2009 American Control Conference
Hyatt Regency Riverfront, St. Louis, MO, USA
June 10-12, 2009

Fault Diagnosis for a Class of Chemical Batch Processes

F. Caccavale and F. Pierri

Abstract – This paper deals with the problem of fault diagnosis for a class of chemical reactions taking place in jacketed batch reactors. An integrated diagnosis scheme, using redundant temperature measurements and a bank of state observers, is adopted to detect, isolate and identify faults. A unified framework is developed to take into account faults affecting sensors, actuators and process. In order to test the effectiveness of the approach, a detailed simulation case study is developed.

Keywords – Fault diagnosis, adaptive observers, chemical batch reactors.

I. Introduction

In chemical processes, the occurrence of faults may affect efficiency of the process (e.g., lower product quality) or, in the worst scenarios, could lead to fatal accidents (e.g., temperature run-away). Hence, in the last two decades, the problem of on-line fault detection and isolation has become a major issue in chemical engineering. Several fault diagnosis (FD) approaches have been proposed for processes operating mainly in steady-state conditions (e.g., continuous reactors). Application of these techniques to batch chemical processes are usually difficult, because of their nonlinear dynamics and intrinsically unsteady operating conditions. Also, in batch processes full state measurements and exact parameters knowledge are usually not available. Actuators (e.g., electric-power failures, pump failures, valves failures), process (e.g., abrupt variation of the heat transfer coefficient, side reactions due to impurities in the raw materials) and sensors are the main sources of failures in chemical processes.

In model-based approaches to FD [1] the measurements of a set of process variables are compared to the corresponding estimates, predicted via the mathematical model of the system. By comparing measured and estimated values, a set of variables sensitive to the occurrence of faults (residuals) are generated; by processing the residuals, the faults can be detected (i.e., the presence of faults can be recognized), isolated (i.e., faulty components are determined) and identified (i.e., magnitude of the faults is estimated). Estimation of monitored process variables requires a model of the system (diagnostic observer) to be operated in parallel to the process. To the purpose, Luenberger observers [2], [3], Unknown Input Observers [4] and Extended Kalmann Filters [5] have been mostly used in fault detection and identification for chemical processes and plants. In [6] a geometric approach for a class of nonlinear systems is presented and applied to a polymerization process. In [7] a robust observer is used for sensor faults detection and isolation in chemical batch reactors, while in [8] the robust approach is compared with an adaptive observer for actuator fault diagnosis. Recently, in [9] the actuator fault detection for continuous reactors is achieved via a nonlinear filter, that uses the available state to simulate the system evolution in the absence of faults. Since perfect knowledge of the model is rarely a reasonable assumption, soft computing methods, integrating quantitative and qualitative modeling information, have been developed to improve the performance of FD observer-based schemes for uncertain systems (see, e.g., [10]). Major contributions to observer-based approaches can be found in [11], where fault isolation is achieved via a bank of observers, while identification is based on the adoption of on-line interpolators (e.g., ANNs whose weights are updated on line).

Most of previous approaches focus on a particular class of failures. A major contribution of this paper is the development of a framework in which diagnosis of both sensor, actuator and process faults can be achieved in an integrated framework. As for sensor faults, the approach in [7] is adopted, i.e., redundant temperature sensors are considered both in the reactor vessel and in the cooling jacket; then, two diagnostic observers are designed to generate a set of residuals achieving fault detection and isolation. The estimates provided by the observers and the corresponding sensor measures are processed so as to recognize the faulty sensor and output an healthy measure. In order to achieve process and actuator fault diagnosis, the healthy measure is used to feed a bank of observers. The first observer in the bank is used to detect the occurrence of process/actuator faults, while the other observers are aimed at isolating and identifying faults via an adaption mechanism. Remarkably, the proposed diagnostic scheme is developed for a wide class of reactive systems, characterized by irreversible non-chain reactions, taking place in jacketed batch reactors. The main structural properties of the algorithms combined in this FD scheme (e.g., estimation errors convergence, faults detectability and isolability) are provided. A simulation case study, referred to a polymerization reactive scheme, is developed to test the effectiveness of the proposed approach in the presence of several classes of faults.

II. Modeling

Let us consider a jacketed batch reactor, in which the following general irreversible non-chain reactions network takes place, where A_i denotes the i-th chemical species, $\nu_{i,h} \geq 0$ is the stoichiometric coefficient of the reaction

The authors are with Dipartimento di Ingegneria e Fisica dell'Ambiente, Università degli Studi della Basilicata, Viale dell'Ateneo Lucano 10, 85100 Potenza, Italy – E-mail: {fabrizio.caccavale}@unibas.it

$A_i \to A_h$ and A_{p+1} is the final product:

$$
\begin{array}{llll}
A_1 \to \nu_{1,2} A_2 & & & \\
A_1 \to \nu_{1,3} A_3 & A_2 \to \nu_{2,3} A_3 & & \\
\vdots & \vdots & & \\
A_1 \to \nu_{1,p+1} A_{p+1} & A_2 \to \nu_{2,p+1} A_{p+1} & \dots & A_p \to \nu_{p,p+1} A_{p+1} .
\end{array}
$$

Assuming first-order kinetics and perfect mixing, the mass balances give, for $h = 1, \dots, p$ (the summation on the right-hand side is absent for $h = 1$)

$$
\dot{C}_h = -k_h(T_r) C_h + \sum_{i=1}^{h-1} \nu_{i,h}\, k_{i,h}(T_r) C_i \,, \tag{1}
$$

where T_r is the reactor temperature ([K]), C_h is the concentration ([mol m^{-3}]) of the chemical species A_h, $k_{i,h}(T_r)$ ($h = 2 \dots p$) is the rate constant of the reaction $A_i \to A_h$, obtained via the Arrhenius law $k_{i,h}(T_r) = k_{0_{i,h}} \exp\left(-E_{a_{i,h}}/RT_r\right)$, $E_{a_{i,h}}$ is the activation energy ([J mol^{-1}]) of each reaction, $k_{0_{i,h}}$ is the corresponding pre-exponential factor ([s^{-1}]) and R is the universal gas constant ([J mol^{-1} K^{-1}]); moreover, the lumped overall rate constants of the reactions of disappearance, $k_i(T_r)$, are defined, for each reactant, as $k_i(T_r) = \sum_{h=i+1}^{p+1} k_{i,h}(T_r)$, which are strictly positive if the corresponding chemical species, A_i, are involved at least in one reaction. It can be shown [13] that the rate constants are bounded, i.e., $0 < \underline{k}_{\,i,h} \le k_{i,h}(T_r) \le \overline{k}_{i,h}$ and $0 < \underline{k}_{\,i} \le k_i(T_r) \le \overline{k}_i, \quad \forall T_r$.

