Detection of Abrupt Changes of Total Least Squares Models and Application in Fault Detection

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***Abstract*—This paper is concerned with detection of parameter changes of total least squares and generalized total least squares models and its application in fault detection and isolation. Total least squares and generalized total least squares are frequently used to model processes when all measured process variables are corrupted by disturbances. It is therefore of practical interest to monitor processes and detect faults using the total least squares and generalized total least squares as well. The local approach for detection of abrupt changes is adopted in this paper as a computational engine for the change detection. The effectiveness and robustness of the proposed algorithm in fault detection and isolation are demonstrated through Monte Carlo simulations, a pilot-scale experiment and sensor validation of an industrial distillation column.**

***Index Terms*—Detection of abrupt changes, fault diagnosis, least squares methods, maximum likelihood detection, singular value decomposition.**

I. INTRODUCTION

THE PROBLEM of linear parameter estimation arises in a broad class of scientific disciplines such as signal processing, automatic control, system theory, general engineering, statistics, physics, economics, biology, medicine, etc. [1]. It starts from a linear (in-parameter) model

$$X_n^T l^{(0)} = 0 \tag{1}$$

where $X_n = [x_1(n), x_2(n), \ldots, x_p(n)]^T$ denotes the process variables that can be measured or can be inferred from other measurements or can be calculated from a nonlinear transformation; all variables are subject to measurement noise; $l^{(0)} = [\beta_1, \beta_2, \ldots, \beta_p]^T$ contains the parameters that characterize the underlying relationship of the process variables.

A basic problem of the estimation is to determine an estimate of the true but unknown parameters vector $l^{(0)}$ from certain measurements $X_1, X_2, \ldots, X_N$. This gives rise to an overdetermined set of N equations

$$\mathcal{X} l^{(0)} = 0$$

where $\mathcal{X} \in R^{N\times p}$ is a matrix that consists of these measurements. It is well known [2], [3] that if the matrix $\mathcal{X}^T\mathcal{X}$ is semi-positive definite, then its eigenvector corresponding to a zero eigenvalue represents a linear relation of the column vectors of the matrix $\mathcal{X}$ that is precisely the parameter vector $l^{(0)}$ shown in (1). If the matrix $\mathcal{X}^T\mathcal{X}$ is positive definite (this is typically due to the effect of measurement noises), the eigenvector corresponding to the smallest eigenvalue is an estimate of $l^{(0)}$. This method of finding linear combinations of the column vectors is known as the total least squares (TLS) [4]–[6].

The method of total least squares has been widely applied in practice, ranging from signal processing [7], biomedical signal processing [1], time series analysis [8], subspace identification [9], [10], frequency domain identification [11], [12] errors-in-variables modeling [13], telecommunications [14], to astronomy [15]. As it is shown in [5] and [16], the method of total least squares is the choice of the parameter estimation if all variables of interest have a linear-in-parameter relation and all measurements are contaminated by noises.

In parallel to parameter estimation of the linear model, (1) is often used as a residual analysis in fault detection and diagnosis [17]. For a process that is experiencing failure, (1) is likely no longer true. A nominal parameter l_0 may be estimated from a training data set when the process is under normal operation. This nominal parameter l_0 is then applied to future measurements to check if (1) still holds for the new measurements. This is one example among many different fault detection algorithms. In general, fault detection and diagnosis is a broad and active area of research. There are a large volume of papers that deal with this subject, see, e.g., [18]–[22] and references therein.

Alternatively, fault detection and diagnosis of a process governed by (1) can be treated as detection of change of the model parameters in $l^{(0)}$. This is also known as detection of abrupt changes and is the focus of this paper. Over the last 20 years, research on the detection of abrupt changes has emerged as an important area in control community due to pioneering work of Basseville *et al.* [24]; see, e.g., [23] and [25] and references therein. We call abrupt change any change in the parameters of the model that occurs either instantaneously or at least very fast with respect to the sampling period of the measurement [23]. Abrupt change by no means implies a large magnitude of the change. Instead, a change with a small magnitude is often the major interest of this subject. Over the past several years, the problems concerned with this subject mainly focused on fault detection and diagnosis, data segmentation, gain updating for adaptive algorithms, and process quality control.

Among various statistics-based detection algorithms, the local approach for detection of abrupt change has recently regained significant interests due to the notable work of Basseville [26] and Zhang *et al.* [27], [28]. The effectiveness and reliability of this approach has been demonstrated by its applications in the monitoring of critical processes such as nuclear power plants, gas turbines, catalytic converter, etc.

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[28]. The local approach has a number of distinct features. Among them are the simplicity yet asymptotically uniformly most powerfulness and capability to detect small changes [26].

As has been discussed, total least squares is the choice of a parameter estimation algorithm if measurement noises appear in all variables of interest. This is also true in process fault detection and isolation where all variables are contaminated by measurement noises. Although the residual analysis is frequently used to detect process fault or validate process models, it is however shown by Basseville [26] that residuals are often not sufficient statistic [26]. Basseville [26] further shows that by utilizing the information of the gradient of the residuals, the local detection algorithm provides more information than the regular residual analysis, and is asymptotically sufficient statistic.

The challenge to local detection approach, however, is often the robustness of the algorithm [26], i.e., how to remain sensitive to small changes while robust to disturbances. This motivates the author to develop a local detection algorithm that is robust to measurement noises and has a potential to be widely applied in process industries. To achieve this objective, a new formulation of the total least squares is derived and is defined as the generalized total least squares (GTLS). It should be pointed out this paper does not intend to produce a new algorithm for parameter estimation. Several alternative algorithms may also yield the same solution in terms of parameter estimation. However, this formulation of the GTLS algorithm does facilitate implementation of the local detection algorithm.

Most recently, a dynamic system fault detection algorithm based on the subspace identification method has been discussed in [26] and [29]. To derive a local detection algorithm, an indirect local equation, that explicitly depends on the observability matrix but implicitly depends on the parameters to be monitored, has been used to replace the singular value decomposition algorithm. In this paper, however, we adopt a different yet a simpler approach by formulating singular value decomposition, which is also required in the total least squares, as a constrained optimization problem. This yields a direct equation that explicitly depends on the parameters to be monitored and thus simplifies the detection algorithm.

The remaining of the paper is organized as follows: Total least squares and its extension to the generalized total least squares are discussed in Section II. Detection algorithm for the generalized total least squares is developed in Section III. Monte Carlo simulation examples are given in Section IV. The proposed algorithm is evaluated by a pilot-scale experiment in Section V. Industrial application is presented in Section VI, followed by concluding remarks in Section VII.

