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Optimal Sensor Network Upgrade for Fault Detection Using Principal Component Analysis

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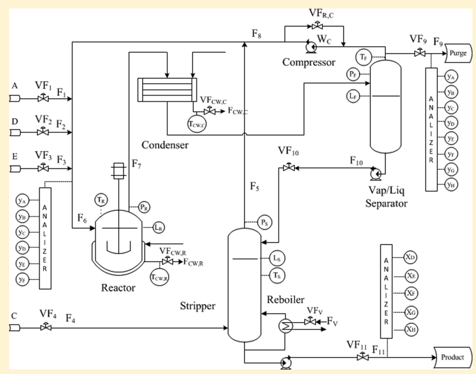
ABSTRACT: The efficiency of a fault monitoring system critically depends on the structure of the plant instrumentation system. For processes monitored using principal component analysis, the multivariate statistical technique most used for fault diagnosis in industry, an existing strategy aims at selecting the set of instruments that satisfies the detection of a given set of faults at minimum cost. It is based on the minimum fault magnitude concept. Because that procedure discards lower-cost feasible solutions, in this work, a new optimal selection methodology is proposed whose constraints are straightaway defined in terms of the principal component analysis's statistics. To solve the optimization problem, a level traversal search with cutting criteria is enhanced taking into account that the fault observability is a necessary condition for fault detection when statistical monitoring techniques are applied. Furthermore, observability and detection degree concepts are defined and considered as constraints of the optimization problems to devise robust sensor structures, which are able to detect a set of key faults under the presence of failed sensors or outliers. Application results of the new strategy to a case study taken from the literature are provided.



1. INTRODUCTION

When an abnormal event occurs in a chemical plant, the process deviates from the normal regime. Early detection and diagnosis of faults while the plant is still operating in a controllable region help prevent the abnormal situation progress and reduce the impact of industrial accidents. All approaches proposed to diagnose faults compare in some way the observed behavior of the process with a reference model. Such behavior is inferred from the measurements obtained by the instruments installed in the plant. Therefore, the efficiency of the fault monitoring system critically depends on the structure of the process sensor network (SN).

At first Raghuraj et al.[1] and Bhushan and Rengaswamy[2] presented directed graphs (DGs)- and signed directed graphs (SDGs)-based approaches, respectively, to design SNs which ensure faults observability and resolution for processes monitored using model-based qualitative methodologies. Next, an instrumentation design strategy, which considers reliability as the primary objective and cost as the secondary one and satisfies the faults observability and resolution criteria, was proposed by Bhushan and Rengaswamy.[3] That technique is not structural as the previous ones because it uses quantitative information regarding process faults and sensors failures probabilities. Later on, Bhushan et al.[4] modified that methodology to take into account the network robustness to errors in the SDG and probability data uncertainties, and Kolluri and Bhushan[5] extended the strategy to solve the instrumentation upgrade and reallocation problems. Other structural techniques use the information contained in the process DG. In this sense, Rodriguez et al.[6] addressed the optimal design of SNs able to resolve a set of key failures under the presence of malfunctioning instruments. With this purpose, the key fault resolution degree concept was defined. All the aforementioned optimization algorithms are solved using mixed integer linear programming codes.

Furthermore, some researchers showed that the installation of an appropriate SN enhances the process fault diagnosis using principal component analysis (PCA). In this regard, Wang et al.[7] proposed to locate sensors using the technique proposed in ref 1 at the design stage. This partially guarantees the detection and isolation of faults when PCA is applied to monitor the system behavior on line. Later on Musulin et al.[8] analyzed the design and upgrade of SNs for processes monitored using that statistical technique. A classic genetic algorithm was applied to obtain the optimal sensor configuration that minimizes a global penalty index made up of the sensor network cost (SNc) and the fault size penalization. This last term was evaluated using the conservative calculus of the minimum fault magnitude (FM) detectable using PCA's statistics, which was provided by Wang et al.[9] Because that calculus is conservative, the strategy may disregard lower-cost feasible solutions; also, it does not deal with the robustness of the sensor structure. The design procedure can be applied to evaluate the performance of SNs of existing plants or simulated ones. In a similar way, the optimization algorithms can be used either to select signals of

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processes with an existing instrumentation network or to decide the best location of sensors if a process dynamic simulation is available at the plant design stage.

