Nonlinear Observer Based Fault Diagnosis for an Innovative Intensified Heat-Exchanger/Reactor

Xue Han, Zetao Li, Boutaib Dahhou, Michel Cabassud and Menglin He

Abstract This paper describes an application of a fault detection and isolation (FDI) scheme for an intensified Heat-exchanger (HEX)/Reactor, where the exothermic chemical reaction of sodium thiosulfate oxidation by hydrogen peroxide is performed. To achieve this, precise estimation of all states of HEX/Reactor, including temperatures and concentrations of different reactants, as well as process fault detection and isolation is completed by a high gain observer. Then, process fault identification is achieved by several banks of interval filters. Finally, an intensified HEX/reactor is used to validate the effectiveness of the proposed strategy. Simulation results are shown to illustrate the performance of the algorithm presented.

Keywords Fault diagnosis · Fault identification · High gain observer · Parameter interval filter · HEX/reactor

1 Introduction

Due to the increasing demand for higher safety and reliability of the dynamic system, fault detection and isolation (FDI) is becoming an effective method to avoid breakdowns and disasters of major systems. In chemical engineering field, an intensified continuous HEX/reactor [1] is a multifunctional device which combines heat exchanger and reactor together. It is much safer according to its outstanding mixing performance and remarkable heat transfer capacity [2]. However, undesirable failures such as thermal runaway still pose a great threat to such intensified process. Therefore, process monitoring provided by fault detection and diagnosis (FDD) method is necessary to improve its performance.

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Extensive review of existing FDD approaches can be found in [3–5]. They are roughly divided into data-based methods and model-based methods. Data-based methods [6–8] only rely on a database of historical data collected under normal operating conditions. While model-based methods require an exact model to estimate process variables. By comparing the measured and corresponding estimated values, a set of deviations (residuals) are generated. After residual evaluation, faults can be isolated and identified. Observer-based approaches, which contribute a lot to model-based methods, are applied to various chemical reactors [9–13]. In addition, the authors of [14, 15], propose a new FDI method based on parameter intervals. The practical domain of the value of each parameter is divided into several intervals, which provides an ideal FDI speed. Since the HEX/Reactor is often connected with field devices (i.e. actuator), [16] focus on the fault diagnosis of such interconnected systems by using invertibility.

However, most of previous model-based FDD approaches focus on either heat exchangers [17, 18], or chemical reactors [10, 19]. Moreover, the referred reactor is a stirred tank with poor heat removal capacity, which increases the risk of out of control and reduction of productivity. The multifunctional HEX/Reactor guarantees a proper temperature for chemical reactions by its excellent capacity of heat exchange. In [10, 13], model-based FDD approaches are proposed for fault diagnosis. Nevertheless, chemical reaction, which affects the temperature in turn, is not considered.

This paper is aimed at proposing an observer-based FDD strategy to solve the fault diagnosis problem on the studied HEX/Reactor. Firstly, an appropriate model of the studied HEX/Reactor is constructed, where both heat exchange and chemical reaction are taken into consideration. Moreover, an observer-based FDD approach is applied to detect and isolate process faults (i.e. fouling within both channels) by only one temperature output. In addition, the output is used to feed a bank of interval filters to provide fault identification.

The rest of this paper is as follows. Firstly, the mathematical model of HEX/Reactor with an exothermic reaction taken place in is presented. Then, the applied FDI method is described in Sect. 3, high gain observer and interval filters are designed to estimate internal states and faulty parameters. Thereafter, Sect. 4 shows the simulation results of the applied FDI scheme. Finally, the conclusion is presented in Sect. 5.