II. Generalized Total Least Squares and Total Least Squares

The following is the assumption of process models to be discussed in this paper. Let Z_n be a vector that corresponds to p measurements sampled at time n, i.e.,

$$Z_n = [z_1(n),\, z_2(n),\, \ldots,\, z_p(n)]^T.$$

The original or noise-free variables are denoted as

$$X_n = [x_1(n),\, x_2(n),\, \ldots,\, x_p(n)]^T.$$

The measurement noises are given by

$$V_n = [v_1(n),\, v_2(n),\, \ldots,\, v_p(n)]^T.$$

Thus, we have

$$Z_n = X_n + V_n. \tag{2}$$

Assume that there exists a unique underlying linear (in parameter) relationship among the original variables

$$X_n^T l^{(0)} = 0. \tag{3}$$

Then the following equation may be used to model the relationship of the actual measured variables:

$$Z_n^T l = r(n) \tag{4}$$

where $r(n)$ is a linear combination of the measurement noises and/or other disturbances and is denoted here as equation error. Estimation of the parameter l may be found by minimizing the following sum of square of the equation error:

$$J = \frac{1}{2N} \sum_{n=1}^{N} r^2(n). \tag{5}$$

However, the parameter vector $l^{(0)}$ that satisfies (3) is not unique. To let the estimation unique, a parameter constraint $l^T l = 1$ may be used, although other constraints are also possible as will be discussed shortly. The solution to the minimization of (5) subject to the constraint $l^T l = 1$ is given by

$$\frac{1}{N} \sum_{n=1}^{N} Z_n Z_n^T l = \lambda l \tag{6}$$

or

$$\mathcal{A} l = \lambda l \tag{7}$$

where $\mathcal{A} = (1/N) \sum_{n=1}^{N} Z_n Z_n^T$ is a nonnegative symmetric matrix. The solution is known as the total least squares (TLS) and is given by the eigenvector (denoted as l_0) of $\mathcal{A}$ which corresponds to the smallest eigenvalue (denoted as λ_0). That is

$$\frac{1}{N} \sum_{n=1}^{N} Z_n Z_n^T l_0 = \lambda_0 l_0 \tag{8}$$

and

$$\lambda_0 = \frac{1}{N} l_0^T \sum_{n=1}^{N} Z_n Z_n^T l_0.$$

TLS is a widely used algorithm for parameter estimation. However, the limitation of this (ordinary) TLS algorithm is consistency[1] problem when the variance of measurement noises $\sum_v = \mathrm{Cov}(V_n) \neq \sigma^2 I$, i.e., when each process variables have different measurement noises and/or mutually correlated.

[1]An estimate of parameter is consistent if it converges to the true parameter when the sample size goes to infinity. See also [30].

To cope with the latter case, a general constraint on the parameters has to be used [16]

$$l^T \mathcal{R} l = 1 \tag{9}$$

where $\mathcal{R}$ is a positive definite symmetric matrix. A general objective function can be written as the following Lagrange equation:

$$J = \frac{1}{N} l^T \mathcal{Z}^T \mathcal{Z} l - \lambda(l^T \mathcal{R} l - 1) \tag{10}$$

where

$$\mathcal{Z} = \begin{bmatrix} Z_1^T \\ \vdots \\ Z_N^T \end{bmatrix}.$$

By defining

$$a = \mathcal{R}^{1/2} l$$

then minimization of (10) is given by the eigenvector corresponding to smallest eigenvalue of a nonnegative symmetric matrix. That is

$$\frac{1}{N} \mathcal{R}^{-1/2} \mathcal{Z}^T \mathcal{Z} \mathcal{R}^{-1/2} a = \lambda a. \tag{11}$$

To achieve a consistent estimate, the matrix $\mathcal{R}$ should be chosen as $k \sum_v$ where k is any positive constant and $\sum_v = Cov(V_n)$. We call this algorithm as the generalized total least squares or GTLS.

The matrix $\mathcal{R}$ consists of correlations of the measurement noises. The correlations of the measurement noises may be obtained through replicate of the experiment [12]. It may also be calculated from steady-state data [16]. If the process is at steady state, the correlation of the measurement noises can be calculated from the steady-state measurements using simple correlation analysis. In the GTLS algorithm, the $\mathcal{R}$ matrix is simply like a tuning parameter of an identification algorithm. A good choice of this tuning parameter will improve the performance of the estimation, while poor choice of $\mathcal{R}$ will not devastate the estimation but may cause a bias of the estimation. However, for the fault detection purpose, this bias may be offset by a bias cancellation scheme as proposed by Zhang *et al.* [28]. This will be discussed in the Section III.

To unify the TLS and the GTLS algorithms under a same framework in order to facilitate implementation of the local detection algorithm as will be discussed in the next section, define

$$\mathcal{Z}' = \begin{bmatrix} Z_1'^T \\ \vdots \\ Z_N'^T \end{bmatrix} \triangleq \mathcal{Z} \mathcal{R}^{-1/2}. \tag{12}$$

This gives rise to

$$\mathcal{R}^{-1/2} \mathcal{Z}^T \mathcal{Z} \mathcal{R}^{-1/2} a = \mathcal{Z}'^T \mathcal{Z}' a = \sum_{n=1}^{N} Z_n' Z_n'^T a. \tag{13}$$

Then (11) can be written as

$$\frac{1}{N} \sum_{n=1}^{N} Z_n' Z_n'^T a = \lambda a$$

which is similar to (6) and the solution a_0 is given by the eigenvector corresponding to the smallest eigenvalue of $(1/N) \sum_{n=1}^{N} Z_n' Z_n'^T$. That is

$$\frac{1}{N} \sum_{n=1}^{N} Z_n' Z_n'^T a_0 = \lambda_0 a_0 \tag{14}$$

and

$$\lambda_0 = \frac{1}{N} a_0^T \sum_{n=1}^{N} Z_n' Z_n'^T a_0. \tag{15}$$

Thus by replacing Z_n with Z_n', the GTLS has the same calculation algorithm as the TLS.

Remark 1: The TLS or GTLS algorithm is different from the least squares or weighted least squares algorithm in the following sense: 1) The model used for the least squares or the weighted least squares is

$$y = \alpha + \beta_1 x_1 + \ldots + \beta_n x_n + e$$

where $x_1, \ldots, x_n$ are known as regressors and are assumed to be free of noise. e is disturbance to the response variable y. However, the assumption of all regressors being noise free is frequently unrealistic. This is the motivation to the development of the total least squares algorithm [5]. 2) In addition, the least squares/weighted least squares and the total least squares/weighted total least squares have different geometric interpretations. Readers are referred to [5] for a more detailed explanation.

