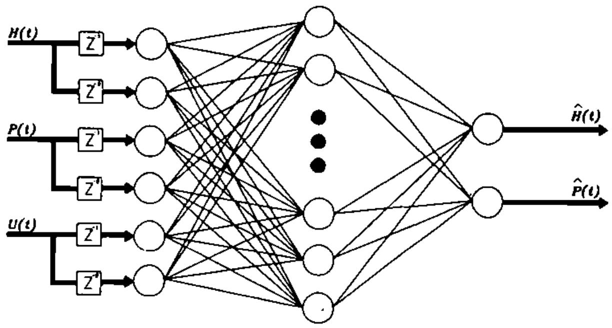

FIGURE 13a The feedforward network used for modeling the storage system I.

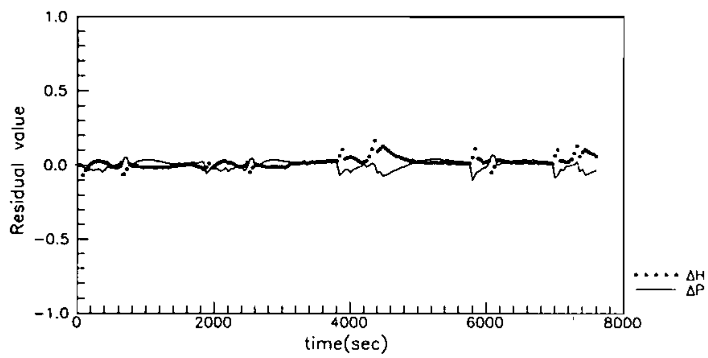

FIGURE 13b The residuals obtained with the short-term prediction approach under the influence of exit pipeline plugging in system I.

Example 5. Fault Diagnosis

The simplified flow diagram of the process studied in this example is given in Figure 7b, i.e. System III. One can see that, using pump No. 1, water can be transferred from reservoir to both tanks, T_1 and T_2, via parallel inlet pipelines. The content in each tank is driven out by gravity. The outlet flow of the first tank is directed to the second tank. The water in the second tank is then discharged back into the reservoir. There are three variables that can be measured on-line, i.e. the outlet pressure of pump No. 1 (P) and the height of liquid level in T_1 and T_2 (H_1 and H_2) respectively. The sampling interval in this case is again 40 seconds.

The hybrid neural network associated with System III was constructed according to Figure 2. The corresponding supervised learning process was terminated when the objective function reached a value less than 0.02. In most cases, the performance of the trained network is quite satisfactory. For the sake of brevity, these results are not included here. The configuration of moving-window FFN in this case is very similar to that used for System I (see Fig. 5). The outputs of this network is naturally related to the faults that can be simulated in System III. The output value 1 signifies that the corresponding fault occurs and 0 means otherwise. There are 6 nodes in the output layer. Their respective physical interpretations are provided in Table II. Notice that, since the symptoms caused by the two faults "a leak in tank T_1" and "a leak in the pipeline between T_1 and T_2" are almost identical, they are combined as fault (vi) here. On the other hand, the residuals associated with the three on-line measurements, i.e. ΔH_1, ΔH_2 and ΔP, and the ON/OFF status of pump No. 1, i.e. U, at consecutive sampling intervals are fed into the input layer of the network. A uniform window size is adopted for these four types of inputs. The number of data points in a window has been varied from 6 to 10 in training and testing. It was found that the network performed satisfactorily with a size of eight. Finally, through extensive computational effort, we have successfully reduced the value of objective function to below 0.025 using seven hidden nodes.

The effectiveness of the proposed moving-window FFN has been verified with untrained on-line data obtained from pilot experiments under normal and abnormal operation modes. The results shown in Figure 14a are associated with normal operation. One can see that, as expected, all six output values stay close to zero with minor fluctuations only at very rare occasions. The diagnostic conclusions presented in Figure 14b to 14g are corresponding to fault (i) to (vi) respectively. These conclusions are generally correct and sufficient for diagnosis purpose. The fact that faults (i) and (ii) are diagnosable is a little surprising. Since the pressure residual is not affected, i.e. $\Delta P = 0$, by partial blockage in either of the inlet pipelines when the pump is switched off, one would expect that this type of faults should be indistinguishable from events such as leakage in the corresponding tank during the same period of time. However, after a closer examination of the interaction among measured variables in this system, it can be concluded that these results are in fact reasonable. Notice that the two inlet pipelines are connected to the same pump. Thus, the occurrence of either one of these faults should affect the levels in both T_1 and T_2. For example, a partial blockage in the pipeline leading to T_1 will cause a decrease in the inlet flow to T_1 and, at the same time, an increase in the input to T_2. As a result, the corresponding pattern of residuals associated with the levels (i.e. $\Delta H_1 < 0, \Delta H_2 > 0$) is sufficient for the identification of fault (i).

