RESIDUAL GENERATION AND DISTURBANCE DE–COUPLING FOR A CHEMICAL PROCESS

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Abstract

The paper presents some results concerning fault diagnosis for dynamic processes using dynamic system identification and disturbance de–coupling techniques. The first step of the considered approach consists of exploiting input–output descriptions of the monitored system. In particular, the disturbance term of that model can be used to take into account unknown inputs affecting the system. The next step of the scheme leads to define a set of relations that can be used as residual signals since they are insensitive to the disturbance term. The proposed fault diagnosis scheme has been tested on an real industrial chemical process in the presence of sensor, actuator and component faults. The results and concluding remarks have been finally reported.

1 Introduction

Since the early 1970's, the problem of reliable fault diagnosis in dynamic processes has received great attention and a wide variety of robust approaches has been proposed and developed. Recently, different analytical redundancy–based methods have been developed to diagnose faults in linear, time-invariant, dynamic systems and a wide variety of model–based approaches has been proposed [12].

There are different model–based approaches to the fault diagnosis problem [9], namely parameter identification [15], parity equations [10], methods in frequency [4] or in state–space domain, such as diagnosis observers [8] and Kalman filters.

Even if analytical redundancy methods have been recognised as a powerful and effective technique for detecting faults, the generation of robust residuals is a critical issue because of the presence of unavoidable modelling uncertainty. The main problem regarding the reliability of fault diagnosis schemes consists of the modelling uncertainties which are due, for example, to process noise, parameter variations and non–linearities.

Model–based methods use a model of the monitored process in order to produce the symptom or residual generator. If the system is not complex and can be described accurately by the mathematical model, fault detection is directly performed by using a simple geometrical analysis of residuals. In real industrial systems however, since the modelling uncertainty is unavoidable, the design of a robust fault diagnosis scheme should consider the modelling uncertainty with respect to the sensitivity of the faults. Several papers addressed this problem. For example, optimal robust parity relations were proposed in [10], and the threshold selector concept was introduced in [6]. One other promising approach is the decoupling between disturbances and residuals achieved by means of a proper observer scheme and design [2, 12]. This approach requires the knowledge of a model of the process under investigation and, in particular, of the disturbance distribution matrix. Thus, modelling [2] or identification [14, 7] procedures can be defined to estimate the disturbance distribution matrix .

A different approach is exploited in the present work. In particular, it is assumed that an input–output discrete–time linear dynamic model (obtained by modelling or identification procedures) can describe the data measured from the monitored system. Moreover, in this model, a disturbance term is introduced to take into account any unknown (or non–measurable) inputs of the real process. By exploiting this disturbance vector, a set of parity relations can be designed to generate residual signals for the detection of faults affecting input and output process measurements. Such residual generator is insensitive to disturbance signal.

The paper is organised as follows. In Section 2 the problem statement is given and described from a mathematical point of view. The robust fault diagnosis scheme is then presented in Section 3. In Section 4, a chemical industrial process used to test the proposed methodology is presented and the results concerning the diagnosis of faults are also reported. Finally, conclusions reported in Section 5 close the paper.

2 Mathematical description

This section addresses the mathematical description of the system under diagnosis and the problem of robust fault detection. In the general framework of linear and time–invariant systems, a discrete–time, input–output model as in Figure (1) has been considered

$$\mathbf{y}^*(t) = \mathrm{G}_u(z)\,\mathbf{u}^*(t) + \mathrm{G}_d(z)\,\mathbf{d}(t), \quad t \geq 0 \tag{1}$$

where $\mathbf{y}^*(t) \in \Re^m$ is the output vector and $\mathbf{u}^*(t) \in \Re^r$ is the control input vector. The term $\mathbf{d}(t) \in \Re^p$ describes disturbances (measurement noise, un–modelled dynamics, etc.) affecting the process. $\mathrm{G}_u(z)$ and $\mathrm{G}_d(z)$ represent the discrete transfer matrices from inputs to outputs and from disturbances to outputs, respectively; z is the forward shift operator, *i.e.* $z\,y(t) = y(t+1)$.