III. Detection of Parameter Changes using Generalized Total Least Squares

Assume that nominal model parameters or parameters before change are given by l_0, and parameters after change given by $l_0 + (\eta/\sqrt{N})$ where η is a vector with the same dimension as l_0 but with an arbitrary direction and a small magnitude. Then the change detection problem can be formulated as the following statistical hypotheses test:

$$H_0\colon l = l_0 \text{ versus } H_1\colon l = l_0 + \frac{1}{\sqrt{N}} \eta.$$

In this section, let us consider detection of parameter changes under the framework of generalized total least squares. The detection problem under the framework of total least squares is a special case of this development.

Define

$$H(Z_n, l) = Z_n' Z_n'^T a - \lambda_0 a \tag{16}$$

where

$$a = \mathcal{R}^{1/2} l. \tag{17}$$

It follows from (14) that

$$\frac{1}{N}\sum_{n=1}^{N}(Z_n' Z_n'^T a_0 - \lambda_0 a_0) = 0. \tag{18}$$

Using (16), (18) can be written as

$$\frac{1}{N}\sum_{n=1}^{N} H(Z_n, l_0) = 0. \tag{19}$$

That is, if there is no change in the model parameters, then (19) should hold for the new data for sufficiently large N.

On the other hand, if there is parameter change in the new data, i.e., $l \neq l_0$, then

$$\frac{1}{N}\sum_{n=1}^{N} H(Z_n, l) \neq 0. \tag{20}$$

The statistic $H(Z_n, l)$ which satisfies (19) and (20) is known as the primary residual [26]. A normalized residual as defined by [26] can be written as

$$\begin{aligned}\xi_N(l) &= \frac{1}{\sqrt{N}}\sum_{n=1}^{N} H(Z_n, l)\\ &= \frac{1}{\sqrt{N}}\sum_{n=1}^{N}(Z_n' Z_n'^T a - \lambda_0 a)\\ &= \frac{1}{\sqrt{N}}\left[\sum_{n=1}^{N}(Z_n' Z_n'^T a) - N\lambda_0 a\right].\end{aligned} \tag{21}$$

Using (13), (21) can be written as

$$\begin{aligned}\xi_N(l) &= \frac{1}{\sqrt{N}}(\mathcal{R}^{-1/2}\mathcal{Z}^T\mathcal{Z}\mathcal{R}^{-1/2}a - N\lambda_0 a)\\ &= \frac{1}{\sqrt{N}}(\mathcal{R}^{-1/2}\mathcal{Z}^T\mathcal{Z}l - N\lambda_0\mathcal{R}^{1/2}l).\end{aligned} \tag{22}$$

In the case of the simple TLS, (22) can be simplified to

$$\xi_N(l) = \frac{1}{\sqrt{N}}(\mathcal{Z}^T\mathcal{Z}l - N\lambda_0 l). \tag{23}$$

Notice that in (18) and equations thereafter, λ_0 is also a parameter estimated from the generalized total least squares but is not treated as a parameter to be monitored, i.e., $\lambda_0 \notin l$, since λ_0 is an estimate of the measurement noise and it may frequently change with time. To avoid frequent alarms due to the change of λ_0, this parameter should therefore be excluded from the parameter set to be monitored. For this purpose, λ_0 may be adapted on-line or calculated from the new data according to (15). Therefore, λ_0 can vary from one set of data to another but this variation will not affect (19) and (20) if the parameter l is not changed.

Remark 2: The nominal parameter l_0 is typically identified from a set of training data. This estimate may not converge to the true parameter $l^{(0)}$ even if the sample size of the training data is infinity. We call this as the bias error. The bias error can be caused by inappropriate choice of the model or incorrect selection of the matrix $\mathcal{R}$ or the correlation between the measurement noises and the process variables. To bypass this problem, a bias cancellation scheme suggested by Zhang *et al.* [28] may be applied. The procedure is summarized as follows.

1) Determine the nominal parameter l_0 which is not necessarily the same as the true parameter $l^{(0)}$.
2) Estimate the bias of the primary residual from a set of training data using
$$h_0 = EH(Z_n, l_0) \approx \frac{1}{K}\sum_{n=1}^{K} H(Z_n, l_0)$$
where K is the sampling size of the training data.
3) Modify the primary residual $H(Z_n, l)$ by subtracting the bias term h_0. This modified primary residual will approximately offset the effect of bias in the parameter estimation.

Although this method may not offset the effect of bias completely, it improves the detection performance significantly [28]. Of course, one should try the best possible identification algorithm to reduce the bias error before he/she resorts to the bias cancellation algorithm.

Now according to Basseville [26], we have

$$\begin{aligned}&\xi_N(l_0) \sim N(0, \Sigma(l_0)) \quad \text{under } H_0\\ &\xi_N(l_0) \sim N(-\mathcal{M}(l_0)\eta, \Sigma(l_0)) \quad \text{under } H_1\end{aligned}$$

where

$$\begin{aligned}\mathcal{M}(l_0) &\approx \frac{\partial}{\partial l}\left[\frac{1}{N}\sum_{n=1}^{N} H(Z_n, l)\right]_{l=l_0}\\ &= \frac{\partial}{\partial l}\left[\frac{1}{N}\sum_{n=1}^{N}(Z_n' Z_n'^T a - \lambda_0 a)\right]_{l=l_0}.\end{aligned} \tag{24}$$

Using (13), (24) writes as

$$\begin{aligned}\mathcal{M}(l_0) &\approx \frac{\partial}{\partial l}\left[\frac{1}{N}(\mathcal{R}^{-1/2}\mathcal{Z}^T\mathcal{Z}\mathcal{R}^{-1/2}a - N\lambda_0 a)\right]_{l=l_0}\\ &= \frac{\partial}{\partial l}\left[\frac{1}{N}(\mathcal{R}^{-1/2}\mathcal{Z}^T\mathcal{Z}l - N\lambda_0\mathcal{R}^{1/2}l)\right]_{l=l_0}\\ &= \frac{1}{N}[\mathcal{R}^{-1/2}\mathcal{Z}^T\mathcal{Z} - N\lambda_0\mathcal{R}^{1/2}].\end{aligned} \tag{25}$$

In the case of the simple TLS, we have

$$\mathcal{M}(l_0) \approx \frac{1}{N}[\mathcal{Z}^T\mathcal{Z} - N\lambda_0 I]. \tag{26}$$

According to [27] $\Sigma(l_0)$ may be approximated by

$$\begin{aligned}\Sigma(l_0) \approx{}& \frac{1}{N}\sum_{n=1}^{N} H(Z_n, l_0)H^T(Z_n, l_0)\\ &+ \sum_{i=1}^{I}\frac{1}{N-i}\sum_{n=1}^{N-i}(H(Z_n, l_0)H^T(Z_{n+i}, l_0)\\ &+ H(Z_{n+i}, l_0)H^T(Z_n, l_0))\end{aligned} \tag{27}$$

where the value I should be properly selected according to the correlation of the signals. Typically, one can gradually increase the value of I until the result converges.