The energy balance in the reactor gives

$$
\dot{T}_r = q(\boldsymbol{x}_M, T_r) - \frac{US\,(T_r - T_j)}{V_r \rho_r c_{pr}} \,, \tag{2}
$$

where $\boldsymbol{x}_M = [C_1 \dots C_p]^T$ is the vector of reactants concentrations, T_j is the temperature of the fluid in the jacket, V_r is the reactor volume ([m^3]), ρ_r is the density of the reacting mixture ([kg m^{-3}]), c_{pr} is the mass heat capacity of the reactor contents ([J kg^{-1} K^{-1}]), U ([J m^{-2} K^{-1} s^{-1}]) is the heat transfer coefficient, S ([m^2]) is the heat transfer area, and q is given by

$$
q(\boldsymbol{x}_M, T_r) = \frac{1}{\rho_r c_{pr}} \sum_{i=1}^{p} \sum_{h=i+1}^{p+1} (-\Delta H_{i,h}) k_{i,h}(T_r) C_i \,, \tag{3}
$$

where $\Delta H_{i,h}$ ([J mol^{-1}]) is the molar enthalpy change of each reaction.

Under the assumption of perfect mixing, the energy balance in the jacket yields

$$
\dot{T}_j = \frac{US\,(T_r - T_j)}{V_j \rho_j c_{pj}} + \frac{(T_{\text{in}} - T_j)}{V_j} F \,, \tag{4}
$$

where V_j is the jacket volume, ρ_j is the density of the fluid in the jacket, c_{pj} is the mass heat capacity of the fluid in the jacket, F ([m^3 s^{-1}]) and T_{in} are the flow rate and the temperature of the fluid entering the jacket, respectively.

In order to rewrite the whole model in the form of state equations, let define the $(p + 2) \times 1$ state vector $\boldsymbol{x} = [C_1 \dots C_p\; T_r\; T_j]^T$, and the control input $u = T_{\text{in}}$. It is assumed that only temperature sensors in the jacket and in the reactor vessel are present. Hence, the output vector is given by $\boldsymbol{y} = [T_r\; T_j]^T = \boldsymbol{x}_E$. Then, Eqs. (1), (2) and (4) can be rewritten in the following state-space form

$$
\begin{cases}
\dot{\boldsymbol{x}} \;=\; \boldsymbol{A}(\boldsymbol{y})\,\boldsymbol{x} + \boldsymbol{b}(\boldsymbol{y}, u) + \boldsymbol{\eta}(\boldsymbol{x}, u) \\
\boldsymbol{y} \;=\; \boldsymbol{C}\,\boldsymbol{x} + \boldsymbol{n} \,,
\end{cases} \tag{5}
$$

where

$$
\boldsymbol{A}(\boldsymbol{y}) = \begin{bmatrix} \boldsymbol{A}_M(\boldsymbol{y}) & \boldsymbol{O}_{p\times 2} \\ \boldsymbol{A}_{M,E}(\boldsymbol{y}) & \boldsymbol{A}_E \end{bmatrix} ,
$$

$\boldsymbol{O}_{p\times 2}$ denotes the $p \times 2$ null matrix, and

$$
\boldsymbol{A}_M(\boldsymbol{y}) = \begin{bmatrix} -k_1(y_1) & 0 & \dots & 0 \\ \nu_{1,2}\, k_{1,2}(y_1) & -k_2(y_1) & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ \nu_{1,p}\, k_{1,p}(y_1) & \nu_{2,p}\, k_{2,p}(y_1) & \dots & -k_p(y_1) \end{bmatrix} ,
$$

$$
\boldsymbol{A}_{M,E}(\boldsymbol{y}) = \begin{bmatrix} a_1(y_1) & \dots & a_p(y_1) \\ 0 & \dots & 0 \end{bmatrix} ,
$$

$$
a_i(\boldsymbol{y}) = \sum_{h=i+1}^{p+1} \alpha_{i,h} k_{i,h}(y_1) \,, \quad \alpha_{i,h} = \frac{(-\Delta H_{i,h})}{\rho_r C_{pr}} \,,
$$

$$
\boldsymbol{A}_E = \begin{bmatrix} -\alpha_r US & \alpha_r US \\ \alpha_j US & -\alpha_j US \end{bmatrix} , \;\; \alpha_* = \frac{1}{V_* \rho_* C_{p*}} , (* = r, j) \,.
$$

The vector $\boldsymbol{b}$ in (5) is defined as follows

$$
\boldsymbol{b}(\boldsymbol{y}, u) = \begin{bmatrix} \boldsymbol{0}_{p\times 1} \\ \boldsymbol{b}_E(\boldsymbol{y}, u) \end{bmatrix} , \quad \boldsymbol{b}_E(\boldsymbol{y}, u) = \begin{bmatrix} 0 \\ \beta_j (u - y_2) \end{bmatrix} ,
$$

with $\beta_j = \dfrac{F}{V_j}$. The output matrix is given by $\boldsymbol{C} = [\boldsymbol{O}_{2\times p} \quad \boldsymbol{I}_{2\times 2}]$, where $\boldsymbol{I}_{2\times 2}$ denotes the (2×2) identity matrix. Finally, the $((p + 2) \times 1)$ vector $\boldsymbol{\eta}(\boldsymbol{x}, u)$ collects all the model uncertainties (e. g., uncertainties on reaction dynamics and/or on parameters values, effects of nonideal mixing and/or heating/cooling, unmodeled heat losses), while the (2×1) vector $\boldsymbol{n}$ represents noise on temperature measurements. The magnitude of uncertainties can be kept bounded if suitable modeling and identification techniques are adopted [14]. Also, sensor noise, as usual, is assumed to be bounded.