Moreover, Li[10] addressed the design of SNs for multistage flash nuclear desalination plants monitored using PCA. First, that author simulated the steady state and dynamic behavior of those plants using the design data. The results showed that the developed dynamic model was able to characterize the system dynamic behavior with reasonably good accuracy to study the control and fault diagnosis of the system. The design of the optimal SN that satisfies the faults observability and resolution was addressed using the formulation based on DGs.[1] Also, reliable sensor structures were obtained following the methodology proposed in ref 3. An integer linear programming greedy search heuristic was developed for solving the optimization problems. The obtained sensor set partially guarantees the detection and isolation of all the faults.[10] A PCA model was built using simulated data of the nominal operation and used to monitor the process on line. The differences between the measurements and their predictions using the PCA model were used for fault isolation. The capability of the monitoring technique to detect failures of certain magnitude was not considered in that work.

In this paper, the optimal upgrade of SNs that are able to detect a set of predetermined process faults using PCA is presented. In contrast to the previous works, the fault detection capability of the network is defined straightaway in terms of the PCA's statistics. Consequently, the procedure has a broad range of application since it can be extended to other statistical monitoring techniques. The availability of a dynamic model of the process, which characterizes the system dynamic behavior with reasonably good accuracy, is required to apply the proposed methodology. Also, this contribution deals with the selection of robust sensor structures, which are able to detect a set of key faults even in the presence of failed sensors or outliers. For this purpose, the detection degree concept is defined in this work. Regarding the solution of the optimization problems, a level traversal search with cutting criteria is used to solve the mixed integer nonlinear formulations. That solution scheme is enhanced by incorporating the fault observability (fault structural determinability) as a linear constraint of the optimization problems given that the fault observability is a necessary condition for the fault detection when PCA is applied.[7] Additionally, the application of the proposed technique to other instrumentation problems is discussed. In this regard, the design case and the selection of signals from a set of existing sensors, which provide information about all the variables affected by the analyzed faults, are considered.

The rest of the paper is structured as follows. In Section 2, a conservative calculus of the minimum FM detectable using PCA is briefly revised. New formulations for selecting SNs able to detect a given set of faults are presented in Section 3. In the next section, a solution strategy based on an improved level traversal search is analyzed. In Section 5, the application results of the technique to a case study taken from the literature are provided. A Conclusions section ends this Article.

2. CRITICAL FAULT MAGNITUDE

This section briefly introduces the conservative calculus of the minimum FM detectable[9] using the PCA technique which is used as a constraint of SN design and upgrade problems.[8] Also, why that value is a conservative estimation is discussed.

Traditionally, PCA-based techniques use two statistics to detect the presence of process failures.[11] These are the hotelling statistic (D) and the squared prediction error (SPE), which are evaluated using the results of the eigendecomposition of the correlation matrix, $\mathbf{R}$, of the normal operating data. These are contained in a matrix $\mathbf{X}$ of dimension (M, N), where M and N represent the number of samples and measurements, respectively.

During the online process monitoring, the standardized measurement vector $\mathbf{x}$ is used to calculate D as follows

$$D = \| \mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x} \|^2 \tag{1}$$

where $\mathbf{\Lambda}$ is the diagonal matrix constituted by the eigenvalues of $\mathbf{R}$ associated with the retained principal components, which are contained in matrix $\mathbf{P}$. That statistic can detect changes in the correlation structure of the data, while observations that indicate a behavior significantly different from the usual one are detected by SPE, which is evaluated as follows:

$$SPE = \|(\mathbf{I} - \mathbf{P}\mathbf{P}^{\mathrm{T}})\mathbf{x}\|^2 \tag{2}$$

The minimum FM detectable using PCA can be estimated using the expression proposed in ref 9. Let us consider that a SN is identified by the binary vector $\mathbf{q}$ of dimension I, such that $q_i = 1$ if the i-th variable is measured and $q_i = 0$ otherwise. Also, let us assume that the matrix $\boldsymbol{\theta}_\mathrm{j}$ of dimension (N, R_j) describes the j-th failure of a given set of J process faults. The variable R_j stands for the number of measured variables affected by the occurrence of the j-th failure, and it should be noticed that $R_j \leq N \leq I$. The n-th row of $\boldsymbol{\theta}_\mathrm{j}$ has a nonzero element if the fault affects the n-th measurement. For example, if $N = 3$, $R_j = 2$, and the measured variables 1 and 3 are affected by the occurrence of the j-th fault, then the elements (1,1) and (3,2) of $\boldsymbol{\theta}_\mathrm{j}$ (3,2) are nonzero. Wang et al.[9] pointed out that a fault subspace, which is roughly defined but contains the essential characteristics of the fault, works well. Those authors also mentioned that matrices ($j = 1. . .J$) can be built using process SDG or numerical simulations. This last approach was used to obtain the $\boldsymbol{\theta}_\mathrm{j}$ ($j = 1. . .J$).[8]