With these results, detection of small changes in the parameter l is asymptotically equivalent to the detection of changes in the mean of a Gaussian vector. The generalized likelihood ratio test detecting unknown changes in the mean of a Gaussian vector is a χ^2 test. It can be shown [26] that the GLR test of H_1 against H_0 can be written as

$$\chi^2_{\text{global}} = \xi_N(l_0)^T \sum^{-1}(l_0)\mathcal{M}(l_0) \times \left(\mathcal{M}^T(l_0)\sum^{-1}(l_0)\mathcal{M}(l_0)\right)^{-1} \times \mathcal{M}^T(l_0)\sum^{-1}(l_0)\xi_N(l_0). \tag{28}$$

If $\mathcal{M}(l_0)$ is a square matrix, then this test can be simplified to

$$\chi^2_{\text{global}} = \xi_N(l_0)^T \sum^{-1}(l_0)\xi_N(l_0) \tag{29}$$

where χ^2_{global} has a central χ^2 distribution under H_0, and a noncentral χ^2 distribution under H_1. The degree of freedom of χ^2_{global} is the row dimension of l. A threshold value χ^2_α can be found from a χ^2 table, where α is the false alarm rate specified by the users. If χ^2_{global} is found to be larger than the threshold value, then a change in the parameter is detected.

Once a change is detected from the model parameters, it may be necessary to isolate which or which set of parameters have changed. This problem is known as isolation problem [26]. Partition l into l_a and l_b, and η into η_a and η_b accordingly. The problem of fault isolation can be formulated as the following hypotheses test:

$$H_0\colon \eta_a = 0 \text{ versus } H_1\colon \eta_a \neq 0 \tag{30}$$

i.e., no change of any of parameters in the parameter subset l_a versus change of at least one parameter in the parameter subset.

Partition the matrix $\mathcal{M}(l_0)$ into two submatrices

$$\mathcal{M}(l_0) = [\mathcal{M}_a, \mathcal{M}_b]$$

which corresponds to the partition of l, i.e. the column dimension of $\mathcal{M}_a$ is the same as the row dimension of l_a and the column dimension of $\mathcal{M}_b$ is the same as the row dimension of l_b.

To perform the minmax test, let $F = \mathcal{M}^T(l_0)\sum^{-1}(l_0)\mathcal{M}(l_0)$ and partition it to

$$F = \begin{bmatrix} F_{aa} & F_{ab} \\ F_{ba} & F_{bb} \end{bmatrix} = \begin{bmatrix} \mathcal{M}_a^T\sum^{-1}(l_0)\mathcal{M}_a & \mathcal{M}_a^T\sum^{-1}(l_0)\mathcal{M}_b \\ \mathcal{M}_b^T\sum^{-1}(l_0)\mathcal{M}_a & \mathcal{M}_b^T\sum^{-1}(l_0)\mathcal{M}_b \end{bmatrix}.$$

Define

$$\tilde{\xi}_a = \mathcal{M}_a^T \sum^{-1}(l_0)\xi_N(l_0)$$
$$\tilde{\xi}_b = \mathcal{M}_b^T \sum^{-1}(l_0)\xi_N(l_0)$$

and

$$\xi_a^* = \tilde{\xi}_a - F_{ab}F_{bb}^{-1}\tilde{\xi}_b$$
$$F_a^* = F_{aa} - F_{ab}F_{bb}^{-1}F_{ba}.$$

Then the minmax test can be written as

$$\chi_a^{2*} = \xi_a^{*T} F_a^{*-1}\xi_a^* \tag{31}$$

where χ_a^{2*} has the χ^2 distribution with the degree of freedom equal to the row dimension of l_a.

In practice it is cautioned by Zhang *et al.* [27] that χ_a^{2*} may not exactly follow the χ^2 distribution. The recommended method by Zhang *et al.* [27] is to compute a minmax test for each possible subvector η_a. Among all these minmax tests, the one having the largest value indicates the nonzero subvector η_a. An obvious advantage of this approach is that no threshold is needed. The downside is that this may involve an extensive computation effort.

The above results on detection and isolation are summarized in the following algorithm.

Algorithm 1

Nominal model parameter l_0 is estimated from a set of training data using the TLS or GTLS algorithm depending on the structure of measurement noises. Then the following detection test can be applied to the new set of data:

1. Calculate the normalized residual $\xi_N(l_0)$ using (22) where λ_0 is calculated using (15).
2. Calculate the primary residual $H(Z_n, l_0)$ using (16).
3. Calculate the gradient $\mathcal{M}(l_0)$ using (25).
4. Calculate the covariance matrix $\Sigma(l_0)$ using (27).
5. Calculate χ^2_{global} using (28) or (29).
6. Select the threshold value from the χ^2 table according to prespecified false alarm rate with the degree of freedom equal to the row dimension of l.
7. If χ^2_{global} is larger than the threshold, issue an alarm and then perform the following isolation test. Otherwise conclude that no change of model parameters is detected.
8. Calculate χ_a^{2*} using (31) for each set of parameters and select threshold values according to the specified false alarm rate.
9. The subset of parameters that has χ_a^{2*} larger than its threshold values are isolated as the parameters that have been changed, or the set of parameters that has the largest χ_a^{2*} is isolated as the parameters that have been changed.

