

MODEL-BASED DATA-DRIVEN APPROACH TO ROBUST FAULT DIAGNOSIS IN CHEMICAL PROCESSES

Silvio Simani* Ron J. Patton**

* *Dipartimento di Ingegneria, Università di Ferrara.
Via Saragat 1, 44100 Ferrara - ITALY.
Phone: +39 0532 293839. Fax: +39 0532 768602.
E-mail: ssimani@ing.unife.it*

** *Department of Engineering, The University of Hull.
Cottingham Road. Hull HU6 7RX, UNITED KINGDOM.
Phone: +44 1482 46 5117. Fax: +44 1482 46 5117.
E-mail: r.j.patton@hull.ac.uk*

Abstract: This paper presents a robust model-based technique for the diagnosis of faults in a chemical process. The diagnosis system is based on the robust estimation of process outputs. A dynamic *non-linear* model of the process under investigation is obtained by a procedure exploiting *Takagi-Sugeno* (T-S) multiple-model fuzzy identification. The combined identification and residual generation schemes have robustness properties with respect to modelling uncertainty, disturbance and measurement noise, providing good sensitivity properties for fault detection and fault isolation. The identified system consists of a fuzzy combination of T-S models to detect changing plant operating conditions. Residual analysis and geometrical tests are then sufficient for Fault Detection and Isolation (FDI), respectively. The procedure here presented is applied to the problem of detecting and isolating faults in a benchmark simulation of a tank reactor chemical process.

Keywords: Analytical redundancy, sensor fault diagnosis, multiple-model, fuzzy system identification, chemical process.

1. INTRODUCTION

Modern chemical plants are large scale, highly complex, and operate with a large number of variables under closed loop control. Early and accurate fault detection and diagnosis for these plants can minimise downtime, increase the safety of plant operations, and reduce manufacturing costs. Chemical processes are becoming more heavily instrumented, resulting in large quantities of data becoming available for use in detecting and diagnosing faults. Exothermic reactions in CSTR are extremely important systems of potential safety problems because the temperature increases rapidly in a short time. Univariate control

charts (Russell *et al.*, 2000) have a limited ability to detect and diagnose faults in such processes due to large correlations in the process data. This has led to a surge of academic and industrial effort concentrated towards developing more effective process monitoring methods.

While techniques based on first-principles models have been around for more than two decades, their contribution to industrial practice has not been pervasive due to the huge cost and time required to develop a sufficiently accurate process model for a complex chemical plant (Russell *et al.*, 2000). The process monitoring techniques that have dominated the literature for the past decade

and have been most effective in practice are based on models constructed almost entirely from process data (Martin *et al.*, 1999; Chen and Patton, 1999; Patton *et al.*, 2000; Patton *et al.*, 2001).

The purpose of this work is to bring an example of data-driven process monitoring technique to practicing engineers.

These fault diagnosis methodologies for dynamic processes have pursued with a wide variety of model-based approaches being proposed (Isermann and Ballé, 1997; Chen and Patton, 1999; Patton *et al.*, 2000). These different methods can be reduced to a few basic approaches such as the parity space (Gertler, 1998), state and output estimation (Isermann, 1984; Patton, 1997), the fault detection filter (Patton, 1997; Chen *et al.*, 1996; Frank and Ding, 1997) and parameter identification (Chen *et al.*, 1996; Patton *et al.*, 2000). All these “model-based” methods require mathematical models of the process, in either state space or input-output form.

Under these assumptions, the paper explores the potential for process fault diagnosis using an output estimation approach in conjunction with a residual processing scheme comprising simple threshold detection. A main issue is the development of FDI residuals which demonstrate individual sensitivity to distinct faults acting in the *non-linear* plant.

It is also a requirement for these residuals to be robust against modelling uncertainty and operating point changes. This is achieved through a special approach in model identification and the use of residuals based on a Takagi-Sugeno multiple-model estimation strategy (Patton *et al.*, 2001).