It should be noted that occasional instances of misdiagnosis can still be observed in the above diagnostic results. From Figure 14b and Figure 14c, one can see that significant oscillation occurs during the initial stage of diagnosis for fault (i) or (ii). This can be attributed to the fact that, in the corresponding experiments, the output voltage of power supply was unstable during the startup period.

A more serious type of misdiagnosis can also be found in Figure 14f and Figure 14g. In the former case, fault (ii) was mistakenly identified instead of fault (v) for a short period of time before switching to the correct conclusion. Similarly, fault (vi) was momentarily replaced by fault (i) as the cause of abnormality during the initial stage of diagnosis in the latter case. It should be emphasized that this type of misdiagnosis is inevitable in our system. These results can be attributed to the fact that the symptoms caused by two different faults are very similar for a short period during operation. Let us use the diagnosis of fault (v) as an example to explain in more detail. First, notice that the pump was not activated initially for about 2000 seconds. Thus, the pressure residuals should be constant at zero during this period and this outcome, i.e. $\Delta P(t) = 0$

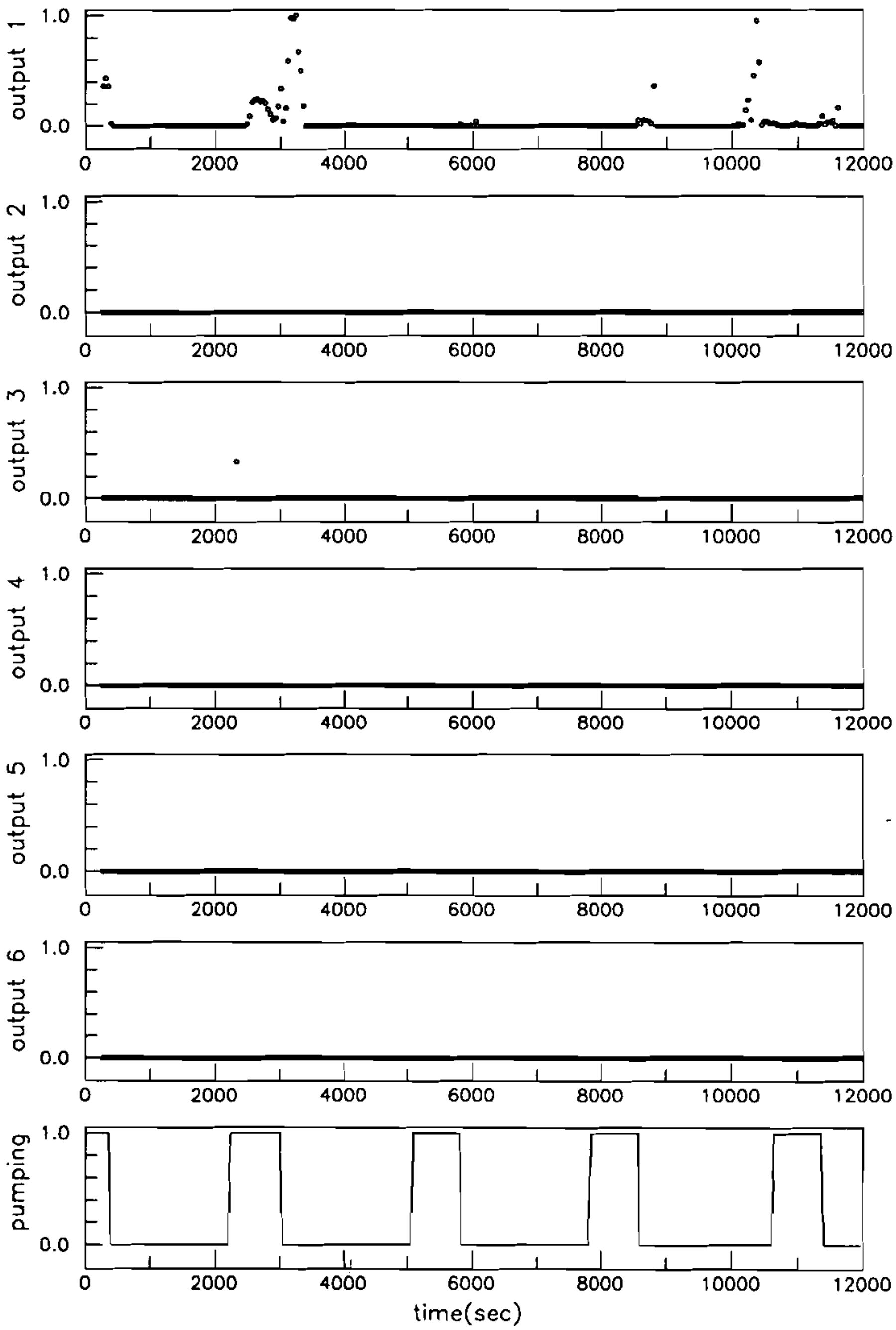

FIGURE 14a Results of fault diagnosis in system III: normal operating conditions.