Figure 1: The monitored system.

The model description in Eq. (1) assumes fault–free system operations and working conditions. As depicted in Figure (1), additive fault occurrence can be modelled by means of the following relations

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

where $\mathbf{f}_u(t)$ and $\mathbf{f}_y(t)$ are the actuator and sensor additive faults, respectively. These vectors may be modelled by step and ramp signals in order to describe the presence of bias or drift on the measurements (abrupt and slowly developing faults). Signals $\mathbf{u}(t)$ and $\mathbf{y}(t)$ represent the input and output measurements, respectively, which have been used for the fault detection task.

Therefore, by neglecting actuator and sensor dynamics, under fault–free assumptions (1), $\mathbf{u}(t) = \mathbf{u}^*(t)$ and $\mathbf{y}(t) = \mathbf{y}^*(t)$.

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 [2], faults affecting output measurements $\mathbf{y}(t)$ can be successfully detected by monitoring both $\mathbf{u}(t)$ and $\mathbf{y}(t)$ signals.

3 Residual Generation

Residuals can be generated using different approaches. In this work, a parity relation scheme is exploited to generate residual signals which are insensitive to a disturbance signal affecting the process under investigation.

In order to introduce and present the residual generation problem, a r inputs $u(t)$, two output $y_1(t)$, $y_2(t)$ ($m = 2$) system (1) with one disturbance $d(t)$ signal ($p = 1$) is considered in this paper. In particular, the model under investigation is depicted in Figure (2).

However, it is worth noting that one cannot de–couple more disturbance p (or fault) signals than the number of outputs m minus one. In particular, in the present work, as an application example with two outputs and one disturbance has been considered, no design freedom are left for fault isolation [1]. On the other hand, in general, the de–coupling of multiple disturbance signals may lead to significant problems, *i.e.* unstable filters and poor noise attenuation.

The extension of the procedure to an arbitrary number $p > 1$ of disturbances or faults will be studied in further works. However, the problem of the sensitivity and robustness in the presence of multiple unknown inputs requires more investigations, as well [1].

Figure 2: The considered system under diagnosis.

In this case, the system represented in Figure (2) is described by the following relations

$$\begin{cases} y_1(t) & = & \mathrm{G}_u^{(1)}(z)\,\mathbf{u}(t) + G_d^{(1)}(z)\,d(t) \\ y_2(t) & = & \mathrm{G}_u^{(2)}(z)\,\mathbf{u}(t) + G_d^{(2)}(z)\,d(t), \quad t \geq 0 \end{cases} \tag{3}$$

where $\mathrm{G}_u^{(i)}(z)$ and $G_d^{(i)}(z)$ ($i = 1, 2$) represent the discrete transfer matrices and the discrete transfer functions from the inputs to the i^{th} output and from the disturbance to the i^{th} output, respectively.

The transfer matrices and the transfer function described in (3) can be written in polynomial forms by defining the following

$$\begin{cases} \mathrm{G}_u^{(1)}(z) = \left[\frac{N_{u_1}^{(1)}(z)}{D_u^{(1)}(z)}, \ldots, \frac{N_{u_r}^{(1)}(z)}{D_u^{(1)}(z)}\right], G_d^{(1)}(z) = \frac{N_d^{(1)}(z)}{D_d^{(1)}(z)} \\ \mathrm{G}_u^{(2)}(z) = \left[\frac{N_{u_1}^{(2)}(z)}{D_u^{(2)}(z)}, \ldots, \frac{N_{u_r}^{(2)}(z)}{D_u^{(2)}(z)}\right], G_d^{(2)}(z) = \frac{N_d^{(2)}(z)}{D_d^{(2)}(z)} \end{cases} \tag{4}$$

where the functions $N_{u_j}^{(i)}(z)$, $N_d^{(i)}(z)$ and $D_{(u)}^{i}(z)$, $D_d^{(i)}(z)$ with ($j = 1, \ldots, r$) are relative prime polynomials representing the numerators and the denominators in descending powers of the shift operator z, respectively.