When the j-th process failure occurs, the vector $\mathbf{x}$ can be defined as follows

$$\mathbf{x} = \mathbf{x}_0 + \boldsymbol{\theta}_\mathrm{j}\mathbf{f}_\mathrm{j} \tag{3}$$

where $\mathbf{x_0}$ is the vector of standardized measurements under normal operation, and $\mathbf{f}_\mathrm{j}$ represents the vector of standardized deviations of all measurements affected by the occurrence of the j-th fault with respect to their normal values. Replacing the definition of $\mathbf{x}$ in eqs 1 and 2, the following expressions are obtained for the statistics:

$$D(\mathbf{q}) = \| \mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x} \|^2 = \| \mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}(\mathbf{x_0} + \boldsymbol{\theta}_\mathrm{j}\mathbf{f}_\mathrm{j})\|^2 \tag{4}$$

$$SPE(\mathbf{q}) = \|(\mathbf{I} - \mathbf{P}\mathbf{P}^{\mathrm{T}})\mathbf{x}\|^2 = \|(\mathbf{I} - \mathbf{P}\mathbf{P}^{\mathrm{T}})(\mathbf{x_0} + \boldsymbol{\theta}_\mathrm{j}\mathbf{f}_\mathrm{j})\|^2 \tag{5}$$

If the triangle inequality of the norm is applied to the expressions of $(D(\mathbf{q}))^{1/2}$ and $(SPE(\mathbf{q}))^{1/2}$ derived from eqs 4 and 5, the following inequalities result

$$\| \mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x} \| \geq |\| \mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x_0} \| - \| \mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\boldsymbol{\theta}_\mathrm{j}\mathbf{f}_\mathrm{j}\||\tag{6}$$

$$\|(\mathbf{I} - \mathbf{P}\mathbf{P}^{\mathrm{T}})\mathbf{x}\| \geq |\|(\mathbf{I} - \mathbf{P}\mathbf{P}^{\mathrm{T}})\mathbf{x_0}\| - \|(\mathbf{I} - \mathbf{P}\mathbf{P}^{\mathrm{T}})\boldsymbol{\theta}_\mathrm{j}\mathbf{f}_\mathrm{j}\||\tag{7}$$

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Under normal operating conditions, $D^{1/2} = \|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x}\|$ and $SPE^{1/2} = \|(\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\mathbf{x}\|$ vary in the ranges $(0, \delta_{D,\alpha})$ and $(0, \delta_{SPE,\alpha})$, respectively, that is $0 \le \|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x_0}\| \le \delta_{D,\alpha}$ and $0 \le \|(\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\mathbf{x_0}\| \le \delta_{SPE,\alpha}$, where $\delta_{D,\alpha}{}^2$ and $\delta_{SPE,\alpha}{}^2$ are the critical values of D and SPE, respectively, and α stands for the significance level of the tests.

Taking into account the previous formulations, the sufficient conditions for fault detection, which are based on the analysis of the square roots of D and SPE values,[9] are

$$\|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\boldsymbol{\theta}_{\mathbf{j}}\mathbf{f}_{\mathbf{j}}\| \ge 2\delta_{D,\alpha} \tag{8}$$

$$\|(\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\boldsymbol{\theta}_{\mathbf{j}}\mathbf{f}_{\mathbf{j}}\| \ge 2\delta_{SPE,\alpha} \tag{9}$$

The application of the triangle inequality of the norm to the left-hand sides of the above equations provides the following inequalities

$$\|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\boldsymbol{\theta}_{\mathbf{j}}\|\,\|\mathbf{f}_{\mathbf{j}}\| \ge \|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\boldsymbol{\theta}_{\mathbf{j}}\mathbf{f}_{\mathbf{j}}\| \ge 2\delta_{D,\alpha} \tag{10}$$

$$\|(\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\boldsymbol{\theta}_{\mathbf{j}}\|\,\|\mathbf{f}_{\mathbf{j}}\| \ge \|(\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\boldsymbol{\theta}_{\mathbf{j}}\mathbf{f}_{\mathbf{j}}\| \ge 2\delta_{SPE,\alpha} \tag{11}$$

from which the j-th minimum FM detectable using both statistics ($\|\mathbf{f}_{\mathbf{D_j}}\|$ and $\|\mathbf{f}_{\mathbf{SPE_j}}\|$) is calculated as follows