Usually, in chemical processes, faults can be classified as process faults, sensor faults or actuator faults.

A sensor fault can be modeled as an unknown additive term in the output equation, i.e.,

$$
\boldsymbol{y} = \boldsymbol{C}\boldsymbol{x} + \boldsymbol{f}_s(t) + \boldsymbol{n} \,, \tag{6}
$$

where the (2×1) vector $\boldsymbol{f}_s(t)$ collects the unknown faults profiles affecting, respectively, the vessel and the jacket temperature measurements.

An actuator fault is generated by a malfunction of the cooling system and may be modeled as an unknown additive term affecting the first equation in (5), due to unexpected variations of the input u with respect to its nominal value (i.e., the value computed by the reactor control system). A process fault may be due to unexpected variations of process parameters (e.g., the heat transfer coefficient, due to foulness on reactor walls) or unknown/neglected dynamics (e.g., side reactions due to impurities in the raw materials). In this paper, only the process faults affecting the dynamics of the state variables $\boldsymbol{x}_E$ are taken into account and are modeled as an additive term affecting the first equation in (5) as well. In sum, the effects of both process and actuator faults on the system dynamics are taken into account via an additive term $\boldsymbol{C}^T\boldsymbol{f}_a(t,\boldsymbol{y},u)$ in the first equation in (5). As customary in the literature (see, e.g., [11]), function $\boldsymbol{f}_a$ is assumed to belong to a finite set of m functions, $\mathcal{F}_a = \{\boldsymbol{f}_{a,1}\ldots\boldsymbol{f}_{a,m}\}$. Each fault function in $\mathcal{F}_a$ is assumed to be linear in a parameter vector $\boldsymbol{\theta}_i$, i.e.

$$\boldsymbol{f}_{a,i}(t,\boldsymbol{y},u) = \boldsymbol{\varphi}_i(t,\boldsymbol{y},u)\boldsymbol{\theta}_i\,, \quad \forall i = 1,\ldots,m\,, \tag{7}$$

where $\boldsymbol{\varphi}_i$ is a known $(2 \times m_i)$ regressor matrix, while $\boldsymbol{\theta}_i$ is a $(m_i \times 1)$ unknown vector of constant parameters. Matrix $\boldsymbol{\varphi}_i$ is assumed norm-bounded for all faults type.

Therefore, in the presence of faults, model (5) becomes

$$\begin{cases} \dot{\boldsymbol{x}} = \boldsymbol{A}(\boldsymbol{y})\boldsymbol{x}+\boldsymbol{b}(\boldsymbol{y},u)+\boldsymbol{C}^T\boldsymbol{f}_a(t,\boldsymbol{y},u)+\boldsymbol{\eta}(\boldsymbol{x},u) \\ \boldsymbol{y} = \boldsymbol{C}\boldsymbol{x}+\boldsymbol{f}_s(t)+\boldsymbol{n}\,, \end{cases} \tag{8}$$

where it is assumed that $\boldsymbol{f}_s(t)$ and $\boldsymbol{f}_a(t,\boldsymbol{y},u)$ are null before the occurrence of a fault at $t = t_f$, i.e., $\boldsymbol{f}_s(t) = \boldsymbol{0}$ and $\boldsymbol{f}_a(t,\boldsymbol{y},u) = \boldsymbol{0}$ for $t < t_f$.

The above model includes the case in which a sensor and a process/actuator fault occur during the same batch operation. Otherwise, occurrence of multiple process/actuator faults (i.e., of different types) and/or of multiple sensor faults (i.e., different sensors are subject to failures) is not considered.

III. Sensor fault diagnosis

It is assumed that a duplex sensor architecture is adopted for the plant. Namely, two temperature sensors (hereafter labeled as $S_{r,1}$ and $S_{r,2}$) providing measurements of T_r, and two providing measurements of $T_\jmath$ (hereafter labeled as $S_{\jmath,1}$ and $S_{\jmath,2}$) are available. Hence, two observers are adopted for sensor fault diagnosis. Observer SM1 uses the measurements provided by $S_{r,1}$ and $S_{\jmath,1}$, i.e., $\boldsymbol{y}_{SM1} = (y_{r,1}\ y_{\jmath,1})^T$. Observer SM2, uses the measurements provided by $S_{r,2}$ and $S_{\jmath,2}$, i.e., $\boldsymbol{y}_{SM2} = (y_{r,2}\ y_{\jmath,2})^T$.

Both the observers have the following form (hereafter $i = 1,2$)

$$\begin{cases} \dot{\widehat{\boldsymbol{x}}}_{SMi} &=& \boldsymbol{A}(\boldsymbol{y}_{SMi})\,\widehat{\boldsymbol{x}}_{SMi}+\boldsymbol{b}(\boldsymbol{y}_{SMi},u)+\boldsymbol{L}_s\widetilde{\boldsymbol{y}}_{SMi} \\ \widehat{\boldsymbol{y}}_{SMi} &=& \boldsymbol{C}\widehat{\boldsymbol{x}}_{SMi}\,, \end{cases} \tag{9}$$

where $\widehat{\boldsymbol{x}}_{SMi}$ denotes the vector of the state estimates; $\widehat{\boldsymbol{y}}_{SMi}$ and $\widetilde{\boldsymbol{y}}_{SMi} = \boldsymbol{y}_{SMi} - \widehat{\boldsymbol{y}}_{SMi}$ denote the vectors of output estimates and output estimation errors, respectively; $\boldsymbol{L}_s$ is a $(p+2)\times 2$ matrix of positive gains defined as follows

$$\boldsymbol{L}_s = \begin{bmatrix} \boldsymbol{L}_M \\ \boldsymbol{L}_E \end{bmatrix}, \quad \boldsymbol{L}_M = \begin{bmatrix} l_1 & 0 \\ l_2 & 0 \\ \vdots & \vdots \\ l_p & 0 \end{bmatrix}, \quad \boldsymbol{L}_E = \begin{bmatrix} l_r & 0 \\ 0 & l_\jmath \end{bmatrix}.$$