From Eqs. (3), by eliminating the unknown signal $d(t)$, the following relation is obtained

$$\begin{aligned} &\frac{D_d^{(1)}(z)}{N_d^{(1)}(z)}\,y_1(t) - \frac{D_d^{(2)}(z)}{N_d^{(2)}(z)}\,y_2(t) + \\ &+\Bigg(\frac{D_d^{(2)}(z)}{N_d^{(2)}(z)}\,\frac{\left[N_{u_1}^{(2)}(z), \ldots, N_{u_r}^{(2)}(z)\right]}{D_u^{(2)}(z)} + \\ &-\frac{D_d^{(1)}(z)}{N_d^{(1)}(z)}\,\frac{\left[N_{u_1}^{(1)}(z), \ldots, N_{u_r}^{(1)}(z)\right]}{D_u^{(1)}(z)}\Bigg)\,\mathbf{u}(t) = 0 \quad . \end{aligned} \tag{5}$$

Relation (5) can be simplified if an multiple input–single output *ARMAX* (Auto–Regressive Moving Average eXogenous) model structure [11] is assumed for the models described by Eqs. (3). In this case, in fact, it can be assumed that $D_u^{(1)}(z) = D_d^{(1)}(z) = D^{(1)}(z)$ and $D_u^{(2)}(z) = D_d^{(2)}(z) = D^{(2)}(z)$, with degrees n_i ($i = 1, 2$), and the corresponding numerators have degrees $n_i - 1$. Therefore, Eq. (5) can be rewritten as

$$\begin{aligned} r(t) = \; & D^{(1)}(z)\, N_d^{(2)}(z)\, y_1(t) - D^{(2)}(z)\, N_d^{(1)}(z)\, y_2(t) + \\ & + \Big(N_d^{(1)}(z) \; \left[N_{u_1}^{(2)}(z), \ldots, N_{u_r}^{(2)}(z) \right] + \\ & - N_d^{(2)}(z) \; \left[N_{u_1}^{(1)}(z), \ldots, N_{u_r}^{(1)}(z) \right] \Big) \, \mathbf{u}(t) = 0, \\ & t \geq 0 \end{aligned} \tag{6}$$

where $r(t)$ represents the residual function computed from the considered system model. Moreover, by using the following notation

$$\begin{aligned} C_{y_1}(z) = \; & D^{(1)}(z)\, N_d^{(2)}(z), \\ C_{y_2}(z) = \; & -D^{(2)}(z)\, N_d^{(1)}(z), \\ \mathbf{C}_u(z) = \; & N_d^{(1)}(z) \; \left[N_{u_1}^{(2)}(z), \ldots, N_{u_r}^{(2)}(z) \right] + \\ & - N_d^{(2)}(z) \; \left[N_{u_1}^{(1)}(z), \ldots, N_{u_r}^{(1)}(z) \right], \end{aligned} \tag{7}$$

relation (6) can be rewritten in the matrix form

$$r(t) = \begin{bmatrix} y_1(t) & y_2(t) & \mathbf{u}(t) \end{bmatrix} \begin{bmatrix} C_{y_1}(z) \\ C_{y_2}(z) \\ \mathrm{C}_u(z) \end{bmatrix} = 0 \tag{8}$$

for $t \geq 0$.

Under the previous assumptions, it can be easily verified that Eq. (6) represents a *causal* filter. However it can be noted that causality conditions are not required if the residual generator of Eq. (6) is used for off–line or batch fault detection operations. However, in order to make the filter causal, the filter polynomials can be written in terms of z^{-1}, which of course is possible.

Relation (6) has been computed under fault–free conditions. Therefore, according to the Eqs. (2), faults affecting the monitored system can be detected, *e.g.*, by comparing the robust residual function $r(t)$ with a fixed threshold ε according to the simple *threshold logic* given below

$$\begin{cases} |r(t)| \leq \varepsilon & \text{for fault–free case,} \\ |r(t)| > \varepsilon & \text{for faulty cases.} \end{cases} \tag{9}$$

If the test is positive (*i.e.* the threshold is exceeded by the residual function $|r(t)|$), it can be hypothesised that a fault is likely. There are many ways of defining residual functions and determining thresholds [2]. As an example, in relations (9) the residual function has been chosen as a norm of the residual $r(t)$ and the threshold ε can be fixed as a constant positive value under fault–free conditions.