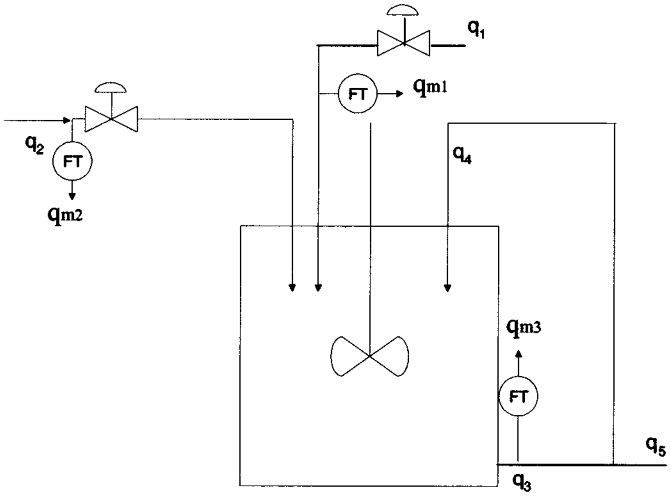

Fig. 1. Schematic of a blending process.

IV. Simulation Example: Process Monitoring and Fault Detection

Example: Consider a blending process (a revised example from Seborg *et al.* [31]) as shown in Fig. 1. Under the normal operating condition, the volume of liquid in the tank can be assumed to be constant since all flow rates q_1, q_2, q_3, q_4, and q_5 are constant subject to small variation. The density of all streams is constant at 90 lb/ft^3. The recycle line is 68.8 ft long and has an inside diameter of 4 in. The tank is 6 ft in diameter and is perfectly mixed. The nominal steady-state values are

$$\bar{q}_1 = 50 \text{ ft}^3/\min \quad \bar{q}_3 = 82 \text{ ft}^3/\min$$
$$\bar{q}_2 = 2 \text{ ft}^3/\min \quad V = 100 \text{ ft}^3$$

q_1, q_2, and q_3 are the only measured variables. The possible faults in the simulation are 1) varying gain of the sensor of q_1; 2) varying gain of the sensor of q_2; and 3) change of the recycling rate. The question is: Can we detect any one of the possible faults with a small magnitude subject to measurement noises? Can we isolate the source of the faults?

The basic equation in this study is the mass balance equation

$$q_1 + q_2 = (1-c)q_3 \tag{32}$$

where c is the recycling rate with a nominal value $c_0 = 0.37$. The measurements of q_1, q_2, and q_3 are contaminated by measurement noise and can be written as

$$q_{m1} = k_1 q_1 + v_1$$
$$q_{m2} = k_2 q_2 + v_2$$
$$q_{m3} = k_3 q_3 + v_3$$

where k_1, k_2, and k_3 are the gains of the flow rate sensors with nominal values equal to one, v_1, v_2, and v_3 are white noises with nominal standard deviation of 0.1. The perturbations through q_1 and q_2 are random signals with the uniform distribution. Their magnitudes vary between 1 and $+1$, which is approximately equivalent to a standard deviation of 0.58. Five scenarios are considered in the simulation: 1) no fault of the process; 2) 10% increase of the sensor gain of q_1; 3) 10% increase of the sensor gain of q_2; 4) 10% increase of the recycle rate; and 5) the standard deviation of measurement noises increases from 0.1 to 0.2 and 0.3, respectively.

A set of training data with a sample size of 1000 is first simulated when no fault occurs in the process. The nominal parameters of (32) are estimated by applying the total least squares to the training data. A total of 100 Monte Carlo simulation runs are then conducted for each scenario and each single run consists of 1000 data points. Results are summarized in Tables I–III which correspond to the standard deviation of measurement noise equal to 0.1, 0.2, and 0.3, respectively. Where in these tables, "Detection rate" represents the successful fault detection rate, "False rate" represents the false alarm rate when in fact there is no fault in the process, and "Isolation rate" represents the successful fault isolation rate. It is observed from these tables that 1) with the noise standard deviation up to 0.2, the detection and isolation performance is near perfect and 2) performance is deteriorated when the noise standard deviation

TABLE I
TLS-Based Detection for Process with 10% Parameter Changes and with Noise Standard Deviation 0.1

Sensor 1 gain	Sensor 2 gain	Recycle rate	Source of fault	Detection rate (%)	False rate (%)	Isolation rate (%)
1	1	0.37	no fault	N/A	2	N/A
1.1	1	0.37	sensor 1	100	N/A	100
1	1.1	0.37	sensor 2	100	N/A	100
1	1	0.407	recycle	100	N/A	100

TABLE II
TLS-Based Detection for Process with 10% Parameter Changes and with Noise Standard Deviation of 0.2

Sensor 1 gain	Sensor 2 gain	Recycle rate	Source of fault	Detection rate (%)	False rate (%)	Isolation rate (%)
1	1	0.37	no fault	N/A	0	N/A
1.1	1	0.37	sensor 1	100	N/A	100
1	1.1	0.37	sensor 2	100	N/A	100
1	1	0.407	recycle	97	N/A	97

TABLE III
TLS-Based Detection for Process with 10% Parameter Changes and with Noise Standard Deviation of 0.3

Sensor 1 gain	Sensor 2 gain	Recycle rate	Source of fault	Detection rate (%)	False rate (%)	Isolation rate (%)
1	1	0.37	no fault	N/A	0	N/A
1.1	1	0.37	sensor 1	82	N/A	82
1	1.1	0.37	sensor 2	66	N/A	66
1	1	0.407	recycle	63	N/A	62

TABLE IV
TLS BASED DETECTION FOR PROCESS WITH 10% PARAMETER CHANGES AND WITH NOISE STANDARD DEVIATION OF 0.3 (SAMPLE SIZE = 1500)

Sensor 1 gain	Sensor 2 gain	Recycle rate	Source of fault	Detection rate (%)	False rate (%)	Isolation rate (%)
1	1	0.37	no fault	N/A	0	N/A
1.1	1	0.37	sensor 1	93	N/A	93
1	1.1	0.37	sensor 2	87	N/A	87
1	1	0.407	recycle	90	N/A	90

TABLE V
COMPARISON BETWEEN TLS- AND GTLS-BASED DETECTION ALGORITHMS FOR PROCESS SUBJECT TO VARYING MEASUREMENT NOISE IN SENSOR 3

Detection method	Sensor 1 gain	Sensor 2 gain	Recycle rate	Source of fault	False rate (%)
TLS	1	1	0.37	no fault	91
GTLS	1	1	0.37	no fault	1

TABLE VI
GTLS-BASED DETECTION FOR PROCESS WITH 10% PARAMETER CHANGES SUBJECT TO VARYING MEASUREMENT NOISE OF SENSOR 3

Sensor 1 gain	Sensor 2 gain	Recycle rate	Source of fault	Detection rate (%)	False rate (%)	Isolation rate (%)
1	1	0.37	no fault	N/A	1	N/A
1.1	1	0.37	sensor 1	100	N/A	100
1	1.1	0.37	sensor 2	100	N/A	100
1	1	0.407	recycle	100	N/A	100

increases to 0.3 which is half of the signal standard deviation. For the same noise standard deviation of 0.3, detection performance is improved by increasing the sample size from 1000 to 1500 as shown in Table IV.