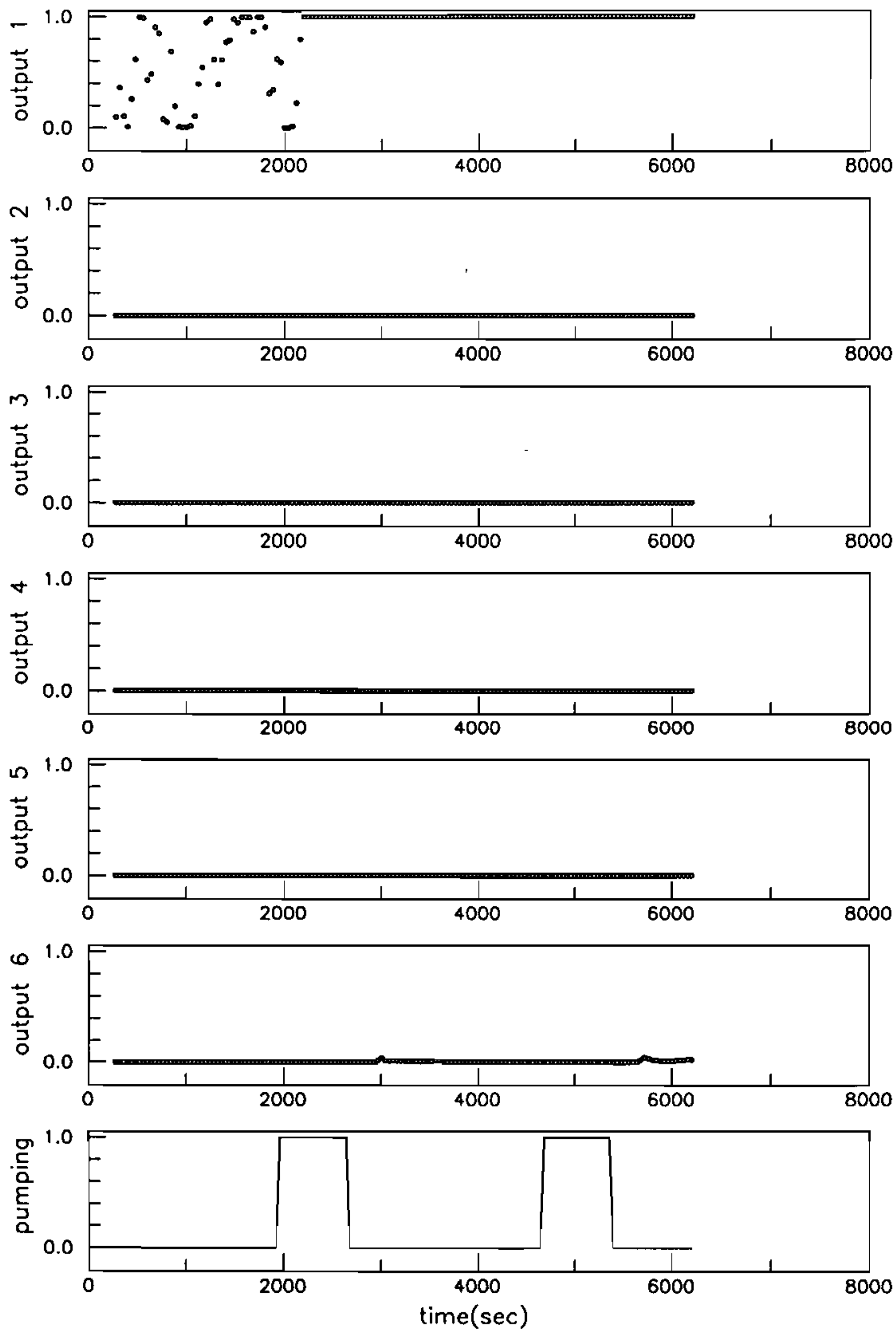

FIGURE 14b Results of fault diagnosis in system III: partial blockage in the inlet pipeline of T_1.