Convergence properties of the state estimation error $\widetilde{\boldsymbol{x}}_{SMi} = \boldsymbol{x} - \widehat{\boldsymbol{x}}_{SMi}$, in the absence of faults, can be analyzed by considering the estimation error dynamics, derived in view of Eqs. (5) and (9)

$$\begin{cases} \dot{\widetilde{\boldsymbol{x}}}_{SMi} &=& \boldsymbol{A}_{s,i}(\boldsymbol{y}_{SMi})\,\widetilde{\boldsymbol{x}}_{SMi} + \boldsymbol{\delta}_{SMi}(\boldsymbol{x},u) \\ \widetilde{\boldsymbol{y}}_{SMi} &=& \boldsymbol{C}\widetilde{\boldsymbol{x}}_{SMi} + \boldsymbol{n}\,, \end{cases} \tag{10}$$

where $\boldsymbol{A}_{s,i} = \boldsymbol{A} - \boldsymbol{L}_s\boldsymbol{C}$ and $\boldsymbol{\delta}_{SMi} = \boldsymbol{\eta} + \boldsymbol{L}_s\boldsymbol{n}$. It can be shown [13] that, in the absence of uncertainties and sensor noise, there exists a set of observer gains such that the state estimation error $\widetilde{\boldsymbol{x}}_{SMi}$ of the observer (9) is globally uniformly convergent to $\boldsymbol{0}$ as $t \to \infty$. Moreover, the convergence is exponential. As for the behavior of the state estimation error in the presence of uncertainties and noise, in [13] it is proven that if $\boldsymbol{\eta}$ and $\boldsymbol{n}$ are bounded (see Section II), then the output estimation error is bounded, i.e.,

$$\exists\, \bar{\mu}_{s,i} > 0\ : \qquad \|\widetilde{\boldsymbol{y}}_{SMi}(t)\| \le \bar{\mu}_{s,i}\,, \qquad \forall t \ge t_0\,, \tag{11}$$

where t_0 is the initial time and the bound $\bar{\mu}_{s,i}$ depends on the initial estimation error, $\widetilde{\boldsymbol{x}}_{SMi}(t_0)$, the magnitude of uncertainties and sensor noise, $\boldsymbol{\eta}$ and $\boldsymbol{n}$, and the largest (negative) eigenvalue of $\boldsymbol{A}_E - \boldsymbol{L}_E$. It is worth noticing that the bound could be, in principle, determined if all the constants needed to compute it are known or, at least, estimated with reasonable accuracy. Nevertheless, such a bound may be quite conservative, and thus, in practice, useless. However, the bound can be reduced if a suitable gain matrix $\boldsymbol{L}_E$ is chosen and a good initial guess of the state is available [13].

Detection of the occurrence of sensor faults can be achieved on the basis of the following residuals:

$$r_{S_r} = \frac{y_{r,1} - y_{r,2}}{\mu_{s,r}}\,, \quad r_{S_\jmath} = \frac{y_{\jmath,1} - y_{\jmath,2}}{\mu_{s,\jmath}}\,, \tag{12}$$

where $\mu_{s,r}$ and $\mu_{s,\jmath}$ are normalization factors to be properly determined by evaluating the effect of noise and disturbances on temperature measurements (in the absence of faults). Hence, if S_r ($S_\jmath$) is affected by a fault, the absolute value of r_{S_r} ($r_{S_\jmath}$) is expected to exceed a certain threshold. The normalization factors are to be selected so as to set the threshold to 1. Hence, a possible choice is given by $2\bar{n}$, since $|y_{*,1}(t) - y_{*,2}(t)| \le 2\bar{n}$ for all t ($* = r,\jmath$).

For isolation purposes (i.e., determination of the faulty sensor), two other residuals must be defined

$$\boldsymbol{r}_{SM1} = \frac{\widetilde{\boldsymbol{y}}_{SM1}}{\mu_{s,1}}\,, \quad \boldsymbol{r}_{SM2} = \frac{\widetilde{\boldsymbol{y}}_{SM2}}{\mu_{s,2}}\,, \tag{13}$$

where $\mu_{s,1}$ and $\mu_{s,2}$ are normalization factors. According to (11), a possible choice for the normalization factors is $\mu_{s,i} = \bar{\mu}_{s,i}$, although they may be chosen by evaluating the effect of uncertainties and sensor noise, e.g., on the basis of available experimental data. By virtue of these normalization factors, the thresholds on the residuals can be set to 1 and the norm of residual vectors can be used to isolate faults. In fact, the output of the SM1 observer is not affected by faults on $S_{r,2}$ and $S_{\jmath,2}$, while the output of the SM2 observer is not affected by faults on $S_{r,1}$ and $S_{\jmath,1}$. Hence, if the norm of $\boldsymbol{r}_{SM1}$ ($\boldsymbol{r}_{SM2}$) exceeds the threshold, a fault is declared on either $S_{r,1}$ or $S_{\jmath,1}$ (either $S_{r,2}$ or $S_{\jmath,2}$), depending on which detection residual (i.e., r_{S_r} or r_{S_J}) exceeds the threshold. In sum, a fault can be declared and, eventually, isolated, provided that simultaneous faults on different sensors do not occur during the same batch operation.

When a sensor fault (occurring at $t = t_f$) affects one of the sensors in the couple $\{S_{r,i}, S_{J,i}\}$ ($i = 1, 2$), the following equality holds

$$\widetilde{\boldsymbol{y}}_{SMi} = \boldsymbol{C}\,\widetilde{\boldsymbol{x}}_{SMi} + \boldsymbol{f}_s(t) + \boldsymbol{n}\,, \quad \forall t \geq t_f\,. \tag{14}$$

As shown in [13], a sufficient condition ensuring correct sensor fault isolation is given by

$$\exists t > t_f\,:\, \left\| \int_{t_f}^{t} \boldsymbol{\Phi}_E(t,\tau)\boldsymbol{L}_E \boldsymbol{f}_s(\tau)d\tau + \boldsymbol{f}_s(t) \right\| \geq \bar{\mu}_{s,i} + \mu_{s,i}\,, \tag{15}$$

where $\boldsymbol{\Phi}_E(t,t_0) = \exp\left((\boldsymbol{A}_E - \boldsymbol{L}_E)(t-t_0)\right)$. In fact, the above condition guarantees that $\|\boldsymbol{r}_{SMi}\| = \|\widetilde{\boldsymbol{y}}_{SMi}\|/\mu_{s,i}$ exceeds 1 at least for a time instant after the occurrence of the fault, thus signaling the presence of the fault. In other words, condition (15) matches with the intuitive idea that faults can be detected only if their magnitude overcomes the effect of the uncertainties. Of course, (15) may result too conservative, especially if the bounds are overestimated; however, it has the merit of showing how sensitivity to faults may be affected by uncertainties and noise.