Let us denote with $n_y = n_1 + n_2 - 1$ the degree of the polynomial $C_{y_i}(z)$ whose coefficients are contained into the vector $\mathbf{c}_{y_i}$, $(i = 1, 2)$ and with $n_u = n_1 + n_2 - 2$ the maximal degree of the polynomial vector $\mathbf{C}_u(z)$, whose coefficients are $\mathbf{c}_u$.

It is worth noting how Eq. (8) leads to an overdetermined set of $N - n_1 - n_2 + 1$ linear equations, where N is the number of considered samples, which can be expressed as [5]

$$\begin{bmatrix} Y_1(N) & Y_2(N) & \mathrm{U}(N) \end{bmatrix} \begin{bmatrix} \mathbf{c}_{y_1} \\ \mathbf{c}_{y_2} \\ \mathbf{c}_u \end{bmatrix} = \mathbf{0}, \tag{10}$$

where

$$Y_i(N) = \begin{bmatrix} y_i(0) & \ldots & y_i(n_y) \\ \vdots & \ddots & \vdots \\ y_i(N - n_y - 1) & \ldots & y_i(N-1) \end{bmatrix} \tag{11}$$

and

$$\mathrm{U}(N) = \left[U_1(N), \ldots, U_j(N), \ldots, U_r(N) \right], \tag{12}$$

with

$$U_j(N) = \begin{bmatrix} u_j(0) & \ldots & u_j(n_u) \\ \vdots & \ddots & \vdots \\ u_j(N - n_y - 1) & \ldots & u_j(N-2). \end{bmatrix}. \tag{13}$$

for $j = 1, \ldots, r$.

From Equations (10), (11) and (12), it follows that it must be $N \geq 4(n_1 + n_2) - 2$ in order to avoid unwanted linear dependence relationships due to limitations in the dimension of the involved vector spaces in relation (10).

By introducing the covariance matrix of the multivariate process $\begin{bmatrix} y_1(\cdot), y_2(\cdot), u_1(\cdot), \ldots, u_r(\cdot) \end{bmatrix}^T$, defined as

$$\begin{aligned} \hat{\Sigma}_N \;\; = \;\; & \frac{1}{N - n_1 - n_2 + 1} \begin{bmatrix} Y_1(N) & Y_2(N) & \mathrm{U}(N) \end{bmatrix}^T \times \\ & \times \begin{bmatrix} Y_1(N) & Y_2(N) & \mathrm{U}(N) \end{bmatrix}, \end{aligned} \tag{14}$$

relation (10) can be rewritten as

$$\mathbf{r}(t) = \hat{\Sigma}_N \begin{bmatrix} \mathbf{c}_{y_1} \\ \mathbf{c}_{y_2} \\ \mathbf{c}_u \end{bmatrix} = \mathbf{0}. \tag{15}$$

It is important to note that Eq. (15) can be used for fault detection purpose. In fact, when the process inputs are persistently exciting of sufficient order, under fault–free conditions, matrix $\hat{\Sigma}_N$ is singular and the vector $\begin{bmatrix} \mathbf{c}_{y_1} & \mathbf{c}_{y_2} & \mathbf{c}_u \end{bmatrix}^T$ represents its null space and $\mathbf{r}(t) = \mathbf{0}$. On the other hand, when a fault occurs, relation (15) does not hold since matrix $\hat{\Sigma}_N$ is not singular.