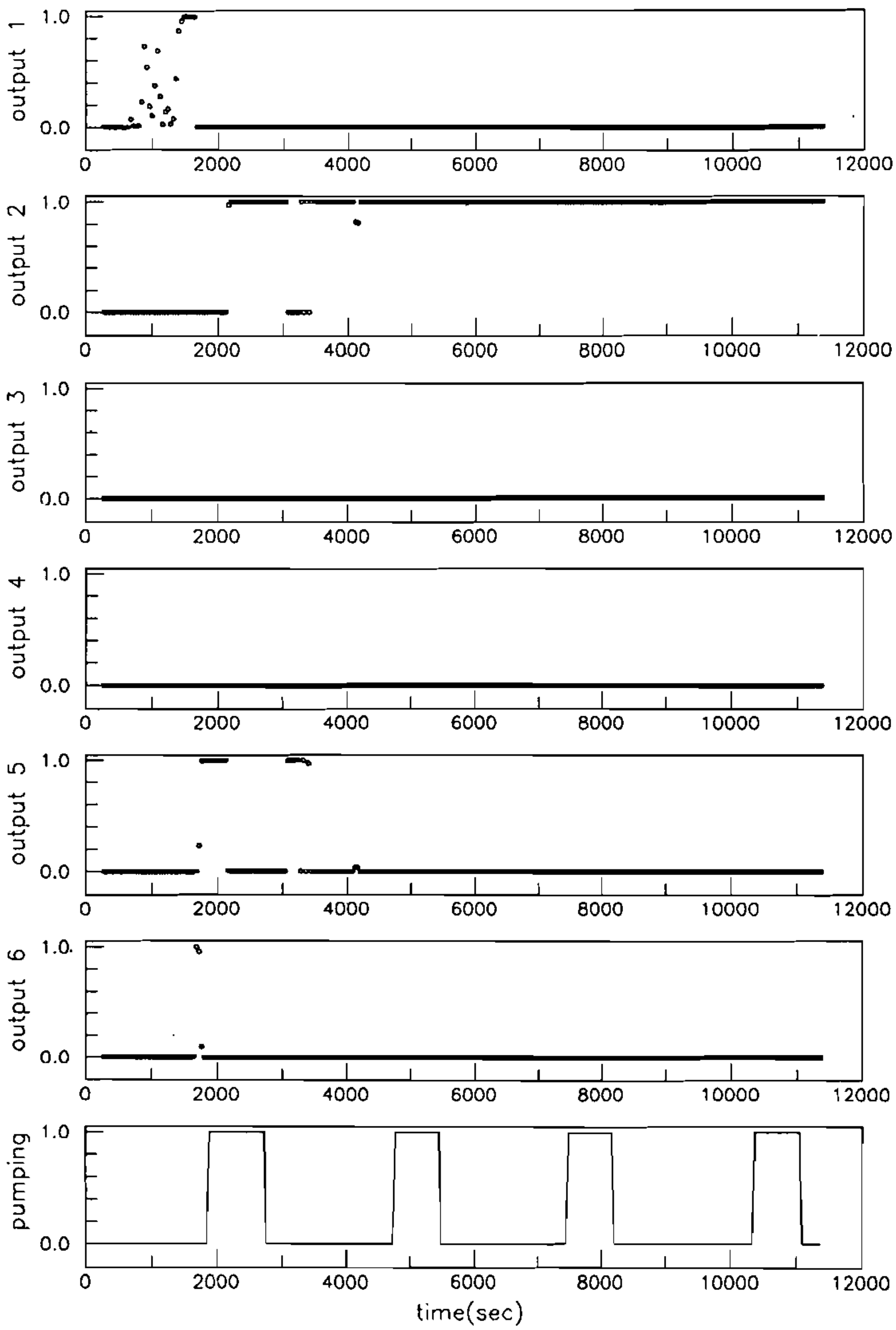

FIGURE 14c Results of applying hybrid network in system III: generalized prediction of the liquid level in T_2.