The proposed method also does not require a deep insight into the monitored process but relies upon the building of input-output relationships through model identification procedures, i.e. Takagi-Sugeno fuzzy non-linear models (Simani *et al.*, 1998; Simani *et al.*, 1999; Patton *et al.*, 2001; Simani *et al.*, 2001).

The identification of locally affine models using the T-S strategy is solved by fuzzy clustering obtained by partitioning the process monitored data into subsets. This estimation technique gives a reliable model of the process being addressed, mainly because the fuzzy modelling approach provides an accurate model in terms of encapsulating different process operating regions.

It is, however, worth noting that when the aim is to apply FDI to continuous systems under steady operating conditions, linear methods, such as ARX, are valid (Simani *et al.*, 2000; Patton *et al.*, 2001). However the complex input-output

behaviour such as multiple steady-states justifies the use of a robust multiple model approach.

The proposed FDI scheme is applied to sensor fault diagnosis in a Continuous Stirring Tank Reactor (CSTR) process model (Russell *et al.*, 2000), the dynamic behaviour of which was obtained using the *non-linear* dynamic fuzzy model identification procedure.

2. MODEL DESCRIPTION

It is assumed that the monitored system, depicted in Figure (1), can be described in fault-free conditions, by a discrete-time, time-invariant, dynamic model of the type (Leontaritis and Billings, 1985a):

$$\mathbf{y}^*(t) = \mathbf{f}(\mathbf{x}^*(t)) \quad (1)$$

where, the NARX (Non-linear AutoRegressive eXogenous input) model (Leontaritis and Billings, 1985b; Ljung, 1999) establishes a relation between the finite past input-output data, represented by the regression vector $\mathbf{x}^*(t) = [\mathbf{u}^*(t-1), \dots, \mathbf{u}^*(t-n), \mathbf{y}^*(t-1), \dots, \mathbf{y}^*(t-n)]$, with pure delay from the input to the output. The vector $\mathbf{y}^*(t) \in \mathbb{R}^m$ contains the outputs of the system, whilst $\mathbf{u}^*(t) \in \mathbb{R}^r$ the control input vector. $\mathbf{f}(\cdot)$ is approximated by using a static non-linear function. The vectors $\mathbf{u}(t)$ and $\mathbf{y}(t)$ are the only available measurements which can be acquired from the input and output sensors. Figure (1) also shows the fault distribution in the monitored system. By neglecting sensor dynamics, the signals $\mathbf{u}^*(t)$ and $\mathbf{y}^*(t)$ can be modelled by the following Equations

$$\begin{cases} \mathbf{u}(t) = \mathbf{u}^*(t) + \tilde{\mathbf{u}}(t) + \mathbf{f}_u(t) \\ \mathbf{y}(t) = \mathbf{y}^*(t) + \tilde{\mathbf{y}}(t) + \mathbf{f}_y(t) \end{cases} \quad (2)$$

where $\mathbf{f}_u(t)$ and $\mathbf{f}_y(t)$ are signal vectors which represent the presence of input and output sensor faults, respectively. Usually the $\mathbf{f}_u(t)$ and $\mathbf{f}_y(t)$ signals are described by step and ramp functions representing abrupt and incipient faults (bias or drift), respectively. In real-world applications, variables $\tilde{\mathbf{u}}(t)$ and $\tilde{\mathbf{y}}(t)$ represent instrument noises.

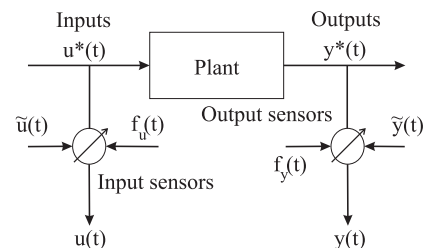


Fig. 1. Monitored system and measurement process structure.