Now consider that the standard deviation of one of the sensors, say q_3, increases from 0.1 to 0.3 while the standard deviation of the remaining two sensors keep the same value of 0.1. In this case, since the sensors have different variance of measurement noises, the detection algorithm based on the generalized total least squares should be used, as the total least squares no longer gives a consistent estimate of the parameters. Table V shows the comparison of the Monte Carlo simulations between TLS and GTLS-based algorithms. The TLS based local detection algorithm gives a false alarm rate of 91% while the GTLS-based local detection algorithm gives a false alarm rate of 1%, indicating importance to take into account of measurement noise structure. Once again, as shown in Table VI the GTLS-based detection algorithm has an excellent detection ability should any of the three faults occur, despite of different measurement variances among the three sensors.

V. EXPERIMENTAL EVALUATION

A "process monitoring and data reconciliation" experiment has been designed to evaluate the performance of the proposed algorithm to verify the energy balance equation. The equipment consists of a cold and hot water stream mixing at a "T" junction as shown in the schematic in Fig. 2. The temperatures and flow rates are measured by thermocouples and orifice meters, respectively. There are two temperature measurement points for the mixed outlet water. Therefore, two control volumes may be used to write energy balance equation. T_4 is measured at a point located immediately after the "T" junction where the hot water and cold water could not have been well mixed. T_5 is measured at a point where a better mixing of the water may be expected. All temperature and flow rate measurements are subject to measurement noises with different variances. The equipment is interfaced to a PC and all variables are logged every 2 s.

In the experiment, the inlet flow rates were kept constant, while the variation occurred in the temperatures of the cold and hot inlet water flows as shown in Fig. 3. These variations serve as natural excitation signals for the model validation. Energy at the ith measurement point is calculated through the equation

$$E_i = 4.18 F_i T_i \qquad i = 1, 2, 4, 5$$

where F_i (KG/h) is the flow rate at the ith measurement point ($F_1 = F_{cw}$, $F_2 = F_{hw}$ and $F_4 = F_5 = F_t$), and T_i (°C) is the temperature measurement at the ith measurement point. The energy balance equations for the two control volumes are given by

$$\text{control volume 1: } E_4 = E_1 + E_2 \tag{33}$$

and

$$\text{control volume 2: } E_5 = E_1 + E_2. \tag{34}$$

The purpose of this experiment is to determine which of the two equations, (33) or (34), is likely to fit the experimental data. The sources of error may be attributed to nonperfect mixing at the measurement points and/or measurement errors. The energy data is zero-mean centered to reduce the effect of any constant error such as bias error in the measurement.

Since each sensor has different measurement noise, the detection algorithm based on the generalized total least squares has to be used. The variance of the measurement noise can be calculated using a section of steady-state data. No training data is required to estimate the nominal model as the theoretical model is known from the energy balance equation. To appreciate the effectiveness of the GTLS algorithm in such cases, the parameters of the balance equations are nevertheless estimated using TLS, GTLS, and least squares (LS) for comparison, and results are shown in Table VII. Clearly, for both control volumes, the GTLS algorithm gives models that are both close to the energy balance equations. Within the two models estimated by the GTLS, the control volume at point T_5 gives an energy balance equation that is closest to the theoretical energy balance equation, indicating a relatively good mixing at this measurement point. These results are also confirmed by the χ^2_{global} values of each control volume. The χ^2_{global} value for the control volume at T_4 is 294.93, while

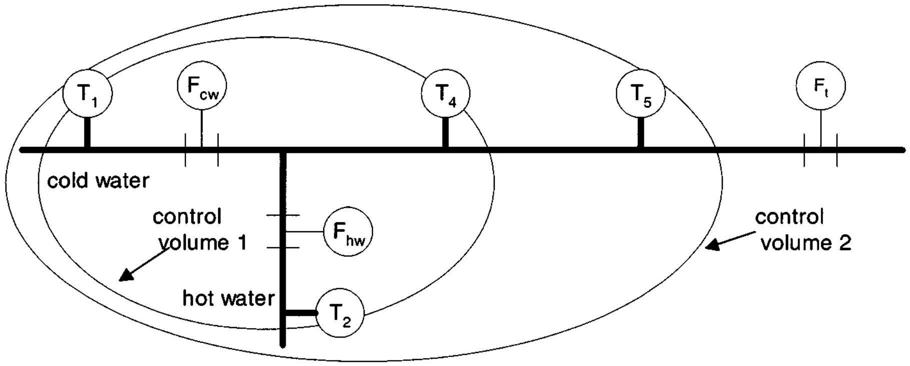

Fig. 2. Schematic diagram of the pilot-scale experiment.

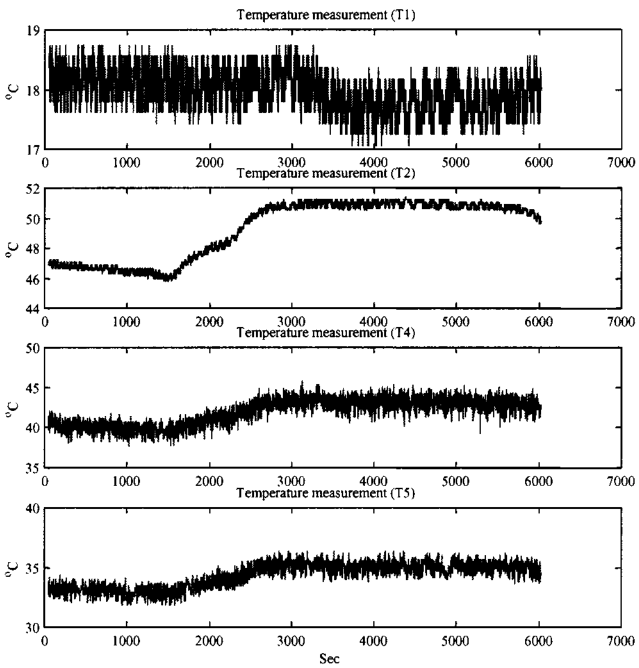

Fig. 3. Temperature trajectories of pilot-scale experiment.