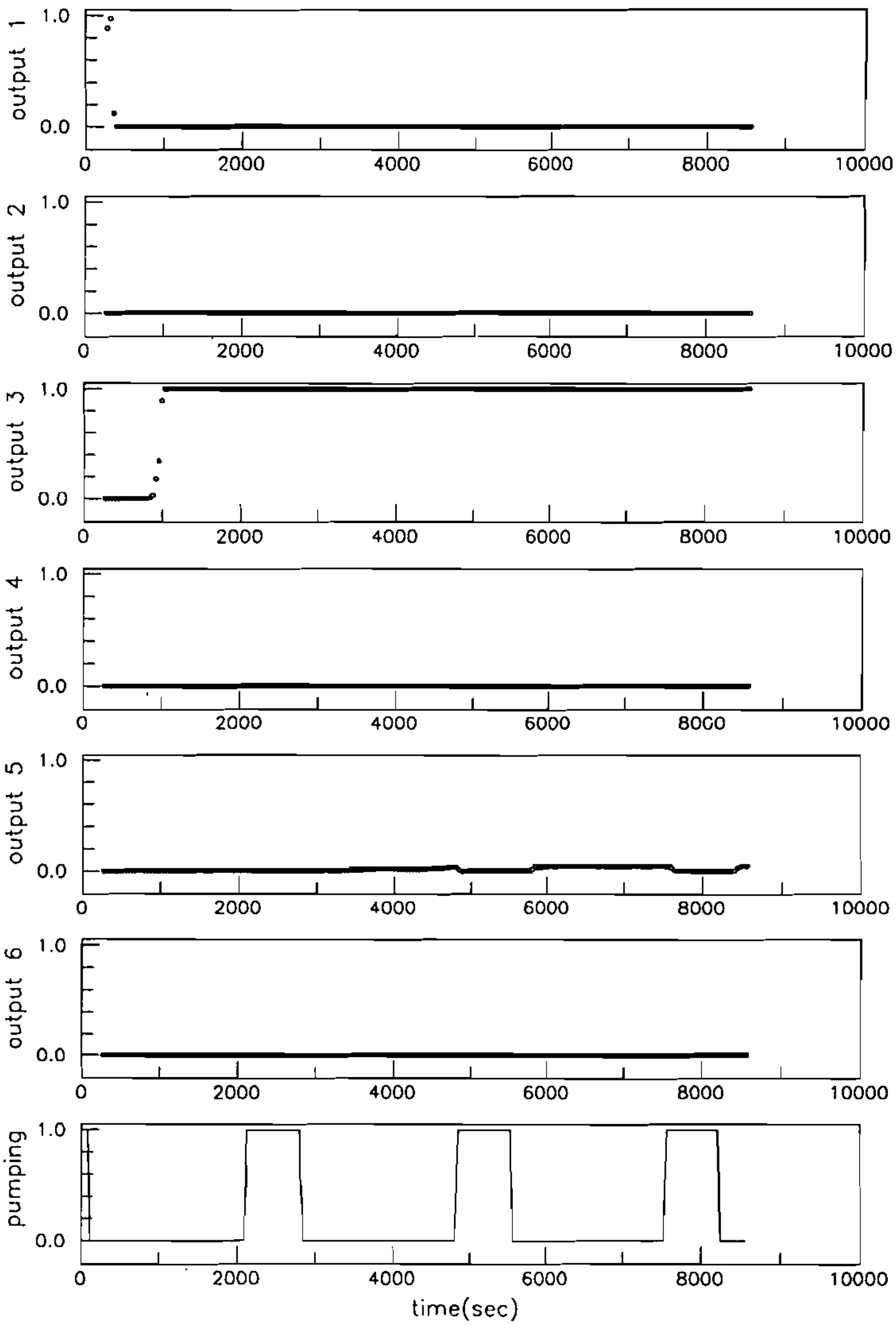

FIGURE 14d Results of fault diagnosis in system III: partial blockage in the pipeline between T_1 and T_2.