Thanks to redundant temperature measurements, the batch can be brought to completion even in the presence of a sensor fault, provided that a suitable voting of the healthy signal is performed. The logic of the *Voter/Monitor* (the sub-system which votes the healthy signal) is described in the following procedure:

Step 1. Compute the detection residuals defined in (12), then:

(i) If the residuals do not exceed the fixed thresholds (no fault condition), vote the signal given by the average of the two sensors (standard duplex measure).

(ii) If a threshold is exceeded (fault condition), check the isolation residuals defined in (13), so as to decide if the faulty signal can be isolated; in this case determine the healthy signal.

Step 2. If, in the case (ii), faults isolation is not achieved (i.e., both $\boldsymbol{r}_{SM1}$ and $\boldsymbol{r}_{SM2}$ are below the respective thresholds), a missed isolation is declared. In this case, the weighted average of the signals provided by the physical and virtual sensor is voted. The weighted average is computed as the arithmetic mean of the measured variable and the output of the sole observer not signaling the occurrence of the fault.

IV. Actuator and Process Fault Diagnosis

The healthy measure, obtained via the diagnostic system described above, is used to feed a bank of $m+1$ observers providing process/actuator fault detection and isolation. One observer plays the role of detection observer, i.e., determines the occurrence of an actuator or process fault. Other m observers, corresponding to the m different fault types, are used for isolation and identification.

The detection observer has the form

$$\begin{cases} \dot{\widehat{\boldsymbol{x}}}_a &= \boldsymbol{A}(\boldsymbol{y})\,\widehat{\boldsymbol{x}}_a + \boldsymbol{b}(\boldsymbol{y},u) + \boldsymbol{L}_a\widetilde{\boldsymbol{y}}_a \\ \widehat{\boldsymbol{y}}_a &= \boldsymbol{C}\,\widehat{\boldsymbol{x}}_a\,, \end{cases} \tag{16}$$

where $\boldsymbol{y}$ is given by the healthy measure voted by the diagnostic system, $\widetilde{\boldsymbol{y}}_a = \boldsymbol{y} - \widehat{\boldsymbol{y}}_a$ and $\boldsymbol{L}_a$ is a matrix gain of the same form as $\boldsymbol{L}_s$. In the absence of faults, the state estimation error dynamics has the same form (10), i.e.,

$$\begin{cases} \dot{\widetilde{\boldsymbol{x}}}_a &= \boldsymbol{A}_a(\boldsymbol{y})\,\widetilde{\boldsymbol{x}}_a + \boldsymbol{\delta}_a(\boldsymbol{x},u) \\ \widetilde{\boldsymbol{y}}_a &= \boldsymbol{C}\widetilde{\boldsymbol{x}}_a + \boldsymbol{n}\,, \end{cases} \tag{17}$$

where $\widetilde{\boldsymbol{x}}_a = \boldsymbol{x} - \widehat{\boldsymbol{x}}_a$, $\boldsymbol{A}_a = \boldsymbol{A} - \boldsymbol{L}_a\boldsymbol{C}$ and $\boldsymbol{\delta}_a = \boldsymbol{\eta} + \boldsymbol{L}_a\boldsymbol{n}$. Convergence and boundedness properties of the state estimation error are the same established in the previous Section. In detail, in the presence of bounded uncertainties and noise, the output estimation error is bounded, i.e.,

$$\exists\, \bar{\mu}_a > 0\,: \qquad \|\widetilde{\boldsymbol{y}}_a(t)\| \leq \bar{\mu}_a\,, \qquad \forall t \geq t_0\,. \tag{18}$$

A fault is declared when the norm of the residual vector

$$\boldsymbol{r}_d = \frac{\widetilde{\boldsymbol{y}}_a}{\mu_a}\,, \tag{19}$$

exceeds a suitably defined threshold. The factor μ_a, as usual, is a normalization factor that has to be selected in such a way that threshold can be set to 1. Of course, a possible choice for the normalization factor μ_a is represented by $\bar{\mu}_a$. A sufficient condition for detectability of a fault occurring at $t = t_f$ is given by [13]

$$\exists t > t_f\,:\, \left\| \int_{t_f}^{t} \boldsymbol{\Phi}_E(t,\tau)\boldsymbol{f}_a(\tau,\boldsymbol{y}(\tau),u(\tau))\,d\tau \right\| \geq \bar{\mu}_a + \mu_a\,. \tag{20}$$

After a fault has been detected, isolation and identification are achieved via m nonlinear adaptive observers. Each observer is designed in such a way to be insensitive to a particular type of fault. In fact, the i-th observer (hereafter $i = 1, \ldots, m$) has the form

$$\begin{cases} \dot{\widehat{\boldsymbol{x}}}_i = \boldsymbol{A}(\boldsymbol{y})\widehat{\boldsymbol{x}}_i + \boldsymbol{b}(\boldsymbol{y},u) + \boldsymbol{L}_{a,i}\widetilde{\boldsymbol{y}}_i + \boldsymbol{C}^T\widehat{\boldsymbol{f}}_{a,i}(t,\boldsymbol{y},u) \\ \widehat{\boldsymbol{y}}_i = \boldsymbol{C}\widehat{\boldsymbol{x}}_i\,, \end{cases} \tag{21}$$

where $\boldsymbol{L}_{a,i}$ is a gain matrix having the same structure as $\boldsymbol{L}_a$ and $\boldsymbol{L}_s$, $\boldsymbol{y}$ is given by the healthy measure voted by the sensor diagnostic system, $\widetilde{\boldsymbol{y}}_i = \boldsymbol{y} - \widehat{\boldsymbol{y}}_i$ and $\widehat{\boldsymbol{f}}_{a,i}$ is an estimate of the i-th fault, that, in view of (7) can be obtained as follows