It is worthwhile noting how the case of *component faults* cannot be described by Eqs. (2). On the other hand, by assuming general detectability conditions (Chen and Patton, 1999), faults affecting output measurements $\mathbf{y}(t)$ can be successfully detected by monitoring both $\mathbf{u}(t)$ and $\mathbf{y}(t)$ signals.

3. DYNAMIC SYSTEM IDENTIFICATION FOR FDI

The FDI approach is implemented by making use of an output estimation method to produce a set of signals from which it will be possible to isolate faults associated with the process. The design of such output predictor requires the knowledge of the process in terms of a dynamic model (1), which is, in particular, in input–output form.

The approach used in this work uses *non-linear* system identification and modelling since the process changes operating regions and it exhibits *non-linear* behaviour, as many batch process operations also do. Non-linear methods such as non-linear observers, extended Kalman filters, fuzzy-logic methods, etc. may be used for dynamic process identification (Simani *et al.*, 2000; Patton *et al.*, 2001). In particular, and in this work, the T–S non-linear fuzzy model is successfully exploited to estimate the outputs of the process.

In the presented application, the *non-linear* dynamic process is therefore described by the composition of several T–S models selected according to the process operating conditions (Patton *et al.*, 2001). The T–S models and, in particular, an appropriate number M of fuzzy subsets are built from the decomposition of input–output data $\mathbf{u}(t)$ and $\mathbf{y}(t)$ ($t = 1, \dots, N$) acquired from a dynamic process. Each subset, R_i , ($i = 1, \dots, M$) represents an operating region of the dynamic process which is approximated by a affine dynamic model. Partitioning of the data set into fuzzy subsets can be achieved, for instance, by using the well-established Gustafson–Kessel (G–K) clustering algorithm (Gustafson and Kessel, 1979; Simani, 2000; Simani *et al.*, 2001), which is implemented in the Fuzzy Modelling and IDentification (FMID) MATLAB Toolbox (Babuška, 2000; Babuška, 1998). Here, each cluster R_i ($i = 1, \dots, M$) obtained by fuzzy partitioning is regarded as a local approximation of the non-linear system. The global equation error model can then be conveniently represented using local affine T–S rules (Takagi and Sugeno, 1985):

$$R_i : \text{If } \mathbf{x}(t) \text{ is } R_i \text{ then } \mathbf{y}_i(t) = \Theta_i^T \mathbf{x}(t) \quad (3)$$

while the global system behaviour is described by a fuzzy fusion of all affine model outputs:

$$\mathbf{y}(t) = \frac{\sum_{i=1}^M \mu_i(\mathbf{x}(t)) \mathbf{y}_i(t)}{\sum_{i=1}^M \mu_i(\mathbf{x}(t))} \quad (4)$$

where $\mathbf{y}(t)$ is the predicted output vector at the instant t . The results of clustering are M , $\mathbf{x}(t) \in \mathfrak{R}^p$ ($p = r \times n \times m \times n$) is a collection of a finite number of inputs and outputs, $\mathbf{x}(t) = [\mathbf{u}(t-1), \dots, \mathbf{u}(t-n), \mathbf{y}(t-1), \dots, \mathbf{y}(t-n)]$ and n is an integer related to the system order. For each operating point i , the model output is described as a fuzzy fusion of the local predicted outputs $\mathbf{y}^{(i)}(t)$ by means of the (multivariate) membership functions:

$$\mu(\cdot) : \mathcal{C} \subset \mathfrak{R}^p \rightarrow [0, 1]. \quad (5)$$

The i^{th} local model (3) is an affine system, whilst its parameters, Θ_i ($i = 1, \dots, M$) and n , can be estimated by using a number of fuzzy identification methods (Simani *et al.*, 1998; Simani *et al.*, 1999; Simani *et al.*, 2001; Patton *et al.*, 2001). The scheme outlined above allows the estimation of non-linear discrete model (4) for the process which has generated the sequences $\mathbf{u}(t)$ and $\mathbf{y}(t)$.