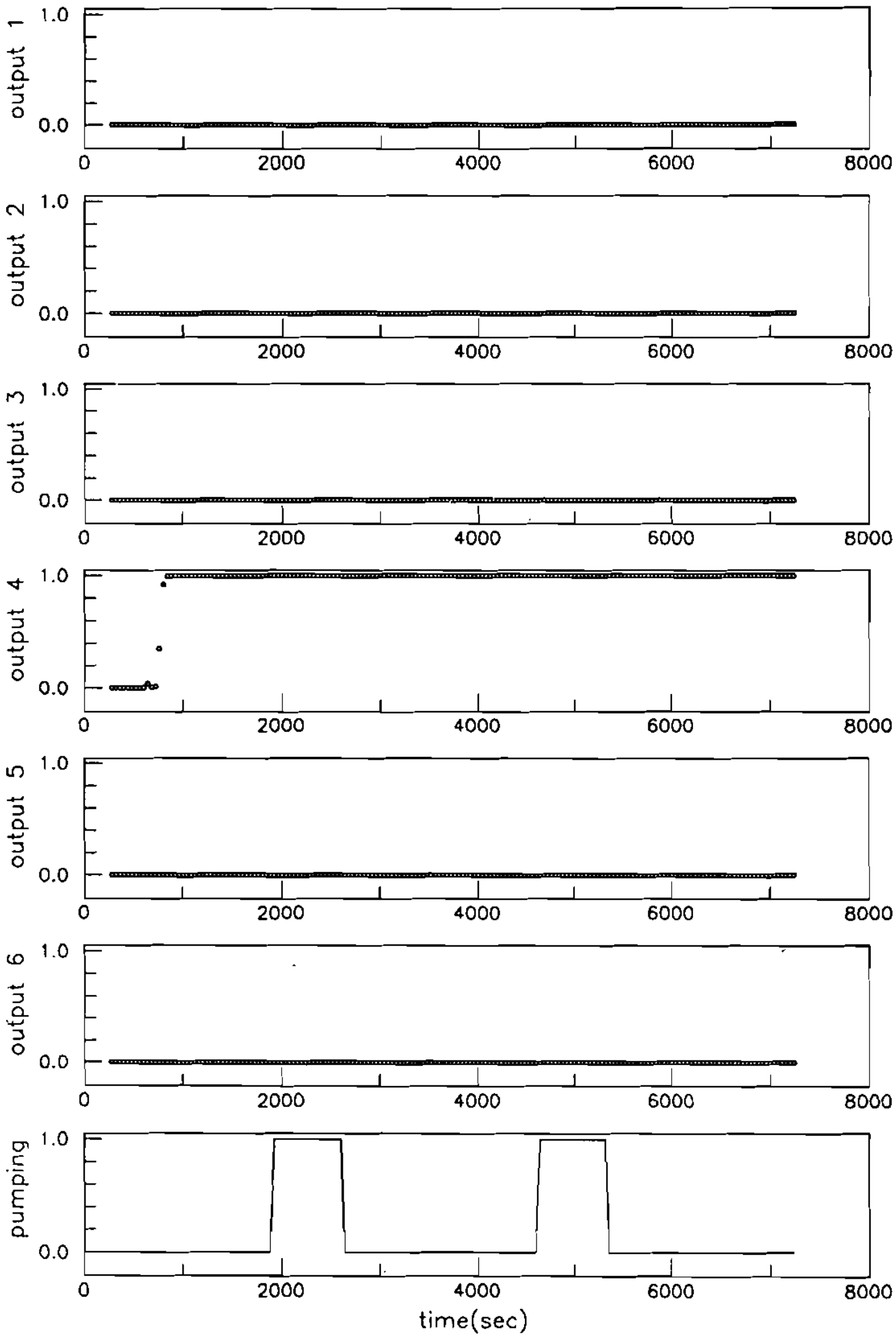

FIGURE 14e Results of fault diagnosis in system III: a leak in the exit pipeline of T_2.