TABLE VII
SUMMARY OF ESTIMATED ENERGY BALANCE EQUATIONS FROM THE PILOT-SCALE EXPERIMENTAL DATA

Control	TLS	$E_4 = 93.98E_1 + 22.01E_2$
Volume	**GTLS**	$\mathbf{E_4 = 0.43E_1 + 1.54E_2}$
at T_4	LS	$E_4 = -0.12E_1 + 1.32E_2$
Control	TLS	$E_5 = 14.51E_1 + 4.09E_2$
Volume	**GTLS**	$\mathbf{E_5 = 1.09E_1 + 1.19E_2}$
at T_5	LS	$E_5 = 0.34E_1 + 0.94E_2$

the χ^2_{global} value for the control volume at T_5 is 86.5. Although both numbers show that the energy balance equations are not perfectly fitted by the data measured at either of the two control volumes, the control volume at T_5 fits the energy balance equation much better than the control volume at T_4, a result that agrees with our expectation.

VI. INDUSTRIAL APPLICATION

This case study focus on sensor validation of an industrial Bitumen column under advanced multivariable model predictive control (MPC) as shown in Fig. 4. As a part of Bitumen separation facilities, Syncrude Canada Ltd. operates a Bitumen column in Fort McMurray, Alberta, Canada. The Bitumen column has eight controlled variables (CVs), five manipulated variables (MVs) and five disturbance variables (DVs). The MPC on the column uses the models embedded in it to predict the process response to the changes in disturbance and manipulated variables and keeps the controlled variables within the setpoint limits by changing the manipulated variables. Unfortunately, the Bitumen column frequently got flooded recently and hence the plant personnel had to manually operate the column when the column got flooded. Without advanced control, production rate and quality could come down considerably. It is observed that the temperature on one of the top trays of the column increases steeply when the column gets flooded and hence is regarded by the plant personnel as a "reliable" observation variable to monitor the flooding status of the column. Some suggested that this flooding observation variable should replace the existing three flooding inferential variables, CV6 (vapor flooding correlation), CV7 (liquid flooding correlation) and CV9 (packing flooding correlation). Since these three flooding inferential variables are strong correlated, an ill-condition control problem could result from the correlation. The question is whether this new observation variable contains all essential information in other three inferential variables and can be used as a single flooding indication variable to replace the three inferential variables.

A set of data was sampled when the column got flooded and then the controller was set to manual operation. The data trajectories of CV6, CV7, CV9, and the flooding observation variable are shown in Fig. 5. All data are zero-mean centered and all units are masked to protect proprietary information. It can be observed from the figure that flooding occurred at about 4300th sample, and the controller was turned off since then. It is clearly observed from this figure that all these flooding indication variables are highly correlated after the column gets flooded. It appears that this observation variable may be used as a substitute to the other three variables.

To check this, consistency of the correlations between the observation variable and other three variables are inspected. We

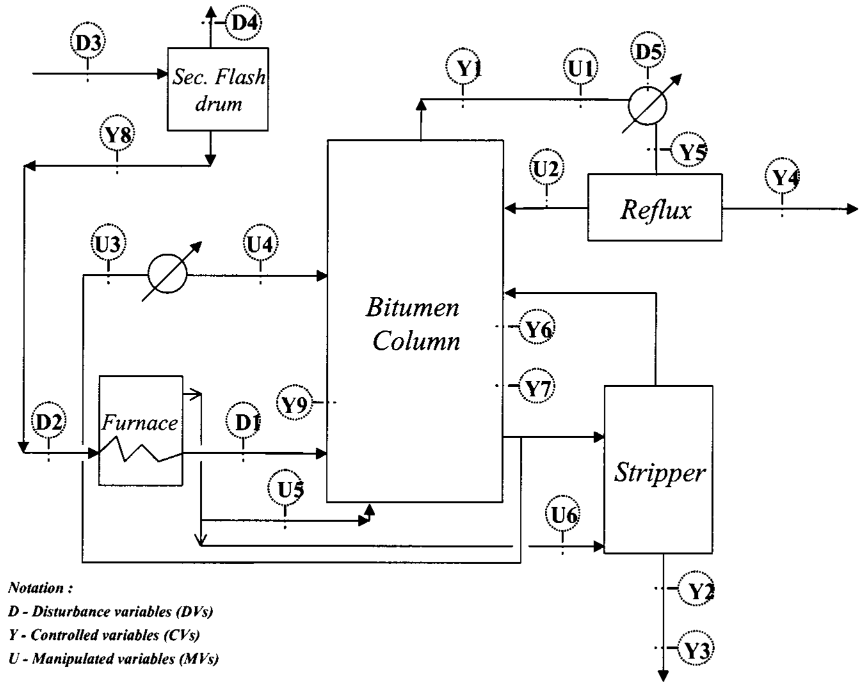

Fig. 4. Schematic diagram of the Bitumen column.

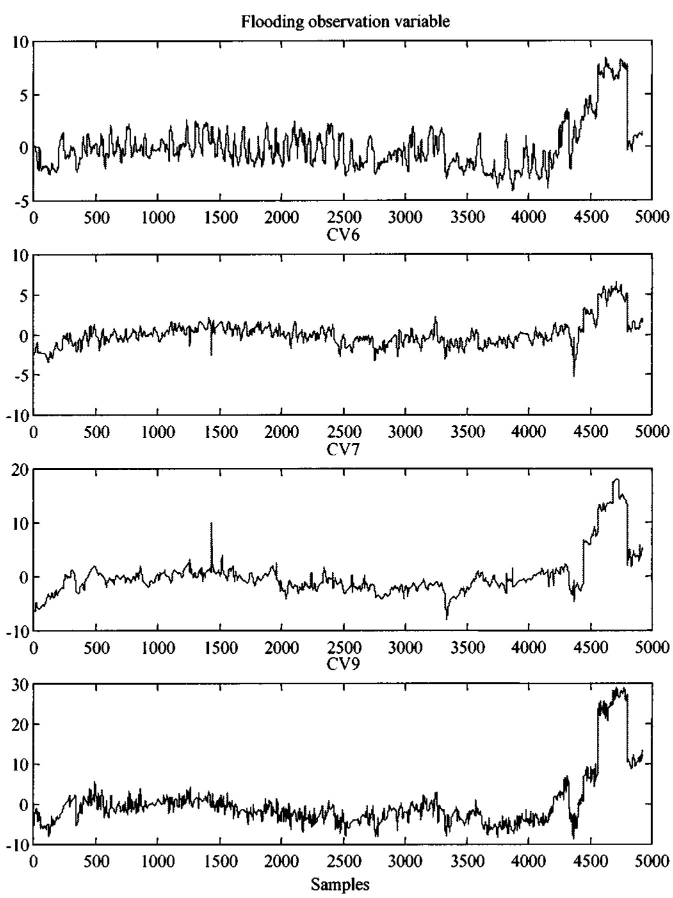

Fig. 5. Data trajectories when the flooding occurred.