$$\widehat{\boldsymbol{f}}_{a,i}(t,\boldsymbol{y},u) = \boldsymbol{\varphi}_i(t,\boldsymbol{y},u)\,\widehat{\boldsymbol{\theta}}_i\,, \tag{22}$$

where $\widehat{\boldsymbol{\theta}}_i$ is an estimate of the unknown parameter vector. The adaptive law for $\widehat{\boldsymbol{\theta}}_i$ is derived by using a Lyapunov synthesis approach [13]

$$\dot{\widehat{\boldsymbol{\theta}}}_i = \lambda_i^{-1}\boldsymbol{\varphi}_i^T(t,\boldsymbol{y},u)\widetilde{\boldsymbol{y}}_i\,, \tag{23}$$

where λ_i is a positive gain. In order to ensure $\widehat{\boldsymbol{f}}_{a,i} = \boldsymbol{0}$ prior to the detection of the fault, the initial value of $\widehat{\boldsymbol{\theta}}_i$ is set to zero and the parameters update is activated only after a fault is detected.

In the presence of the i-th fault (i.e., $\boldsymbol{f}_a = \boldsymbol{f}_{a,i}$) the state estimation error, $\widetilde{\boldsymbol{x}}_i$, of the i-th observer (21) is given by

$$\begin{cases} \dot{\widetilde{\boldsymbol{x}}}_i = \boldsymbol{A}_{a,i}(\boldsymbol{y})\,\widetilde{\boldsymbol{x}}_i + \boldsymbol{C}^T\boldsymbol{\varphi}_i(t,\boldsymbol{y},u)\widetilde{\boldsymbol{\theta}}_i + \boldsymbol{\delta}_{a,i}(\boldsymbol{x},u) \\ \widetilde{\boldsymbol{y}}_i = \boldsymbol{C}\widetilde{\boldsymbol{x}}_i + \boldsymbol{n}\,, \end{cases} \tag{24}$$

where $\widetilde{\boldsymbol{x}}_i = \boldsymbol{x} - \widehat{\boldsymbol{x}}_i$, $\widetilde{\boldsymbol{\theta}}_i = \boldsymbol{\theta}_i - \widehat{\boldsymbol{\theta}}_i$, $\boldsymbol{A}_{a,i} = \boldsymbol{A} - \boldsymbol{L}_{a,i}\boldsymbol{C}$ and $\boldsymbol{\delta}_{a,i} = \boldsymbol{\eta} + \boldsymbol{L}_{a,i}\boldsymbol{n}$. In the absence of uncertainties and sensor noise, if the rate constants are bounded, there exists a set of observer gains such that the state estimation error $\widetilde{\boldsymbol{x}}_i$ of the observer (21) is globally uniformly convergent to $\boldsymbol{0}$ as $t \to \infty$ and the parameter estimation error $\widetilde{\boldsymbol{\theta}}_i$ is uniformly bounded for every t. Remarkably, in the presence of bounded uncertainties and sensor noise, boundedness of $\widetilde{\boldsymbol{\theta}}_i$ is no longer guaranteed. A sufficient condition to achieve boundedness is given by the persistency of excitation [15], which is often difficult to meet in practice. Otherwise, the update law (23) can be modified by adopting the so-called projection operator [16].

To achieve faults isolation, the following residuals are computed

$$\boldsymbol{r}_{a,i} = \frac{\widetilde{\boldsymbol{y}}_i}{\mu_{a,i}}, \quad i = 1,\ldots,m \tag{25}$$

where, as usual, $\mu_{a,i}$ are normalization factors selected in such a way to set the thresholds to 1. If the i-th fault occurs, the norms of all the residuals but the residual $\boldsymbol{r}_{a,i}$ exceed their thresholds.

It is worth remarking that, when a fault different from the m types considered in the design of the bank of observers occurs, it can be only detected but not isolated and identified.

In [13] is shown that, in the presence of bounded uncertainties and noise, a bound on the output estimation error can be found , i.e.,

$$\exists\, \bar{\mu}_{a,i} > 0 : \qquad \|\widetilde{\boldsymbol{y}}_i(t)\| \le \bar{\mu}_{a,i}\,, \tag{26}$$

provided that the fault estimation error $\boldsymbol{\varphi}_i\widetilde{\boldsymbol{\theta}}_i$ is guaranteed to be bounded. If $\bar{\mu}_{a,i}$ can be estimated, it represents a possible choice for the normalization factor $\mu_{a,i}$.

In the presence of the the same fault, the state estimation error, $\widetilde{\boldsymbol{x}}_l$, of the l-th observer ($l \ne i$) is given by

$$\begin{cases} \dot{\widetilde{\boldsymbol{x}}}_l = \boldsymbol{A}_{a,l}(\boldsymbol{y})\,\widetilde{\boldsymbol{x}}_l + \boldsymbol{C}^T\Big(\boldsymbol{\varphi}_i(t,\boldsymbol{y},u)\boldsymbol{\theta}_i - \boldsymbol{\varphi}_l(t,\boldsymbol{y},u)\widehat{\boldsymbol{\theta}}_l\Big) \\ \qquad\quad + \boldsymbol{\eta}(\boldsymbol{x},u) \\ \widetilde{\boldsymbol{y}}_l = \boldsymbol{C}\widetilde{\boldsymbol{x}}_l + \boldsymbol{n}\,. \end{cases} \tag{27}$$

A sufficient condition for isolability of the i-th type of process/actuator fault is given by the two inequalities

$$\forall\, l = 1,\ldots,m\ (l \ne i)\,, \quad \exists t > t_f\ :$$

$$\left\|\int_{t_f}^{t}\boldsymbol{\Phi}_E(t,\tau)\Big(\boldsymbol{\varphi}_i(\tau,\boldsymbol{y},u)\boldsymbol{\theta}_i - \boldsymbol{\varphi}_l(\tau,\boldsymbol{y},u)\widehat{\boldsymbol{\theta}}_l\Big)d\tau\right\| \ge \bar{\mu}_{a,l} + \mu_{a,l}, \tag{28}$$

and

$$\|\widetilde{\boldsymbol{y}}_i(t)\| \le \bar{\mu}_{a,i}\,, \quad \forall t > t_f\,, \tag{29}$$

since they guarantee that all the residuals $\|\boldsymbol{r}_{a,l}(t)\| = \|\widetilde{\boldsymbol{y}}_l(t)\|/\mu_{a,l}$ ($l \ne i$) exceed their respective thresholds at least for a time instant, while the i-th residuals keeps below its threshold.