Finally, the system resulting from the non-linear fuzzy system (4) identification approach will be used as one-step-ahead output predictor, as depicted in Figure (2), for the residual generation task.

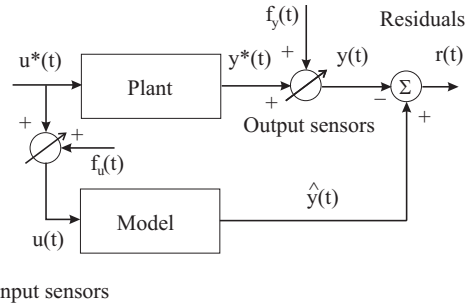


Fig. 2. The residual generation scheme.

4. APPLICATION EXAMPLE

The aim of the study presented in this paper is to develop a general procedure for the diagnosis of sensor faults in chemical processes. In particular, the monitored process is a model of a CSTR, where the reaction is exothermic $A \rightarrow B$ (A reactant, B product). The main variables are: reactor temperature $T(t)$, concentration of A , C_{af} , in feed stream, volumetric flow rate, F , (volume/time) and concentration of A , C_a , in reactor. The process objective is to maintain the concentration C_a controlling the coolant flow, $q(t)$. The importance of this case study is that there are many examples of reactors in industry like polymerisation reactor. Some of them with complex kinetic but with

similar properties behaviour as examined in this paper. The CSTR with cooling jacket is shown in Figure (3).

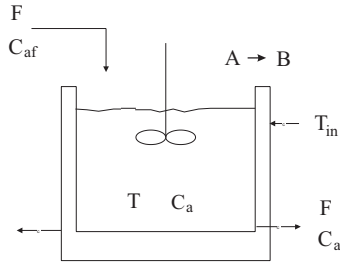


Fig. 3. Schematic of the CSTR process.

The process has $r = 1$ control input $q(t) = u(t)$, (coolant flow, $\frac{l}{min}$). Two output measurements ($m = 2$), $C_a(t) = y_1(t)$ (concentration, $\frac{mol}{l}$) and $T(t) = y_2(t)$ (temperature, Kelvin degrees) can be acquired from the simulator in Figure (3). Constant physical properties and constant boundary pressures of all input and output streams are assumed. The non-linear equations describing the plant are recalled in (Russell *et al.*, 2000).

The dynamic SIMULINK simulator was used to generate both process normal operating and faulty data. A sampling rate of 0.1s was used to acquire a number of $N = 7500$ data sequences with noise and disturbances ($\tilde{\mathbf{u}}(t)$, $\tilde{\mathbf{y}}(t)$) due to measurement uncertainty. The measurement signal noise levels are flow $\pm 3\%$, temperature $\pm 0.5K$ and concentration $\pm 0.5\%$. Figure (4) shows the input and the outputs of the plant.

The process monitoring method presented in this work has been tested on the data collected from the process simulation for the CSTR process. The plant has been widely used by the process monitoring community as a benchmark or source of data for comparing various diagnosis approaches (Russell *et al.*, 2000).

The system was exploited here in order to provide a realistic industrial process for evaluating process control and monitoring methods. The test process is based on a simulation of an actual chemical process where the components, kinetics, and operating conditions have been modified for proprietary reasons. Mode details about the process are described in (Russell *et al.*, 2000).

It can be noted how the CSTR behaves in a non-linear manner (non-stationary manner) during changes of operating conditions (Russell *et al.*, 2000). It is in these situations that T-S models can be used to enhance the FDI capabilities.