use the first 2000 data as a training data set to calculate the correlations and build models between the observation variable and other three variables, respectively. Nonlinear transformations of the variables are also considered in the model building, but not much improvement from the nonlinear transformation is observed. The linear models are therefore used and verified over the remaining data including the data sampled when the column gets flooded. The proposed local detection algorithm is applied to the data to detect change of the model parameters and thus validate consistency of the models over all sampled data. Since the three inferential variables CV6, CV7, and CV9 are calculated from their inferential models, no measurement error is expected. Therefore, a suitable monitoring scheme would be the GTLS-based detection algorithm where the measurement variance of the observation variable is chosen to be one, and variances of the remaining three variables are chosen to be near zero.

To compare both TLS and GTLS-based detection algorithms, result calculated using the TLS based detection algorithm is also shown in Fig. 6, and result calculated using the GTLS-based detection algorithm is shown in Fig. 7. It appears from both figures that all of the three linear models between the observation variable and the other three variables hold consistently until the column gets flooded. Models are clearly changed once the column gets flooded. A noticeable difference may also be observed between the results of TLS-based validation and GTLS based validation, particularly after the column gets flooded, indicating once again importance to take disturbance structure into account. Nevertheless, both results show changes of all three models after the flooding. This indicates that the observation variable should not be used to replace the other three variables as a general flooding indication variable. Alternative methods must be sought to improve the early flooding detection performance in order to prevent flooding. Based on this recommendation, a subsequent analysis on the early fault detection has been performed and yielded a conclusion that the the flooding

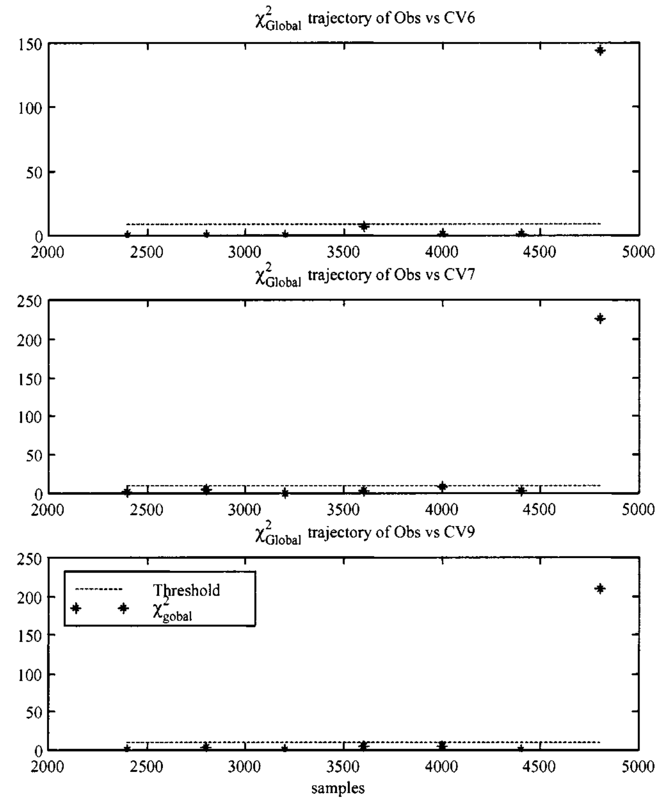

Fig. 6. Change detection using the TLS-based detection algorithm.

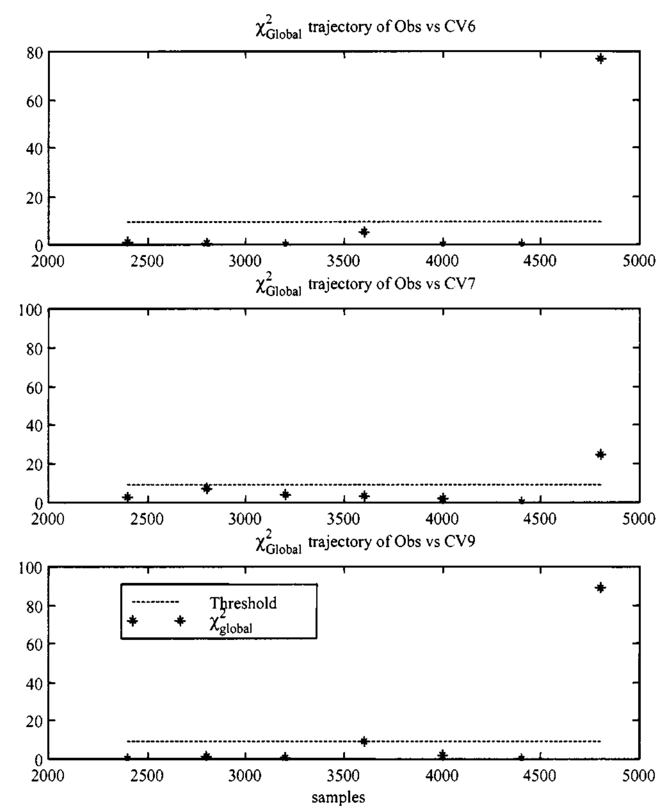

Fig. 7. Change detection using the GTLS-based detection algorithm.

may be better monitored and detected by using a model-based local approach. Further recommendations have been reported in [32].

VII. Conclusion

A local detection algorithm based on the total least squares and generalized total least squares has been derived in this paper. The total least squares and generalized total least squares models are frequently used to model processes when all measurement variables are corrupted by disturbances. It is therefore of practical interest to use the total least squares and the generalized total least squares to monitor the processes as well. By using the local detection algorithm derived from the generalized total least squares algorithm, it is shown that the robustness of the detection algorithm to the disturbances can be improved compared to using the total least squares. The proposed algorithm has been verified through Monte Carlo simulations, evaluated in a pilot-scale experiment, and applied to sensor validation for an industrial Bitumen column.

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