A final issue to be considered regards decoupling of sensor fault diagnosis from process/actuator fault diagnosis. Namely, in order to make the observer (9), adopted to generate the sensor fault isolation residuals, insensitive to process/actuator faults, the observer dynamics (9) is modified as

$$\begin{cases} \dot{\widehat{\boldsymbol{x}}}_{SMi} = \boldsymbol{A}(\boldsymbol{y}_{SMi})\,\widehat{\boldsymbol{x}}_{SMi} + \boldsymbol{b}(\boldsymbol{y}_{SMi},u) \\ \qquad\qquad + \boldsymbol{L}_s\widetilde{\boldsymbol{y}}_{SMi} + \boldsymbol{C}^T\widehat{\boldsymbol{f}}_a(t,\boldsymbol{y},u)\,, \\ \widehat{\boldsymbol{y}}_{SMi} = \boldsymbol{C}\widehat{\boldsymbol{x}}_{SMi}\,, \end{cases} \tag{30}$$

where $\boldsymbol{C}^T\widehat{\boldsymbol{f}}_a(t,\boldsymbol{y},u)$ is an estimate of the isolated process/actuator fault, i.e., if the i-th fault has been detected and isolated, then $\widehat{\boldsymbol{f}}_a(t,\boldsymbol{y},u) = \widehat{\boldsymbol{f}}_{a,i}(t,\boldsymbol{y},u)$.

V. CASE STUDY

A case study has been developed to test the effectiveness of the proposed approach on a simulation model built in the Matlab/Simulink© environment. A reaction process for the production of resol-type phenolic resins has been considered. This reaction under upset conditions, such as loss of cooling, can accelerate and cause temperature and pressure to increase (*run away* conditions) [17]. Here, a detailed model (89 reaction and 13 compounds) of the reaction process is used to build a realistic simulation model, while the simplified reaction scheme $A_1 \to A_2 \to A_3 \to A_4$, which has been identified in [14], is used to design the control scheme and the diagnostic observers, where A_1 represents the phenol, A_2 is a mixture of mono- and dimethylolphenols, A_3 is the trimethylolphenol and A_4 is a mixture of poliphenols.

The model-based temperature controller proposed in [12] is adopted. A first-order linear dynamics (with a time constant equal to $\tau = 3$ [s]) between the commanded control input (computed by the controller) and the real temperature of the water entering the jacket is introduced, but not modeled in the design of the controller and of the observers.

The relevant parameters of the reactor and jacket models are summarized in Table I.

Parameter	value
$k_{0_{1,2}}$, $k_{0_{2,3}}$, $k_{0_{3,4}}$	$2.41 \cdot 10^7$, $1.20 \cdot 10^4$, $1.23 \cdot 10^2$ [s^{-1}]
$E_{a_{1,2}}$, $E_{a_{2,3}}$, $E_{a_{3,4}}$	77.8, 58.3, 43.8 [kJ mol^{-1}]
$\Delta H_{1,2}$, $\Delta H_{2,3}$, $\Delta H_{3,4}$	-40.6, -10.5, -21.4 [kJ mol^{-1}]
U	0.72 [kJ s^{-1} K^{-1} m^{-2}]
S	15.96 [m^2]
F	0.1 [m^3 s^{-1}]
V_r, V_j	6, 1.73 [m^3]
$\rho_r\, c_{pr}$	$1.9 \cdot 10^3$ [kJ m^{-3} K^{-1}]
$\rho_j\, c_{pj}$	$4.19 \cdot 10^3$ [kJ m^{-3} K^{-1}]
$C_1(0)$, $C_2(0)$, $C_3(0)$	4200, 0, 0 [mol m^{-3}]
$T_r(0)$, $T_j(0)$	293, 310 [K]

TABLE I

SIMULATION PARAMETERS.

Three actuator/process faults have been considered in the simulations (i.e., m=3): variation of the heat transfer coefficient (fault type 1), fault on the heat isolation of the cooling jacket (fault type 2) and fault on the cooling system, i.e., actuator fault (fault type 3). The gain matrices of all the diagnostic observers have been set as

$$\boldsymbol{L}_s = \begin{bmatrix} \boldsymbol{L}_M \\ \boldsymbol{L}_E \end{bmatrix}, \ \boldsymbol{L}_M = \begin{bmatrix} 1 \cdot 10 & 0 \\ 5 \cdot 10^2 & 0 \\ 1 \cdot 10^{-1} & 0 \end{bmatrix}, \ \boldsymbol{L}_E = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}.$$

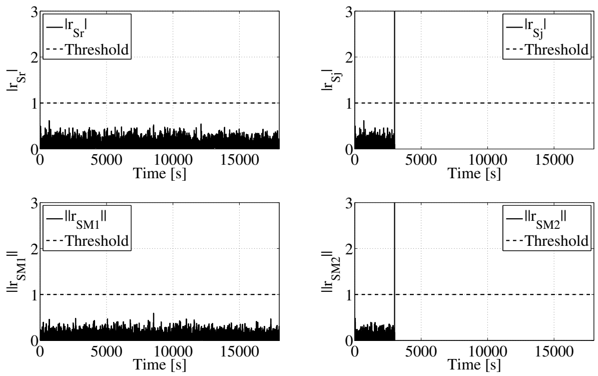

Fig. 1. Sensor $T_{j,2}$ and cooling system faults: detection and isolation residuals for the sensor fault.

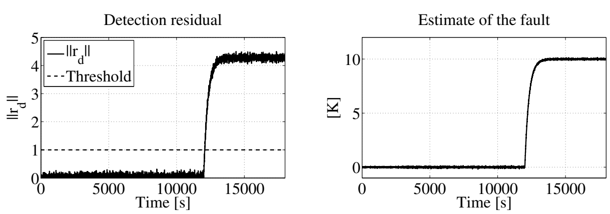

Fig. 2. Sensor $T_{j,2}$ and cooling system faults: detection residual and estimate of the actuator fault.