The CSTR simulator contains several pre-programmed faults. Some of these faults are known, and other are unknown. Abrupt failure dynamics can be associated with a step change in process variables. On the other hand, slow developing

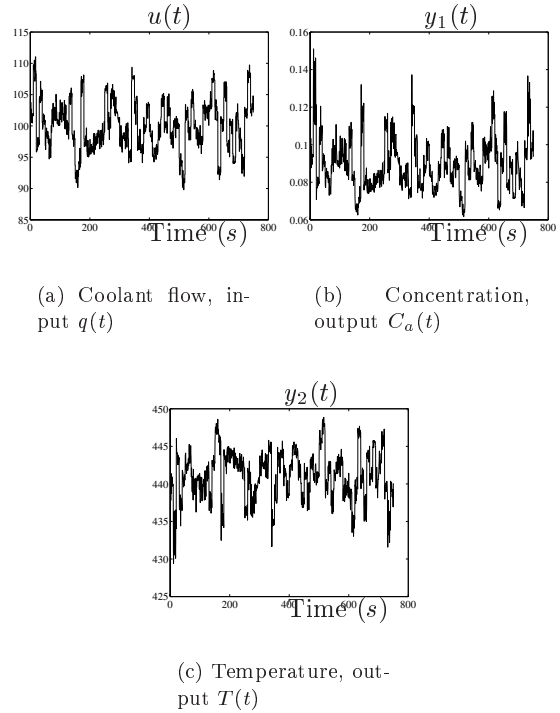


Fig. 4. Input and output measurement.

faults can be associated with an increase in the variability of some process variables, e.g. a slow drift in the reaction kinetics.

The sensitivity and robustness of the process monitoring method can also be investigated by simulating the process under various fault conditions. The simulation program allows the faults to be implemented either individually or in combination with one another. In this paper, as an example, a fault case affecting the output temperature $T(t)$ sensor for the measurement of $y_2(t)$ will be considered in this study.

Under this assumption, in order to diagnose single sensor faults, the non-linear fuzzy system (4) for the prediction of the $\mathbf{y}(t)$ outputs has to be identified. The estimation errors, or residual, concerning the diagnosis of the outputs $\mathbf{y}(t)$ are estimated by the system. The symptom signals are therefore expressed as $r_i(t) = y_i(t) - \hat{y}_i(t)$, which represents the difference between the estimated $\hat{y}_i(t)$ and the measured output, $y_i(t)$, with $i = 1, 2$, i.e. the i^{th} component of the output vector $\mathbf{y}(t)$. According to the residual generation scheme depicted in Figure (2), output estimates $\hat{y}_i(t)$ can therefore be generated by the output estimator for the model (4) (Babuška, 1998).

Figure (5) compare the estimated and measured output $y_1(t)$ and $y_2(t)$, respectively, when the non-linear fuzzy model (4) was identified on the basis of the different operating conditions of the plant. Because of the accuracy of the identified fuzzy model (4), it is shown how the measured and

estimated outputs cannot be distinguished. Here, a 2nd order ($n = 2$) T-S fuzzy model ($r = 1$, $m = 2$) of the fuzzy output models of 2nd order for $M = 3$ clusters and driven by $u(t)$ input was identified for both the outputs with a per cent reconstruction error of less than $J = 0.1\%$ (Simani *et al.*, 2000; Patton *et al.*, 2001).

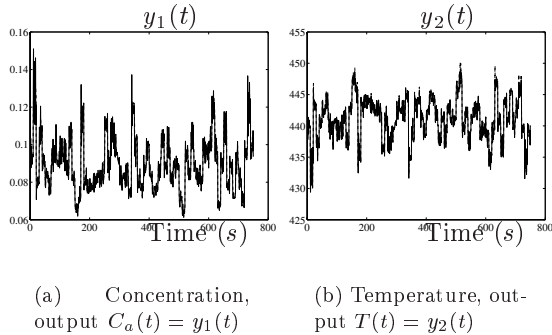


Fig. 5. Measured (continuous line) and predicted (dashed line) temperature outputs $y_1(t)$ and $y_2(t)$.