2 Modelling of the Intensified HEX/Reactor

2.1 Physical Structure of the Intensified HEX/Reactor

The intensified HEX/Reactor considered in this paper is assembled by three process plates and four utility plates, which are both engraved into 2 mm square cross-section channels (shown in Fig. 1). Steel between channels, which acts as the heat exchange media, are called plate wall. The cell-based structure and flow configuration are

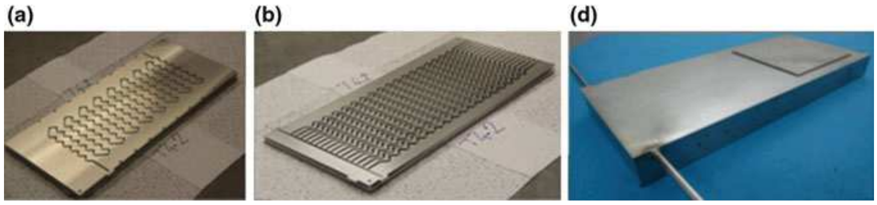


Fig. 1 **a** Process channel; **b** utility channel; **c** the physical HEX/Reactor [20]

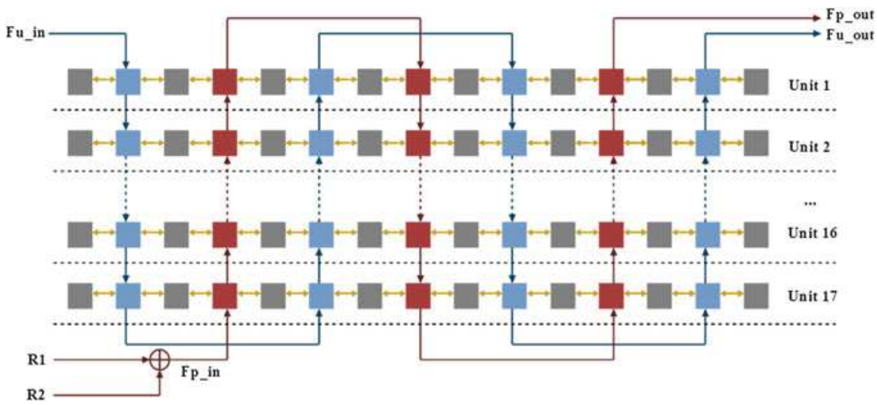


Fig. 2 Description of cells diving and flow configuration

shown in Fig. 2. The process flow Fp_in, which is combined by two (or several) feeding lines (reactant R1 and reactant R2 in Fig. 2), circulates in a single channel, within which the reaction is taken place. The utility fluid Fu_in (water in most cases) flows in parallel zigzag type channels so as to take reaction heat away. The temperature of each cell is influenced by the former and latter cell connected. Note that conductive heat exchange is only considered in horizontal direction.

2.2 *Mathematical Modelling*

The modelling of each cell is based on the expression of mass and energy balance. Each cell is assumed homogenous and no back mixing. In addition, the exothermic reaction of sodium thiosulfate oxidation by hydrogen peroxide is conducted in the pilot. The reaction equation is:

$$2Na_2S_2O_3 + 4H_2O_2 \rightarrow Na_2S_3O_6 + Na_2SO_4 + 4H_2O$$

The concentration of reactants plays an important role in heat generation during the reaction process, and will further result in temperature change. They are also considered as internal states. To sum up, the dynamic of the pilot can be expressed as follows:

$$\begin{aligned}
\dot{T}_p &= \frac{F_1 + F_2}{V_p}\left(T_{p_in} - T_p\right) + \frac{h_p A_p}{\rho_p V_p C p_p}\left(T_w - T_p\right) \\
&\quad + \frac{\Delta H r_j}{\rho_p C p_p} k_j^0 \exp\left(-\frac{E_j^a}{R\left(T_p + 273.15\right)}\right) C_1 C_2 \\
\dot{T}_u &= \frac{F_u}{V_u}\left(T_{u_in} - T_u\right) + \frac{h_u A_u}{\rho_u V_u C p_u}(T_w - T_u) \\
\dot{T}_w &= \frac{h_p A_p}{\rho_p V_p C p_p}\left(T_p - T_w\right) + \frac{h_u A_u}{\rho_u V_u C p_u}(T_u - T_w) \\
\dot{C}_1 &= \frac{F_1 + F_2}{V_p}\left(C_{1_in} - C_1\right) - 2k_j^0 \exp\left(-\frac{E_j^a}{R\left(T_p + 273.15\right)}\right) C_1 C_2 \\
\dot{C}_2 &= \frac{F_1 + F_2}{V_p}\left(C_{2_in} - C_2\right) - 4k_j^0 \exp\left(-\frac{E_j^a}{R\left(T_p + 273.15\right)}\right) C_1 C_2
\end{aligned} \tag{1}$$

where state vector is $x = \left[T_p\ T_u\ T_w\ C_1\ C_2\right]^T$. T, C represent temperature (°C) and concentration (mol m^{-3}). The index p, u, w represent process plate, utility plate and plate wall. The initial temperature T_{p_in}, T_{u_in} and T_w are 17.6, 39.7 and 25 °C. Inlet concentrations of reactants C_{1_in} and C_{2_in} are both set at 9% in mass. 1 and 2 represent the reactants $Na_2S_2O_3$ and H_2O_2 respectively. The input vector $u = \left[F_1\ F_2\ F_u\right]^T$, stands for volumic flow-rate (m^3 s^{-1}) of the reactants and utility fluid. Input vector is fix at $\left[2.5833 \times 10^{-6}, 1.3056 \times 10^4, 3.1389 \times 10^{-5}\right]^T$. Output $y = T_p^k$ is the outlet temperature. ρ (kg m^{-3}), V (m^3), A (m^2) and Cp (J kg^{-1} K^{-1}) are density, volume, heat exchange area and specific heat of material respectively. The index $\boldsymbol{j}$ stands for reaction $\boldsymbol{j}$. ΔHr (J mol^{-1}) is the heat generated. k^0 (mol m^{-3} s^{-1}) is pre-exponential factor. E^a (J mol^{-1}) is activation energy. R (J mol^{-1} K^{-1}) is perfect gas constant. For the reaction concerned, $\Delta Hr = 5.86 \times 10^5, k^0 = 8.13 \times 10^8, E^a = 7.6123 \times 10^4, R = 8.314$. For the given HEX/Reactor, heat transfer process is divided in two parts: one is the convective heat exchange between process channel and plate wall, the other is between utility channel and plate wall. The nominal values of heat transfer coefficients (J m^{-2} K^{-1} s^{-1}) are $\left[h_p\ h_u\right]^T = \left[1.0636 \times 10^4, 1.1426 \times 10^3\right]^T$.

3 Fault Detection and Diagnosis Scheme

3.1 Description of the Proposed FDI Method

For the intensified HEX/Reactor, a bank of observers is constructed to generate a bank of residuals. One of the observers serves as the detection and isolation observer. Once the residual exceeds to threshold, the procedure of fault identification is triggered by an alarm of fault. Then, other q observers, corresponding to q different fault types and values, act as interval filters to generate several residuals aiming at identifying the fault.

3.2 High Gain Observer Design

The model proposed in Eq. (1) is shortly express as:

$$\begin{aligned} \dot{x} &= f(x,\theta) + g(x)u \\ y &= h(x,\theta) \end{aligned} \tag{2}$$

where $\theta = \left[h_p^k \ h_u^k \right]^T$ is the parameter vector. $f(\cdot)$, $g(\cdot)$ and $h(\cdot)$ are smooth vector fields, their first partial derivatives on x and θ are continuous, bounded, Lipschitz in x and θ. In order to estimate all of the states in the presented model (2), a high gain observer presented in [21] is designed as follows:

$$\begin{aligned} \dot{\hat{x}} &= f\big(\hat{x},\theta^{0b}\big) + g\big(\hat{x}\big)u - \Phi^{*-1}\big(\hat{x},\theta^{0b}\big)\Delta_\theta K_0\big(\hat{y}-y\big) \\ \hat{y} &= h\big(\hat{x},\theta^{0b}\big) \end{aligned} \tag{3}$$

where y is the output vector of the system (2), $\hat{y}$ is the output vector of the observer. $\hat{x}$ is the observer state vector, θ^{0b} is the observer parameter vector, $\Phi^{*-1}\big(\hat{x}\big)$ is the inversion of the Jacobian matrix of the nonlinear change of coordinates $\Phi(x(t)) = \left[h(x(t)) \ L_f h(x(t)) \ \ldots \ L_f^{n-1} h(x(t)) \right]^T$. $L_f h(x)$ is the Lie derivative of $h(\cdot)$ along $f(\cdot)$. $\Delta_\theta = diag\left[\theta \ \theta^2 \ \ldots \ \theta^n\right]$, θ is an arbitrary positive constant. $K_0 = \left[k_1 \ k_2 \ k_3 \ k_4 \ k_5\right]^T$ is the observer gain. It is calculated by $K_0 = S^{-1}C_0^T$, where S is a symmetric positive definite matrix which satisfies the algebraic Lyapunov equation $A_0^T S + S A_0 + S - C_0^T C_0 = 0$, with $A_0 = \begin{bmatrix} 0_{4\times1} & I_{4\times4} \\ 0_{1\times1} & 0_{1\times4} \end{bmatrix}$, $C_0 = \left[1 0_{1\times4}\right]$, I represents identity matrix. The estimation error $e_x = \hat{x} - x$ of the observer (3) is globally uniformly convergent to zero when $t \to \infty$ in the absence of uncertainties. Furthermore, the convergence is exponential.

Define that:

$$e_y = \hat{y} - y \tag{4}$$

$$r_y(t) = \frac{d\|e_y\|}{dt} = \frac{d\|\hat{y} - y\|}{dt} \tag{5}$$

As long as the norm of the residual vector $r_y(t)$ exceeds the suitable threshold $supr_y(t)$, a fault is detected. According to the different performance of $r_y(t)$, the fault is isolated.

3.3 Fault Identification

When a fault is detected and isolated, a procedure of fault identification is triggered. The practical domain of the value of each system parameter is partitioned into several intervals as in [14]. For instance, parameter θ_j is divided into q intervals, where the value of the faulty parameter is contained in one of the intervals, their bounds are presented by: $\theta_j^0, \theta_j^1, \ldots, \theta_j^i, \ldots, \theta_j^q$. The boundaries of the ith interval are θ_j^{i-1} and θ_j^i, which is also denoted by θ_j^{ai} and θ_j^{bi}. In this paper, the boundary of each interval is calculated by the percentage changes of the nominal value, rather than an accurate value of the parameter. To verify if the faulty parameter is contained in an interval, a parameter interval filter, which is consisted of two observers corresponding to upper and lower bounds, is built for this interval. Each observer serves two neighboring intervals. To illustrate this procedure, the ith interval of parameter θ_j is discussed. Considering the model (2), the parameter filter for the ith interval $\left[\theta_j^{ai}, \theta_j^{bi}\right]$ of parameter θ_j is given as follows:

$$\begin{aligned} \dot{\hat{x}}_j^{ai} &= f\left(\hat{x}_j^{ai}, \theta_j^{oba}\right) + g\left(\hat{x}_j^{ai}\right)u - \Phi^{*-1}\left(\hat{x}_j^{ai}, \theta_j^{oba}\right)\Delta_\theta K_0\left(\hat{y}_j - y\right) \\ \hat{y}_j^{ai} &= h\left(\hat{x}_j^{ai}, \theta_j^{oba}\right) \end{aligned} \tag{6}$$

$$\begin{aligned} \dot{\hat{x}}_j^{bi} &= f\left(\hat{x}_j^{bi}, \theta_j^{obb}\right) + g\left(\hat{x}_j^{bi}\right)u - \Phi^{*-1}\left(\hat{x}_j^{bi}, \theta_j^{obb}\right)\Delta_\theta K_0\left(\hat{y}_j - y_j\right) \\ \hat{y}_j^{bi} &= h\left(\hat{x}_j^{bi}, \theta_j^{obb}\right) \end{aligned} \tag{7}$$

where $\theta_j^{oba} = \begin{cases} \theta_j^0, & t < t_f \\ \theta_j^a, & t > t_f \end{cases}$, $\theta_j^{obb} = \begin{cases} \theta_j^0, & t < t_f \\ \theta_j^b, & t > t_f \end{cases}$, fault occurs at $t = t_f$.

Define the identification index of this parameter filter: $v_j^i(t) = sgn\left(\varepsilon_j^{ai}\right)sgn\left(\varepsilon_j^{bi}\right)$, where $\varepsilon_j^{ai} = \hat{y}_j^{ai} - y$, $\varepsilon_j^{bi} = \hat{y}_j^{bi} - y$. When the fault occurs, if the value of faulty parameter is contained in $\left[\theta_j^{ai}, \theta_j^{bi}\right]$, $v_j^i(t)$ should equal to -1 after a short transient time, and fault signature sends 1. Oppositely, if $v_j^i(t)$ remains 1, the faulty parameter is not contained in this interval, and the corresponding fault signature sends 0. If the fault lies in the ith interval, the value of the estimated faulty parameter is obtained by:

$$\hat{\theta}_j = \frac{1}{2}\left(\theta_j^{ai} + \theta_j^{bi}\right) \tag{8}$$

4 Simulation Results and Discussion

To validate the effectiveness of the proposed approach, a case study is developed in this paper. All related experimental data is given in [20], and the normal values of the operating conditions used in simulation are presented in Table 1 and Sect. 2.

In this study, two kinds of process faults are considered, the deviation of h_p or h_u from their nominal values. Temperature of the outlet process fluid is assumed to be the only available measurement and the only criteria of fault diagnosis.

As shown in Table 2, the dividing rule of an interval is according to the percentage variation of the nominal value. The limited range of interval for heat transfer coefficient is [100%, 20%], i.e., the value of the faulty parameter decreases from the nominal value to 20% of the nominal value. Since it takes about 230 s for the HEX/Reactor to achieve its thermal equilibrium, the fault is introduced at t = 250 s. The heat transfer coefficient decreases to 70% of the nominal value. Residuals generated by detection observers are shown in Fig. 3. For the studied model, the reduction

Table 1 Physical data of the pilot

Constant	Description	Value	Units
V_p	Volume of process plate	2.68×10^{-5}	m^3
ρ_p, ρ_u	Density of process/utility plate	10^3	kg m^{-3}
Cp_p, Cp_u	Specific heat of process/utility plate	4.186×10^3	J kg^{-1} K^{-1}
A_p	Heat exchange area of process plate	2.68×10^{-2}	m^2
V_u	Volume of utility plate	1.141×10^{-4}	m^3
A_u	Heat exchange area of utility plate	4.564×10^{-1}	m^2
V_w	Volume of plate wall	1.355×10^{-3}	m^3
ρ_w	Density of plate wall	8×10^3	kg m^{-3}
Cp_w	Specific heat of plate wall	5×10^2	J kg^{-1} K^{-1}

Table 2 Interval bounds for heat transfer coefficients

No. of interval	1	2	3	4	5
h_p (%)	100	80	60	40	20
h_u (%)	100	80	60	40	20

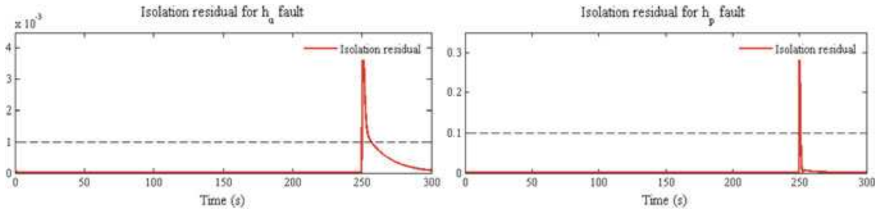
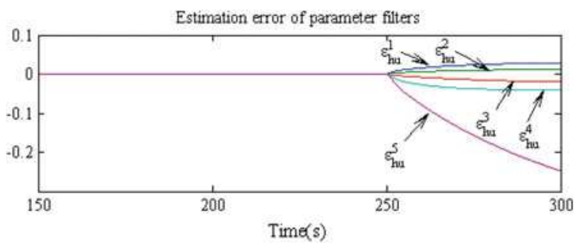


Fig. 3 Isolation residual for heat transfer coefficient h_u (*left*) and h_p (*right*)

of h_p has an influence on heat exchange between process plate and plate wall, which affects the temperature of process fluid directly. The decrease of h_u influences the heat exchange between utility plate and plate wall, and further affects process fluid temperature indirectly by heat exchange procedure, i.e., output temperature changes slightly as a fault occurs on h_u, while it changes greatly as a fault occurs on h_p. Therefore, the residual vector $r_y(t)$ in Eq. (5) performs differently. Then, the thresholds vary according to the type of fault. In the studied case, when the faulty parameter is h_p, the threshold is much bigger than that of a fault occurs of h_u. When a fault happens, residual goes over the corresponding threshold, and the fault is detected. Moreover, the fault is isolated by the performance of residual vector $r_y(t)$.

Once the fault is detected and isolated, a bank of parameter interval filters begins to work to identify the exact value of the faulty parameter. When h_u changes, the corresponding estimation error of each parameter filter is shown in Fig. 4. It is obviously that $v_{hu}^2(t) = sgn\left(\varepsilon_{hu}^2\right)sgn\left(\varepsilon_{hu}^3\right) = -1$, i.e. faulty parameter stays in interval 2. The performances of fault signatures are shown in Fig. 5. Since both the faulty parameters are defined as 70% of their nominal value, the fault signature 1 is sent by interval 2 at about t = 251 s, whose bounds are 80% of nominal value and 60% of nominal value. Other fault signatures stay at 0, which means the faulty parameter is not contained in these intervals. Then, the value of faulty parameter is identified by the upper and lower bounds of interval 2: $\hat{h}_u = \frac{1}{2}(80\% + 60\%) \times h_u$, $\hat{h}_p = \frac{1}{2}(80\% + 60\%) \times h_p$. Even though there exists estimation errors, they can be narrowed by diving in more intervals.

Fig. 4 Estimation error of each parameter filter when h_u is faulty



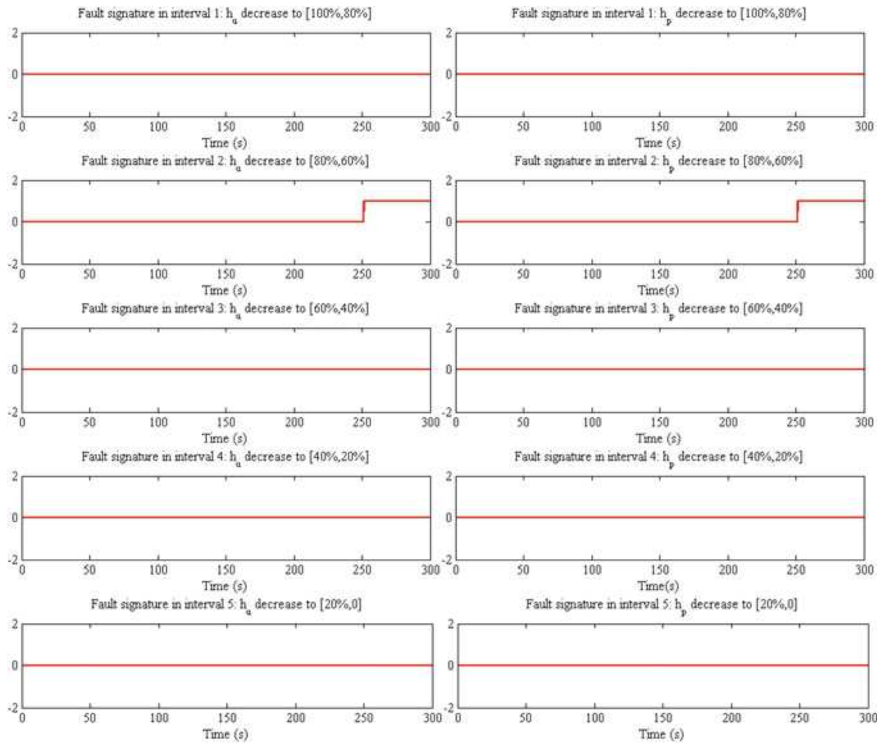


Fig. 5 Fault signatures sent by parameter filters of h_u (*left*) and h_p (*right*)

5 Conclusion

In this paper, a model-based FDI approach is applied to an intensified HEX/Reactor with an exothermic reaction taken place in. High gain observer is constructed to serve as detection and isolation observer for process fault detection and isolation. When a fault is detected, identification procedures are triggered. A bank of intervals is divided according to the value of the process parameters. And interval filters are designed to provide fault identification. Then, the presented FDI method is applied to an intensified HEX/Reactor. The effectiveness of the proposed approach is confirmed by the simulation results. Moreover, the ideal isolation speed and the estimation value of the faulty parameter provide support for the following controller reconfiguration in fault tolerant control system.

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