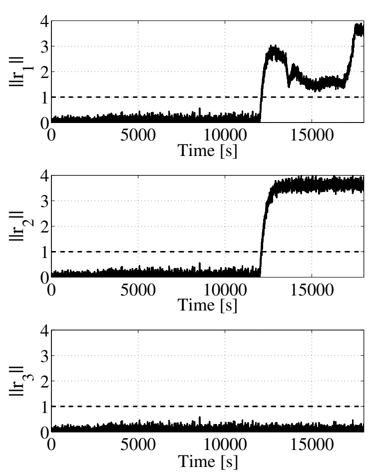

Fig. 3. Sensor $T_{j,2}$ and cooling system faults: isolation residuals for the actuator fault.

A simulation in which both a sensor and an actuator fault occur during the same batch has been developed. First, an abrupt freezing of the measured signal of sensor $T_{j,2}$ occurs at time $t_{f,1} = 3000$ [s]; then, an actuator fault, with magnitude of 10 [K], affecting the cooling system occurs at time $t_{f,2} = 12000$ [s]. Figure 1 shows that the residuals $\boldsymbol{r}_{SMi}$ $(i = 1, 2)$, r_{S_r} and r_{S_j} are able to detect and isolate the sensor fault. Figure 2 shows that the actuator fault is correctly detected (i.e., the norm of the detection residual vector $\boldsymbol{r}_d$ exceeds its threshold) and identified (i.e., the magnitude of the fault is correctly estimated). Figure 3 reports the isolation residuals: only the norm of residual $\boldsymbol{r}_3$ remains always below the threshold, therefore the fault is isolated as a fault of third type.

Finally, it can be noticed that residuals $\boldsymbol{r}_{SMi}$, r_{S_r} and r_{S_j} are insensitive to the actuator fault, while residuals $\boldsymbol{r}_d$ and $\boldsymbol{r}_l$ $(l = 1, 2, 3)$ are insensitive to the sensor fault.

REFERENCES

[1] R.J. Patton, P.M. Frank, R.N. Clark, "Issues in Fault Diagnosis for Dynamic Systems,", Springer-Verlag, London, UK, 2000.

[2] R. Tarantino, F. Szigeti, E. Colina-Morles, "Generalized Luneberger Observer-Based Fault Detection Filter Design: An Industrial Application," *Control Engineering Practice*, vol. 8, pp. 665-671, 2000.

[3] M. Witczak, J. Patton, J. Korbicz, "Fault detection with observers and genetic programming: application to the DAMADICS benchmark problem," In *Proceeding of the 5th IFAC symposium on fault detection, supervision and safety for technical processes*, pp. 1203–1208, 2003.

[4] O.A.Z. Sotomayor, D. Odloak, "Observer-based fault diagnosis in chemical plants," *Chemical Engineering Journal*, vol. 112, pp. 93–108, 2005.

[5] Y. Huang, G.V. Reklaitis, V. Venkatasubramanian, "A Heuristic Extended Kalmann Filter Based Estimator for Fault Identification in a Fluid Catalytic Carcking Unit," *Ind. Eng. Chem. Res.*, vol. 42, pp. 3361–3371, 2003.

[6] P. Kaborè, S. Othman, T.F. McKenna,H. Hammouri, "Observer-Based Fault Diagnosis for a Class of Nonlinear Systems – Application to a Free Radical Copolymerization Reaction," *International Journal of Control*, vol. 73, pp. 787–803, 2000.

[7] F. Pierri, G. Paviglianiti, F. Caccavale, M. Mattei "Observer-based sensor fault detection and isolation for chemical batch reactors," *Engineering Applications of Artificial Intelligence*, vol. 21, pp. 1204-1216, 2008.

[8] F. Pierri, G. Paviglianiti, "Observer-based actuator fault detection for chemical batch reactors: a comparison between nonlinear adaptive and $\mathcal{H}_\infty$ -based approaches" In *Proc. of the Mediterranian Control Conference*, Athens, Greek, 2007.

[9] P. Mhaskar, A. Gani, N.H. El-Farra, C. McFall, P.D. Christofides, J.F. Davis, "Integrated Fault-Detection and Fault-Tolerant Control of Process Systems," *AIChE Journal*, vol. 52, pp. 2129–2148, 2006.

[10] R.J. Patton, F.J. Uppal, C.J. Lopez-Toribio, "Soft Computing Approaches to Fault Diagnosis for Dynamic Systems: A Survey," *Preprints of the 4th IFAC Symposium on Fault Detection Supervision and Safety for Technical Processes*, Budapest, H, 298-311, 2001.

[11] X. Zhang, M.M. Polycarpou, T. Parisini, "A Robust Detection and Isolation Scheme for Abrupt and Incipient Faults in Nonlinear Systems," *IEEE Transactions on Automatic Control*, vol. 47, pp. 576–593, 2002.

[12] F. Caccavale, M. Iamarino, F. Pierri, V. Tufano, "A Controller-Observer Scheme for Temperature Control of Non-Chain Reactions in Batch Reactors," *International Journal of Adaptive Control and Signal Processing*. vol. 22, pp. 627–651, 2008.

[13] F. Caccavale, F. Pierri, M. Iamarino, V. Tufano, "An Integrated Approach to Fault Diagnosis for a Class of Chemical Batch Processes," *Journal of Process Control*, 2008, DOI: 10.1016/j.jprocont.2008.11.003.

[14] F. Caccavale, M. Iamarino, F. Pierri, V. Tufano, "Kinetic Model Reduction for Control of Phenol-Formaldehyde Reactive System," *Proceedings of EUROSIM/UKSim 2008*, Cambridge, UK, April 2008.

[15] K.J. Åström and B. Wittenmark, *Adaptive control (2nd Edition)*, Addison-Wesley, 1995.

[16] P.A. Ioannou and J. Sun, *Robust Adpative Control*, Prentice Hall, Upper Saddle River, NJ, 1996.

[17] E. Kumpinsky, "A study on resol-type phenol-formaldehyde runaway reactions," *Ind. Eng. Chem. Res.*, vol. 33, pp. 285–291, 1994.