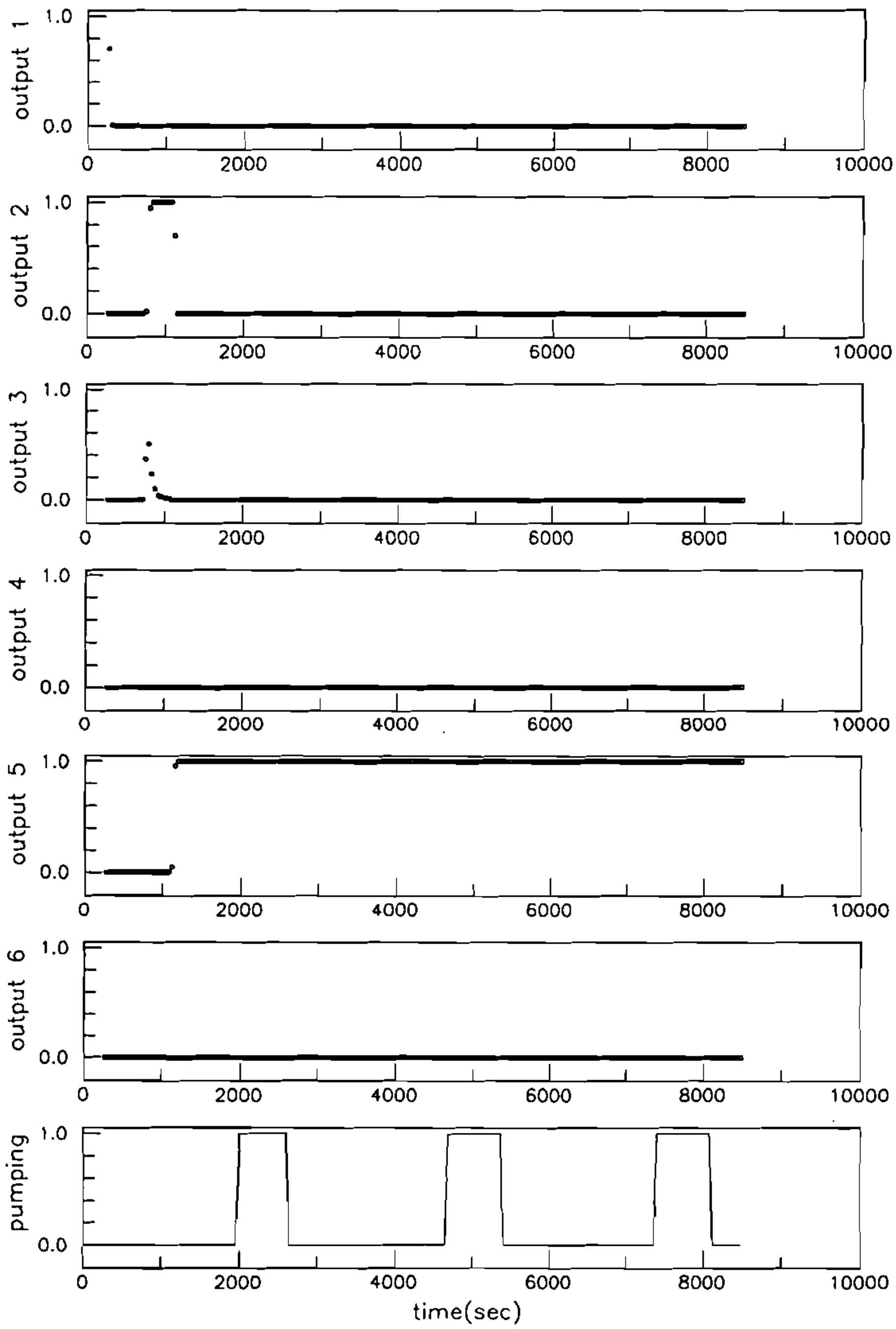

FIGURE 14f Results of fault diagnosis in system III: a leak in the storage tank T_2.

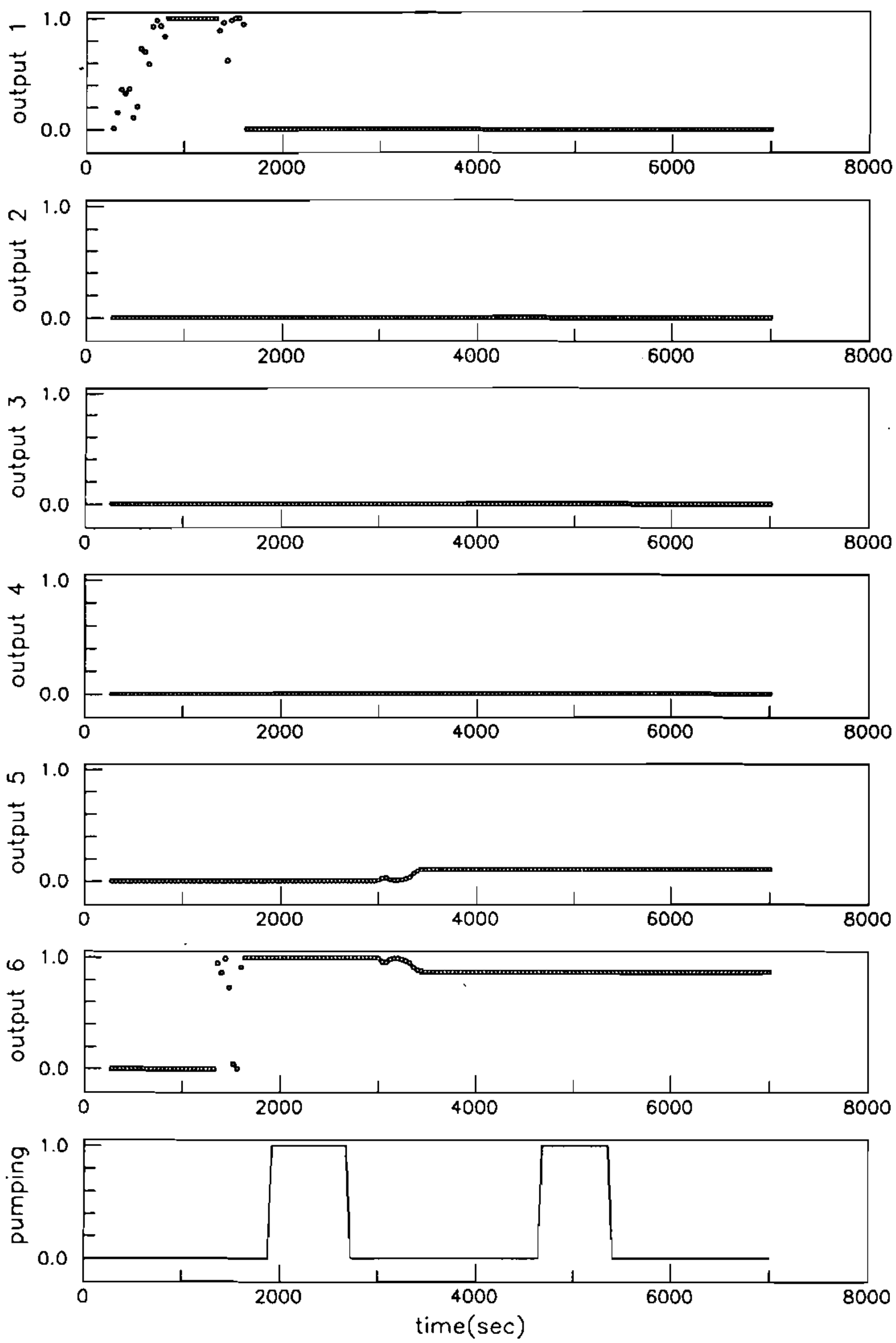

FIGURE 14g Results of fault diagnosis in system III: a leak in the pipeline between T_1 and T_2.