Moreover, for this example, the Variance Accounted For (VAF) value (Babuška, 1998; Patton *et al.*, 2001) was approximately 98.7% for the first output $y_1(t)$ and about 97.9% for the second one, $y_2(t)$. This implies that the percentage of data described by fuzzy rules (3) can be regarded as being a representative value. According to Figure (2), it is worthy to note that the model was used in “full simulation” since it is driven by $u(t)$ only, in order to generate the estimate of the output $y_2(t)$. For this model, a number of working points $M = 3$, were used in order to obtain an accurate non-linear description of the behaviour of the system under investigation.

Once the residual signal for $y_2(t)$ is generated, the detection of a fault due to temperature thermocouple sensor which fails high starting at $t = 350$ s can be performed. Fault-free (continuous line) and faulty residual (dashed line) are shown in Figure (6) when a fault of the 5% affects the temperature sensor. Such value represents the minimum detectable fault when an accuracy of $J = 0.1\%$ is achieved by the identified model.

Results shown in Figure (6) were obtained using the linear model (4) of the monitored system. Because of the residual dynamics, a simple geometrical analysis, such as a fixed threshold logic can be exploited in order to detect actuator faults. Clearly, suitable threshold values have to be set under fault-free conditions.

From a physical point of view, the presented fault case involves a step change in the reactor temperature T measurement. The significant effect of the fault on $y_2(t)$ signal is therefore to induce a step change in the coolant water flow rate. By means

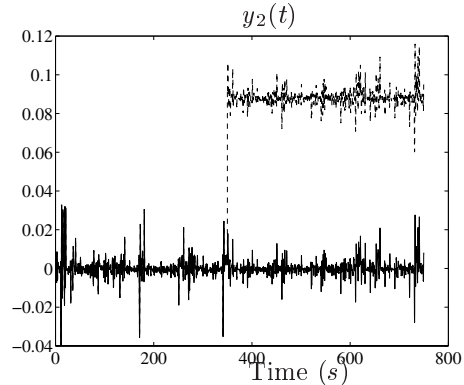


Fig. 6. Fault free and faulty residual for the monitored $y_2(t)$ signal.

of the control input $u(t)$, the control loop tries to compensate for the change and the temperature in the reactor tends to return to its setpoint. Detecting and diagnosing such a fault could be a challenging task, since failure effects are hidden by the control loop system.

In general, in order to *detect* sensor faults on the i^{th} output component, the estimator for the i^{th} output, fed by the input $\mathbf{u}(t)$ and to predict the output measurement most sensitive to the fault considered, need to be identified (Simani *et al.*, 2000; Patton *et al.*, 2001).

Moreover, in order to *isolate* faults, when the process develops a malfunction, it is important to know exactly which faults have occurred or which parts of the system caused the problem. The residuals were computed as the difference between the faulty outputs and the corresponding signals predicted by the non-linear T-S fuzzy model of the CSTR (4). In this paper, the sensor fault isolation task can be successfully achieved by using the non-linear T-S fuzzy predictor of Figure (2), as well. The mutual isolation of both the output sensor faults can also be obtained since only a single fault affects the residual function $r_i(t)$ of the estimator driven by the input $u(t)$.

The detection capabilities of the proposed strategy for identification and diagnosis of faults on the sensors and related problems appear to be promising for diagnostic applications to chemical processes.

5. CONCLUSIONS

A design method for FDI in sensor related faults in a Continuous Stirred Tank Reactor have been described. The study of the fault diagnosis performance has shown that the proposed method, which does not require a detailed mechanistic model, can provide an output predictor through a fuzzy system identification method which can then be used in FDI.

In order to investigate the diagnostic effectiveness of the FDI system in the presence of sensor faults, several malfunctions were simulated in the CSTR model. The minimal detectable faults for this industrially related diagnostic application and the existence of multiple steady-state behaviour of the process where there may be more than a possible value of the output variable for the same input variable justify the use of the T-S fuzzy approach.

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