$$\|\mathbf{f}_{\mathbf{j}}\| \ge \|\mathbf{f}_{\mathbf{D_j}}\| = 2\sigma_{\max}{}^{-1}(\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\boldsymbol{\theta}_{\mathbf{j}})\delta_{D,\alpha} \tag{12}$$

$$\|\mathbf{f}_{\mathbf{j}}\| \ge \|\mathbf{f}_{\mathbf{SPE_j}}\| = 2\sigma_{\max}{}^{-1}((\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\boldsymbol{\theta}_{\mathbf{j}})\delta_{SPE,\alpha} \tag{13}$$

where $\|\mathbf{f}_{\mathbf{j}}\|$ is the fault vector norm, $\|\mathbf{f}_{\mathbf{D_j}}\|$ is the critical fault magnitude (CFM) in the principal components subspace, $\|\mathbf{f}_{\mathbf{SPE_j}}\|$ is the CFM in the residual subspace, and $\sigma_{\max}$ (**arg**) is the maximum singular value of the matrix argument. For Wang et al.'s approach,[9] the statistic's CFM represents the minimum FM that it detects.

It should be noticed that the CFM calculations are conservative. For normal operating conditions, $D^{1/2}$ values range from 0 to $\delta_{D,\alpha}$, that is $0 \le \|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x_0}\| \le \delta_{D,\alpha}$. Because the norm of the vector $(\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x_0})$ is assumed exactly equal to $\delta_{D,\alpha}$, the CFM of D is the upper bound of the minimum FM detectable using this statistic.[9] Furthermore, if α is reduced and $\delta_{D,\alpha}$ increases, the CFM also increases. The same analysis can be performed for SPE.

3. OPTIMAL SELECTION OF SENSOR STRUCTURES FOR FAULT DETECTION PURPOSES

In this section, new formulations for the optimal selection of sensor configurations from a fault detection perspective are proposed. At first, the constraints that guarantee the detection of J faults when the process is monitored using PCA are considered. Both the FD restrictions[8] and the ones introduced in this work are presented. Then, the fault detection degree (DD) concept is defined and the constraints that should be satisfied to fulfill the detectability of a key faults set even in the presence of failed sensors are established. Finally, new optimization problems for instrumentation selection are formulated.

3.1. Fault Detection Constraints. On the basis of the formulations presented in ref 9, the j-th minimum critical fault magnitude ($MCFM_j$), which is the minimum FM that can be detected using the sensor configuration $\mathbf{q}$ when the process is monitored using PCA is defined[8]

$$\mathrm{MCFM}_j(\mathbf{q}) = \min\{\|\mathbf{f}_{\mathbf{D_j}}\|, \|\mathbf{f}_{\mathbf{SPE_j}}\|\} \tag{14}$$

It was considered that a SN is able to detect the occurrence of the j-th process fault if

$$\mathrm{MCFM}_j(\mathbf{q}) \le f_{\sup_j}(\mathbf{q}) \quad j = 1\cdots J \tag{15}$$

To evaluate $f_{\sup_j}(\mathbf{q})$, process deviation limits (PDLs) for all the variables are initially set. Those values should not be surpassed to avoid the occurrence of undesirable events during process operation. Then, the vector $\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}}$ ($j = 1. . .J$) of dimension I is evaluated by simulation. It represents the standardized measurement vector that would be obtained when one or more measurements reach their respective PDLs and all the variables are measured ($N = I$). If $x_j^{PDL}(i) > 3$, then the i-th variable is affected by the occurrence of the j-th failure.[8] On the basis of this information, the cause−effect matrix of the process, $\mathbf{A}$ (I,J), is stated. It is made up of binary elements such that $a_{ij} = 1$ if the i-th variable is affected by the occurrence of the j-th fault, and $a_{ij} = 0$ otherwise. The j-th column of $\mathbf{A}$, $\mathbf{a_j}$, is a binary vector that represents all the variables which reveal the j-th failure if they are measured. Also, a vector $\mathbf{f}_{\mathbf{j}}^{\mathbf{0}}$ is defined such that if $x_j^{PDL}(i) > 3$ then $\mathbf{f}_{\mathbf{j}}^{\mathbf{0}}(i)$ is the standardized variation of the i-th variable with respect to its normal value, and $\mathbf{f}_{\mathbf{j}}^{\mathbf{0}}(i) = 0$ otherwise. For a given SN, this vector is used to set a limit for the j-th FM, $f_{\sup_j}(\mathbf{q})$, which should not be exceeded due to operational and safety issues and is expressed as

$$f_{\sup_j}(\mathbf{q}) = \|\mathbf{f}_{\mathbf{j}}^{\mathbf{o}} * \mathbf{q}\| \tag{16}$$

where "∗" represents the element by element product between the two vectors.