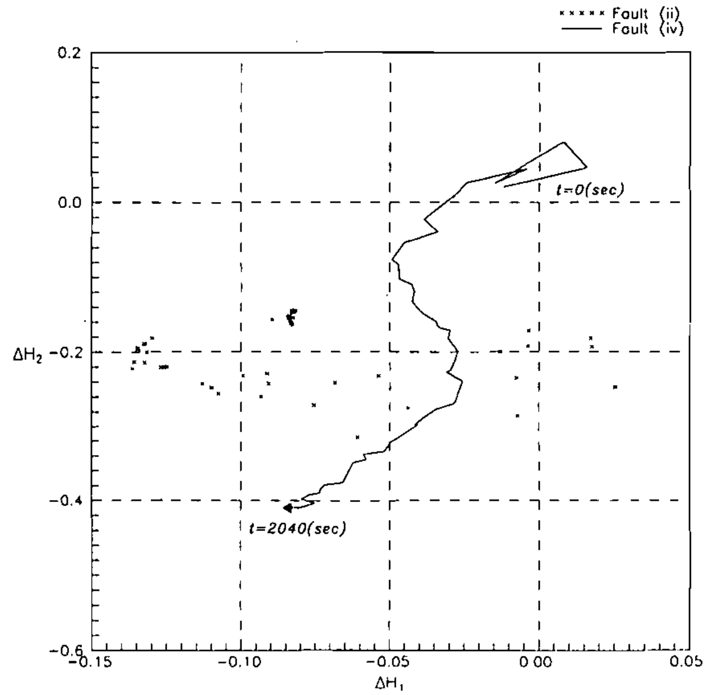

FIGURE 15 The Initial residual trajectory corresponding to fault (v) in system III.

for $0 \leqslant t \leqslant 2000$, can be produced by either fault (ii) or (v). In Figure 15, the trajectory of ΔH_1 versus ΔH_2 corresponding to fault (v) is plotted for the same period against a background of the training data used for fault (ii) when the pump is turned off. One can see clearly that the residual pattern generated after the introduction of fault (v) "walks" into a region which has already been classified as fault (ii). As a result, the unavoidable mistake was committed temporarily in diagnosis.

CONCLUSIONS

Effective neural-network-based techniques have been developed in this study for fault detection and diagnosis in batch and semi-batch processes. The principal difference between this paper and the published works which also address the problem of fault identification from transient data (e.g. Watanabe *et al.*, 1989; Vaidyanathan *et al.*, 1990) is that the external inputs to the given process are no longer assumed to be constant. As a result, it is necessary to first generate residuals associated with the on-line measurements and then locate the fault origins accordingly. This turns out to be the major point of departure from the previous approaches.

The proposed fault monitoring system consists of two neural networks connected in series, i.e, a hybrid network and a moving-window FFN. The former is capable of predicting the normal long-term behavior of realistic batch and semi-batch systems in which various types of fast equilibrium and slow dynamic relations may exit simultaneously. The outputs of this network are the reference values for computing residuals which, in turn, can be used for fault detection via statistical tests. Once the existence of a fault is confirmed, the latter network can then be implemented to map the corresponding residual pattern to its origin.

Extensive experimental studies have also been carried out in this work. Based on the test data we have produced so far concerning the hybrid networks, one can conclude that the accuracy demonstrated in their predictions definitely meets the need for a reliable fault detection scheme in the fault monitoring system. Also, from the diagnostic results presented in this paper, one can see that the moving-window FFN is in general able to correctly identify the residual pattern caused by a single fault origin. Although, in several cases, misdiagnosis appeared at occasional instances during the initial stage, this network always yielded the correct results eventually within a short period of time.

NOMENCLATURE

$\mathbf{f}_1, \mathbf{f}_2$	The descriptive functions of the process
$\mathcal{F}_1, \mathcal{F}_2$	The alternative descriptive functions of the process
H_1, H_2	The heights of water levels in tanks T_1 and T_2 respectively
$\Delta H_1, \Delta H_2$	The residuals of H_1 and H_2 respectively
n_d	The number of training data sets
n_0	The number of nodes in the output layer
p	The discharge pressure of pump
$\mathbf{p}$	The vector of unknown parameters
P	The normalized discharge pressure
ΔP	The residual associated with P
t	The present time
$\mathbf{x}_1, \mathbf{x}_2$	The vector of system outputs
$\hat{\mathbf{x}}_1, \hat{\mathbf{x}}_2$	The vector of estimated outputs
$\Delta \mathbf{x}$	The vector of residuals
$\mathbf{u}$	The vector of system inputs
U	The ON/OFF status of the pump

Greek Symbols

ε_{ij}	The training errors
τ	The dummy index of time intervals

Abbreviations

ANN	Artificial neural network
ERN	External recurrent neural network
FFN	Feedforward neural network
PDF	Probability density function

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