Instead of monitoring $\mathbf{r}(t)$, as reported in (9), a different residual function may be represented [3] by the minimal singular value $\underline{\sigma}(\cdot)$ of the matrix $\hat{\Sigma}_N$, *i.e.* $\underline{\sigma}(\hat{\Sigma}_N)$. The fixed threshold ε is related to the minimal singular value of $\hat{\Sigma}_N$ matrix computed in fault–free conditions. Therefore, the fault detection criterion may consist of performing a test by monitoring the changes of $\underline{\sigma}(\hat{\Sigma}_N)$, as follows

$$\begin{cases} \underline{\sigma}(\hat{\Sigma}_N) \leq \varepsilon & \text{for fault–free case} \\ \underline{\sigma}(\hat{\Sigma}_N) > \varepsilon & \text{for faulty cases} \end{cases} \tag{16}$$

for increasing values of N. The threshold ε is fixed on the basis of the value of $\underline{\sigma}(\hat{\Sigma}_N)$ in fault–free conditions. In such a case, this value is differently affected by noise and non–linearity of the process.

It is worth noting that the fault detection method described by Eq. (16) does not depend on the model parameters of the process under diagnosis since it is based only on the check of the singularity of $\hat{\Sigma}_N$ matrix. Relation (16) can be therefore exploited for both model–based and *model–free* fault detection.

However, if there is more than on fault in the process, relation given by Eq. (16) cannot be exploited for isolation purpose. On the other hand, under this condition, the relation of Eq. (8) could be modified for obtaining isolation properties [10, 2].

4 Chemical Process Fault Diagnosis

The aim of the study presented in this paper is to develop a general procedure for the diagnosis of faults in a chemical process. In particular, the monitored process is a real Continuous Stirring Tank Reactor (CSTR), where the reaction between reactant and product is exothermic. The main variables are: reactor temperature $T(t)$, feed stream reactant concentration $C_{af}(t)$, volumetric flow rate $F(t)$ (volume/time), reactor reactant concentration $C_a(t)$ and reactor impurity concentrations $d(t)$.

The process objective is to maintain the reactor concentration $C_a(t)$ controlling the coolant flow $q(t)$ ($\frac{l}{min}$) in despite of reactor impurity concentration $d(t)$. The importance of this case study is that there are many examples of reactors in industry like polymerisation reactor [13]. Some of them with complex kinetic but with similar properties behaviour as examined in this paper. The CSTR model with cooling jacket is shown in Figure (3).

Figure 3: Schematic of the CSTR process.

The system has $r = 3$ control inputs $\mathbf{u}(t) = [q(t), C_{af}(t), F(t)]$. 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 plant depicted in Figure (3). The disturbance $d(t)$ vector ($p = 1$) represents reactor impurities and fouling [13]. Constant physical properties and constant boundary pressures of all input and output streams are assumed. Both process normal operating time series and faulty data have been measured from the real process. A sampling rate of 6s was used to acquire a number of $N = 7500$ actual data sequences. The measurements acquired from the actual chemical process have been modified for proprietary reasons.

The CSTR process is affected by several 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 faults can be associated with an increase in the variability of some process variables, *e.g.* a slow drift in the reaction kinetics.

In this work, two fault cases regarding *(a)* the coolant flow $q(t)$ actuator and *(b)* the output temperature $T(t)$ sensor for the measurement of $y_2(t)$ have been considered. Figure (4) sketches the simplified block diagram of the process.

Therefore, in such fault scenario, in order to successfully perform the fault detection task, two output measurements, $y_1(t)$

Figure 4: Block diagram of the CSTR process.

and $y_2(t)$, are exploited.

They are shown in Figures (5(a)) and (5(b)), where continuous lines represent the fault–free signals while the dashed ones depict the faulty signals. Both the faults affect the output measurements starting at the instant $t = 400$.

(a) (b)

Figure 5: (a) The first and (b) the second monitored process outputs.

It is important to note that, in general, in order to achieve the maximal fault detection capability, the measurement corresponding to the most sensitive output $y_i(t)$ to a fault signal has to be selected. Moreover, with reference to this case study, two signals are enough to accomplish fault isolation, as well [14].

Hence, the design of the residual generators presented in Section 3 requires the knowledge of two ARMAX MISO (three inputs and one output) models (3). The i–th submodel ($i = 1, 2$) is driven by both $\mathbf{u}(t)$ and $d(t)$ and gives the i–th output $y_i(t)$.