Because the CFMs of both statistics are involved in the calculation of the FM-based restrictions, some solution vectors $\mathbf{q}$, which are certainly able to detect process faults, are discarded, as it was indicated in the previous section. That is, the use of the assumptions $\|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x_0}\| = \delta_{D,\alpha}$ and $\|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x_0}\| = \delta_{SPE,\alpha}$ affects the solution of the optimization problem. Therefore, different constraints are proposed to quantify the capability of a SN to detect process failures in this work. Those are straightaway defined in terms of D and SPE, as it is explained next.

The j-th fault should be detected before one or more variables affected by its occurrence reach their respective PDLs, but if this undesirable situation occurs and only N process variables are measured, the standardized measurement vector is a subvector of $\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}}$, denoted as $\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL*}}$, and the statistics values are

$$D_j(\mathbf{q}) = \|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL*}}\|^2 \tag{17}$$

$$\mathrm{SPE}_j(\mathbf{q}) = \|(\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL*}}\|^2 \tag{18}$$

Therefore, the SN represented by the vector $\mathbf{q}$ is able to detect the j-th fault before a dangerous event takes place if at least one of the two statistics, calculated using the eqs 17 and 18, exceeds its critical value. That is, if the following constraint is satisfied:

$$[(D_j(\mathbf{q}) \ge \delta_{D,\alpha}{}^2(\mathbf{q})) \vee (\mathrm{SPE}_j(\mathbf{q}) \ge \delta_{SPE,\alpha}{}^2(\mathbf{q}))] \quad j = 1\ldots J \tag{19}$$

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In this work, the fault detection constraints are defined in particular for the PCA's statistics, but the same approach can be used to state those restrictions for other statistical monitoring techniques.

3.2. Fault Detection Degree Constraints. To enhance the ability of the SN to detect key process failures even under the presence of failed sensors, the detection degree (DD) of a key fault (KF) is defined as an extension of the resolution degree[6] concept.

A SN has a DD equal to g_s for the s-th key fault (s-KF) if this failure remains detectable even when g_s observations, contained in the set of measurements affected by that fault occurrence, are not available. In this case, there are $t_s = (R_s!)/(g_s!(g_s - R_s)!)$ sensor configurations of dimension $(R_s - g_s)$ that are able to detect the s-KF when PCA is applied, where R_s is the number of variables affected by the s-KF. Therefore, t_s conditions for each KF should be satisfied to guarantee that the SN is able to cope with the malfunctioning of g_s sensors. This is mathematically formulated as follows

$$\{[D_s^r(\mathbf{q}) \geq (\delta_{D,\alpha}^r(\mathbf{q}))^2] \vee [\mathrm{SPE}_s^r(\mathbf{q}) \geq (\delta_{SPE,\alpha}^r(\mathbf{q}))^2]\}$$
$$r = 1\dots t_s; \quad s = 1\dots S \tag{20}$$

where S is the number of KFs, $D_s^r(\mathbf{q})$ and $SPE_s^r(\mathbf{q})$ represent the statistics values when the r-th sensor configuration is analyzed for the s-KF, and $(\delta_{D,\alpha}^r(\mathbf{q}))^2$ and $(\delta_{SPE,\alpha}^r(\mathbf{q}))^2$ stand for their critical values.

In this work, similar constraints are also formulated to devise more robust SNs when the FM approach is applied to analyze the FD ability of an instrumentation system. In this case, the DD restrictions are expressed as follows

$$\mathrm{MCFM}_s{}^r(\mathbf{q}) \leq f_{\sup s}^r(\mathbf{q}) \quad r = 1\dots t_s; \quad s = 1\dots S \tag{21}$$

where $\mathrm{MCMF}_s^r(\mathbf{q})$ and $f_{\sup s}^r$ are the *MCFM* and the upper FM for the r-th SN associated with the s-KF, respectively.

3.3. Formulations for the Optimal Upgrade of Measurements. In this subsection, different instrumentation selection problems are stated using the previously defined constraints. Problems based on *MCFM*-calculations are also formulated because their solutions are compared with those obtained using the new constraints in the next section.

At first, the upgrade problem is addressed. