Robust Nonlinear Fault Detection Applied to Chemical Processes

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Abstract—This paper proposes a robust fault detection system that can be applied to nonlinear chemical processes. A nonlinear state estimator which is able to handle both parameter estimation and parameters with uncertainties is designed. The detection process is created by examining changes in the controlled outputs with respect to set point, followed by probing variations in the parameters that are estimated. A steam generator system is used to validate this approach where a process fault is considered.

I. INTRODUCTION

A successful model-based fault diagnosis technique depends on a sufficiently accurate model of the system. Uncertainties in the model lead to false alarms or failures in detection. These issues make applying model-based techniques to nonlinear processes difficult. The majority of chemical processes have many uncertainties in their parameters due to their complexity. Research that addresses this problem consists of designing observers capable of parameter estimation [1]. However, restrictions surrounding the observability of these parameters limit this approach. Examples of chemical applications that use nonlinear fault diagnosis found in the literature are: CSTR [2], distillation columns [3] and polymerization reactors [4].

Model-based fault diagnosis techniques are typically divided into three main parts [5]: (1) fault detection, which determines the presence of faults in the system and the time of detection; (2) fault isolation, where the nature and location of the fault is determined; (3) fault identification, which determines the size and time-variant behavior of the fault. This paper focuses on the design of a robust fault detection (RFD) system that can be applied to nonlinear chemical processes by using a state estimator capable of dealing with both bounded uncertainties and estimation of the model parameters. Traditionally, the fault detection mechanism is based on detecting abnormal changes between an observer, or state estimator estimates, and the measured signals from the plant. One disadvantage of this approach is that once faults are detected, the observer is not able to follow the behavior of the faulty system. When the nonlinear system has to operate in closed-loop control, the observer may be unnecessary, since the faults can be detected when the controlled outputs are unable to follow the trajectory of the set points. In the new approach proposed here, where the state estimator is able to follow the faulty system, the mechanism of detection is based on detecting both the abnormal deviations between the controlled outputs and the set point trajectories and the variations of the estimated parameters from their normal values. Current robust fault detection techniques that deal with parameter uncertainty are based on the sliding mode concepts in which sliding observers are formulated for restrictive nonlinear systems. Examples of these fault detection techniques based on residual generation can be found in [6], [7] and [8]. Also, linear sliding observers are used in [9] by transforming the nonlinear model. In this paper, the sliding mode concepts are applied to deal with the bounded uncertainties of some parameters of the model that cannot be estimated and to simplify the complexity of the fault free model with algebraic nonlinear functions that have bounded uncertainty in its parameters.

The paper is organized as follows: the second section presents a brief description of a steam generator system followed by a brief analysis of the main characteristics of its dynamic model. The third section presents the fault detection system in which an algorithm for the nonlinear state observer is presented. Next, in the fourth section, the model-based technique is validated using a steam generator model with simulations during normal operation and under a process fault. Comparisons with both an extended Kalman filter (EKF) and Moving Horizon Estimation (MHE) are presented. Finally, the conclusions of this paper are contained within the fifth section.

II. STEAM GENERATOR PROCESS

A. Brief Description of the Process

Figure 1 shows the P&ID diagram of the steam generator. This model is used in applications of fault diagnosis [5], [10]. Modifications have been carried out in the control system, where PI controllers are used instead of on/off controllers, and in the nonlinear thermodynamical properties listed in the Appendix.

This paper focuses on the dynamic of the boiler, which possesses the more severe nonlinearities. The boiler system has four inputs: (1) the flow of feed water, $F_{AL}$ [kg/s], which is proportional to the opening of the control valve $V_1$; (2) the heater control signal $u_{TH}$; (3) the steam flow in the boiler output, $F_{GV}$ [kg/s], which is proportional to the opening of the control valve $V_2$; (4) the temperature of the feed water,
$T_{AL}$ [°C]. Three measurable outputs are considered: (1) the water volume of the boiler, $L$ [l]; (2) the pressure in the boiler $P_{GV}$ [bar]; (3) the temperature of the metal body of the boiler, $T_{MG}$ [°C]. The system’s model contains three state variables: (1) the mass of the water-steam mixture in the boiler, $M_{GV}$ [kg]; (2) enthalpy in the boiler, $H_{GV}$ [J]; (3) the temperature of the metal body of the boiler, $T_{MG}$ [°C]. Two PI controllers maintain the pressure and level in the boiler within a desired range. The pressure in the boiler is controlled by manipulating the thermal resistor, which has a maximum power of 55 [KW], while the level in the boiler is controlled by operating the control valve $V_1$, which transfers water from the storage tank. Additionally, the steam flow is controlled by using control valve $V_2$ which is operated in manual mode. The differential equations that represent the behavior of the boiler are:

$$rac{dM_{GV}}{dt} = F_{AL} - F_{GV}$$

$$rac{dH_{GV}}{dt} = u_{TH} P_{TH} + c_{pe} T_{AL} F_{AL} + V \frac{dP_{GV}}{dt} - F_{GV} h_v - K_{GM} (T_{GV} - T_{MG})$$

$$T_{MG} = C_{GM} (K_{GM} (T_{GV} - T_{MG}) - K_{ex} (T_{MG} - T_{ex}))$$

$$y(t) = [(1 - X) M_{GV} v_L P_{GV} T_{MG}]^T$$

where the parameters ($V$, $C_{pe}$, $P_{TH}$, $K_{GM}$, $K_{ex}$, $C_{GM}$ and $T_{GV}$) and the thermodynamical properties ($h_{GV}$, $v_{GV}$, $h_L$, $h_v$, $v_L$ and $v_{GV}$) are defined in the Appendix. The polynomials of the thermodynamical properties were fitted by using the data provided by the International Association for the Properties of Water and Steam (IAPWS) [11].

The outputs of the model are given by equation 4. Also, equations 5 and 6 are used to model the two-phase water-steam mixture. By using these equations, both the pressure $P_{GV}$ of the boiler and the steam quality $X$ are obtained by solving the polynomials of equations 7 and 8 respectively.

$$h_{GV} = \frac{H_{GV}}{M_{GV}} = h_v (P_{GV}) \cdot X + h_L (P_{GV}) \cdot (1 - X)$$

$$v_{GV} = \frac{V}{M_{GV}} = v_v (P_{GV}) \cdot X + v_L (P_{GV}) \cdot (1 - X)$$

$$(h_{GV} - h_L) (v_v - v_L) - (v_{GV} - v_L) (h_v - h_L) = 0$$

$B$. Characteristics of the Nonlinear Process

The previous subsection presents three interesting characteristics of the nonlinear model. The first characteristic is related to the modeling of the water-steam mixture, where the thermodynamical properties are used in equations 5 and 6. Figure 2 shows a typical trajectory of the boiler pressure, $P_{GV}$, which is obtained by solving the polynomial given in equation 7. Based on this pressure trajectory, that is the function of the state variables $M_{GV}$ and $H_{GV}$, a noninvertible characteristic can be found. For instance, if the pressure of the boiler is 7.5 [bar], (grey plane shown in Figure 2) then the pressure value can be obtained from three different values in the state variables, $M_{GV}$ and $H_{GV}$. This fact makes it very difficult to derive a nonlinear function that approximates the trajectory of the pressure in terms of the state variables. Therefore, it is a formidable task to analyze the properties of the model, such as observability and controllability, while also using the model as a state estimator.

The second characteristic is related to the uncertainty of some parameters of the model. For instance, in equations 2 and 3, the parameters $K_{GM}$ and $K_{ex}$ are difficult to determine. As a result, errors in the prediction of outputs can lead to false alarms. Finally, the third characteristic is related to the stability of the system. Equation 1 of the system is unstable in open loop, forcing the system to be analyzed under closed-loop control. This violates causality assumptions in system identification [12], [13].

III. FORMULATION OF THE ROBUST FAULT DETECTION SYSTEM

Figure 3 illustrates the architecture of the robust fault detection system. This system is divided into two components: a discrete robust observer and a fault detector. In order to deal with bounded uncertainties in the parameters of the model, the discrete observer is based on the sliding observers theory [14] whereby it is demonstrated that the robust performance of these type of observers is possible in the presence of
parameter inaccuracies. The sliding observer is designed such
that it drives the states to a particular surface, called the
sliding surface. Once this surface has reached the sliding
motion, which is generated by using a switching function, it
is ensured that the states will remain close to the surface.
The sliding observer is based on the linear Utkin
observer [14], which has been extended to nonlinear systems.
Furthermore, the observer proposed also allows parameter
estimation wherein an extended Luenberger observer in
combination with the sliding motion guarantee a robust
estimation.

The nonlinear model, presented in Section II, can be
formulated as a differential algebraic equation (DAE) which
is summarized in equations 9 through 11.

\[
\frac{dx}{dt} = f(x,u,\theta,p_d,q) \tag{9}
\]

\[
q(\theta,p_d) = 0 \tag{10}
\]

\[
y = h(x,\theta,p_d,q) \tag{11}
\]

where:
- \( f(\cdot) \) is the nonlinear state equation function
- \( q(\cdot) \) is a nonlinear function that can be used in equa-
tions 9 and 11
- \( h(\cdot) \) is the nonlinear output function
- \( p_d \) are the parameters that cannot be estimated and these
  are defined as \( p_d = \bar{p}_d + \delta p_d \). Each of these parameters
  are assumed to have bounded uncertainty defined by
  \( |\delta p_d| \leq \varepsilon \)
- \( \theta \) are bounded parameters that can be estimated by
  the observer. The parameters are assumed fixed (not
time-variant) but unknown. The maximum limits of
these parameters are defined by \( \theta_{\text{min}} < \theta < \theta_{\text{max}} \).

As the observer executes parameter estimation, the state
variables are augmented with the estimated parameters, \( \theta \),
\( \tilde{x} = [x\quad \theta]^T \). Thus, equations 12 through 15
become equations 12 through 11.

\[
\frac{d\tilde{x}}{dt} = \tilde{f}(\tilde{x},u,p_d,q) \tag{12}
\]

with
\[
\tilde{f}(\tilde{x},u,p_d,q) = \begin{bmatrix} f(x,u,\theta,p_d,q) \ 0 \end{bmatrix}^T \tag{13}
\]

\[
q(\tilde{x},p_d) = 0 \tag{14}
\]

\[
y = h(\tilde{x},p_d,q) \tag{15}
\]

A simple discrete version of these equations can be written
as follows:

\[
\tilde{x}_k = \tilde{x}_{k-1} + T_s \cdot \tilde{f}(\tilde{x}_{k-1}, u_{k-1}, p_d, q) \tag{16}
\]

\[
q(\tilde{x}_{k-1}, p_d) = 0 \tag{17}
\]

\[
y = h(\tilde{x}_{k-1}, p_d, q) \tag{18}
\]

where \( T_s \) is the sample time.

A. Robust Observer Algorithm

The prediction of the states can be achieved by using the
following algorithm at each time step:

Step 1: Approximate values of the state vector \( \tilde{x}_{k-1} \)
are obtained by using both the value of the a priori state estimate
\( \hat{x}_{k-1} \) and equation 16.

\[
\tilde{x}_k = \hat{x}_{k-1} + T_s \cdot \tilde{f}(\hat{x}_{k-1}, u_{k-1}, p_d, q) \tag{19}
\]

Step 2: Estimates of measurement vector \( \hat{y}_k \)
are obtained by replacing equation 19 in equation 18.

\[
\hat{y}_k = h(\tilde{x}_k, p_d, q) \tag{20}
\]

Step 3: The nonlinear state equation and output functions
are linearized around the current estimated state, \( \tilde{x}_{k-1} \), as in
equations 21 and 22.

\[
A_{[i,j]} = \frac{\partial f_{i}}{\partial x_{j}} \bigg|_{\tilde{x}_{k-1},u_{k-1}} \quad A \in \mathbb{R}^{nxn} \tag{21}
\]

\[
C_{[i,j]} = \frac{\partial h_{i}}{\partial x_{j}} \bigg|_{\tilde{x}_{k-1},u_{k-1}} \quad C \in \mathbb{R}^{pxn} \tag{22}
\]

Thus, the linear nominal system, at each time step, can be
written as in equation 23 whereby non-external disturbances
are considered.

\[
x_k = Ax_{k-1} \tag{23}
\]

\[
y_k = Cx_k
\]

Step 4: The gains that are used in the proposed nonlinear
state estimator are calculated in this step. These gains are
computed based on the linearized model of equation 23
which is obtained at each time step. The state estimator in
the linear domain has the following form:

\[
\tilde{x}_k = A\tilde{x}_{k-1} + K_k e_{k-1} + T_c^{-1} \begin{bmatrix} -L_k \hat{y}_k \\ \hat{y}_k \end{bmatrix} \tag{24}
\]

\[
\hat{y}_k = Cx_k
\]

where \( K_k \) corresponds to the Luenberger gain and \( L_k \) is the
sliding gain. Further details of equation 24 will be presented
below. The errors \( e_{yk} \), which is the difference between
the measurement vector \( y_k \) and the estimates of the outputs.
\( \hat{y}_k \) and \( e_{x_k} \), the difference between the true states \( x_k \) and estimates \( \hat{x}_k \), are defined in equations 25 and 26 respectively.

\[
\begin{align*}
   e_{y_k} &= y_k - \hat{y}_k \\
   e_{x_k} &= x_k - \hat{x}_k
\end{align*}
\]

\( K_k \) is determined such that the eigenvalues of the error \( e_{x_k} \), given by equation 27, have strictly negative real parts. This error is derived by using equations 23, 24 (without considering the contribution of the sliding term), 25 and 26.

\[
e_{x_k} = (A - K_k C)e_{x_{k-1}}
\]

In order to obtain the sliding gain \( L_k \), a sliding surface, \( S(t) \), is defined as follows:

\[
S(t) = \{ \hat{x}_k \in \mathbb{R}^n : e_{y_k} = 0 \}
\]

The matrix \( A \) of equation 23 is transformed such that the error \( \chi_{k-1} \) becomes:

\[
\begin{bmatrix}
   \hat{z}_k \\
   \hat{y}_k
\end{bmatrix} =
\begin{bmatrix}
   A_{11} & A_{12} \\
   A_{21} & A_{22}
\end{bmatrix}
\begin{bmatrix}
   \chi_{k-1} \\
   \hat{y}_{k-1}
\end{bmatrix} + T_c K_k e_{y_k} + \begin{bmatrix}
   -L_k y_k \\
   v_k
\end{bmatrix}
\]

where each row of the discontinuous vector \( v_k \in \mathbb{R}^{n \times 1} \), in which \( p \) corresponds to the number or measurable outputs, is defined by:

\[
v_i = M_i \text{sign}(y_i - \hat{y}_i) \quad i = 1, ..., p
\]

\( M_i \) is chosen in order to match all the bounded uncertainties that were defined in the model parameters.

Equation 31 shows the error between the transformed estimates and true states.

\[
\begin{bmatrix}
   e_{y_k} \\
   e_{\chi_k}
\end{bmatrix} =
\begin{bmatrix}
   A_{11} & A_{12} \\
   A_{21} & A_{22}
\end{bmatrix}
\begin{bmatrix}
   e_{\chi_{k-1}} \\
   e_{\hat{y}_{k-1}}
\end{bmatrix} + T_c K_k e_{y_k} - \begin{bmatrix}
   -L_k y_k \\
   v_k
\end{bmatrix}
\]

After some finite time when the states have reached the sliding surface, as defined by equation 28, the errors \( e_{y_{k-1}} \) and \( e_{\chi_k} \) become 0. Equation 31 then reduces to:

\[
e_{\chi_k} = (A_{11} - L_k A_{21}) e_{\chi_{k-1}}
\]

The matrix \( L_k \in \mathbb{R}^{(n-p) \times p} \) is obtained such that the eigenvalues of equation 32 have strictly negative real parts.

**Step 5:** A posteriori estimate \( \tilde{x}_{k} \), or a correction of the values \( \chi_{k-1} \), is obtained by using equation 33 that is similar to the observer model presented in equation 24. However, the difference lies in the error of the outputs \( e_{\hat{y}_k} \), which is defined as the difference between the measurement vector \( y_k \) and the approximate measurement vector \( \hat{y}_k \) obtained in step 2.

\[
\tilde{x}_k = \hat{x}_k + K_k e_{\hat{y}_k} + T_c^{-1} \begin{bmatrix}
   -L_k y_k \\
   v_k
\end{bmatrix} e_{\hat{y}_k}
\]

The gains \( K_k \) and \( L_k \) are calculated by using equations 27 and 32. Finally, the states that correspond to the parameters of the model are verified such that they are inside the limits defined previously.

**B. Fault Detector System**

As it is shown in Figure 3, to perform the detection of the process fault, differences in the controlled variables with set point trajectories are verified, followed by an examination of the changes in the parameter values that were estimated from the normal operation trends. This procedure will be clarified in Section IV.

**IV. Simulation Results**

Figure 4 shows the pressure and volume trajectories of the boiler respectively, where random noise has been included in solving the model formulated in equations 1 through 8. Four steps are used to define the model for the robust observer. First, instead of using equation 7, which is a high order polynomial, an explicit function that solves for the pressure \( P_{GV} \) is defined as in equation 34 and corresponds to the function \( q \) defined in 14. Second, an observability analysis is done in order to define the parameters of the nonlinear model that can be estimated. For this model \( K_{GM} \) and \( K_{ex} \) were the parameters selected. Third, the maximum values of these parameters are defined in equations 35 and 36. Finally, both the bounded uncertainties of the parameters that are not able to be estimated and \( M_i \) values are defined.

\[
P_{GV} = b_1 + b_2 M_{GV} + b_3 H_{GV}
\]

In equation 34, the parameters \( b \) are defined as \( b = [11.96, -0.23, 2.78e^{-7}]^T \) with the following bounded uncertainties: \( |\delta b_1| \leq 4 \), \( |\delta b_2| \leq 0.1 \) and \( |\delta b_3| \leq 1e^{-07} \). The value of \( M_i \) of equation 30 will be estimated have the following limits:

\[
0 \leq K_{ex} \leq 10
\]

\[
0 \leq K_{GM} \leq 2100
\]

Figure 5 shows the estimate of the pressure \( P_{GV} \) where the mean absolute percentage error (MAPE), defined in equation 37, obtained was 1.53 [%]. The blue (thick) line
represents the real trajectory of the pressure, which is obtained by solving equations 1 through 8. The red (thin) line has an oscillatory trajectory around the operation points of pressure, which represent the sliding motion of the observer. The green (dash) line corresponds to the estimated trajectory of pressure which is a filtered version of the oscillatory red line.

\[ MAPE = \left| \frac{Y_{\text{real}} - \hat{Y}}{Y_{\text{real}}} \right| \times 100\% \quad (37) \]

Figure 6 shows the estimated trajectory of parameter \( K_{ex} \). The black (thick) line is the estimated parameter, which results from filtering the oscillatory trajectory given by the red (thin) line trajectory. Because of the sliding motion, the oscillation presented is within the limits defined previously in equation 35 for this parameter.

A gas leak is introduced in the system at \( t = 1,000 \text{ [s]} \). Figure 7 shows the estimated trajectories. As a result of the fault, the pressure value, blue (thick) line, falls at \( t = 1,000 \text{ [s]} \) and separates from the set point trajectory. The observer is able to follow the pressure trajectory, green (dash) line, with a MAPE error equal to 2.17 [\%].

Figure 8 shows the coefficient \( K_{ex} \) trajectory, black (thick) line, in the presence of a gas leak fault. In this case, changes in the value of this coefficient from the nominal value have occurred and the fault is detected as a result. The fault is first detected from the deviation of the pressure values to the set point trajectory and then verified once changes in the parameter value have been detected. The fault is detected at \( t = 1,085 \text{ [s]} \).

Finally, Figure 9 shows the pressure estimates of both an extended Kalman filter (EKF), red (dash) line, and a Moving Horizon Estimation filter (MHE), black (thick) line, without parameter estimation. The performance of these filters are evaluated under the gas leak case. Before the fault occurs, the trajectories of the pressure estimates have bigger errors than the estimates of the proposed robust observer (shown in Figure 7), stemming from the approximation of the pressure function defined in equation 34.
The average heat capacity of the metal,

\[ v = \frac{1}{\rho c_p} \]

The specific heat of the feedwater flow,

\[ m_{\text{metal}} \]

The geometric volume of the boiler,

\[ \text{Volume} = \frac{V_{\text{boiler}}}{\rho} \]

The mixture to the metal body of the boiler,

\[ \text{Mixture} = \frac{m_{\text{mixture}}}{\rho_{\text{mixture}}} \]

To detect process faults by using the non-faulty (nominal) model. Finally, this approach was validated by using a steam process factor approach to closed-loop identification, "International Journal of Chemical Reactor Engineering, vol. 6, pp. 801–818, 2008.

Therefore, these parameter estimations cannot be used to detect faults.

V. CONCLUSIONS

A robust fault detection system, by using the normal operation model, was designed. The state estimator is based on the theory of sliding modes combined with the extended Luenberger observer. As a result, this estimator is capable of dealing with bounded uncertainties in the parameters of the model as well as parameter estimation in presence of noise. The changes in the parameter values can be used to detect process faults by using the non-faulty (nominal) model. Finally, this approach was validated by using a steam generator model.

APPENDIX

PARAMETERS AND THE THERMODYNAMICAL PROPERTIES OF THE STEAM GENERATOR

\[ K_{GM} \]

\[ K_{C0} \]

\[ h_{GV} \]

\[ v_{GV} \]

\[ T_{GV} \]

The temperature of the boiler, \( T_{GV} \) [°C], is

\[ T_{GV} = -8.569e^{-3} P_{GV}^2 + 0.336 P_{GV} - 4.805 P_{GV}^3 \\
+ 34.357 P_{GV} + 65.533 \]

The specific enthalpy of liquid, \( h_L \) [kJ/kg], is

\[ h_L = -3.578e^{-2} P_{GV}^4 + 1.402 P_{GV} - 20.077 P_{GV}^2 \\
+ 144.7 P_{GV} + 273.96 \]

The specific enthalpy of steam, \( h_v \) [kJ/kg], is

\[ h_v = -4.068e^{-4} P_{GV}^3 + 2.205e^{-2} P_{GV}^2 - 0.472 P_{GV} \\
+ 5.094 P_{GV}^2 - 29.552 P_{GV} + 96.438 P_{GV} + 2599.3 \]

The specific volume of liquid, \( v_L \) [m³/kg], is

\[ v_L = -3.591e^{-7} P_{GV}^2 + 1.246e^{-5} P_{GV} + 1.039e^{-3} \]

The specific volume of steam, \( v_v \) [m³/kg], is

\[ v_v = -3.290e^{-5} P_{GV}^3 + 1.600e^{-3} P_{GV} - 3.008e^{-2} P_{GV} \\
+ 0.271 P_{GV} - 1.211 P_{GV} + 2.489 \]

REFERENCES