The residual signal $r(t)$ in Eq. (8) can be generated and therefore the threshold test (9) may be performed. For the considered subsystems $n_{y_1} = n_{y_2} = 6$ and $n_u = 5$ since $n_1 = 3$ and $n_2 = 4$.

Figure (6(a)) depicts the value of the residual $r(t)$ computed in faulty conditions (dashed line) which is compared with the value of $r(t)$ itself in healthy conditions (continuous line).

A fault $f_y(t)$ of 10% on the maximal value of $y_2(t)$ signal causes a change in the residual $r(t)$ computed by relation (8).

In order to determine the threshold above which the fault is detectable, the simulation of different amplitude faults signals has to be performed since the threshold value depends on the residual amounts. In the test (9), a $\varepsilon = 5 \times 10^{-5}$ can be fixed according to the maximal value assumed by $|r(t)|$ in fault–free conditions. Moreover, such fault $f_y(t)$ also affects the value of the minimal singular value of $\hat{\Sigma}_N$, as depicted in Figure (6(b)).

The value of the residual $\underline{\sigma}(\hat{\Sigma}_N)$ computed in faulty conditions (dashed line) by using a growing window is compared with its value in healthy conditions (continuous line). The threshold in Eq. (16) was fixed in fault-free conditions as well as by imposing an acceptable false–alarms rate.

The starting value of $N = 50$ was used to calculate $\hat{\Sigma}_N$ matrix.

The fixed threshold $\varepsilon = 4 \times 10^{-5}$ was chosen in relation (16) according to the minimal singular value of $\hat{\Sigma}_N$ matrix com-

(a) (b)

Figure 6: (a) The residual signals $r(t)$ computed from Eq. (8) and (b) from relation (15).

puted in fault–free conditions.

Finally, Table (1) summarises the performance of fault detection techniques and collects the minimal detectable fault on the sensor $T(t)$ ($f_y(t)$) and the actuator $q(t)$ ($f_u(t)$) signals, when the value of $r(t)$ in Eq. (8) and $\underline{\sigma}(\hat{\Sigma}_N)$ are monitored, respectively.

The minimal detectable fault values in Table (1) are expressed as percentage of the maximal signal values and are relative to the case in which the occurrence of a fault must be detected as soon as possible.

Residual type	$f_u(t)$	$f_y(t)$
$r(t)$ of Eq. (8)	30%	15%
$\underline{\sigma}(\hat{\Sigma}_N)$	6%	3%

Table 1: Minimum detectable faults.

The minimal detectable faults obtained by using test (16) are lower than the ones obtained by means of test (9). This improvement was obtained by an increased computational cost and the complexity of the fault detection technique. Moreover, the improved fault sensitivity of the covariance matrix eigenvalue is due to the fact that it relies on a series of observations rather than a single one, thus involving residual filtering.

From a physical point of view, the presented fault cases involve a change in both the reactor temperature $T(t)$ measurement and the actuator signal $q(t)$. The significant effect of these faults is therefore to induce a change in the coolant water flow rate. By means of the control input $u_1(t) = q(t)$, the control loop tries to compensate for the variation and the temperature in the reactor tends to return to its setpoint. Diagnosing such a fault could be a challenging task, since fault effects are hidden by the control loop system.

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 Conclusion

The complete design procedure for the fault diagnosis of an industrial chemical process was described in this work. The fault detection task is performed by using a residual generation method via a parity relation scheme with a disturbance de–coupling approach. The proposed method may not require any physical knowledge of the process under observation since a model of the monitored system can be obtained by means of system identification scheme. The presented residual generation procedure was tested by using data from an industrial chemical process. As an example, actuator and sensor faults on the process were considered. The results obtained by this approach show the effectiveness of the proposed fault detection method. In the first stage of this work, a multiple input and two output model in the presence of one disturbance signal was considered in order to sketch the fault diagnosis approach. Moreover, measurement noise signals, were not taken into account. Finally, investigations regarding the isolation of multiple faults and studies concerning residual generator robustness properties will be addressed by future works.

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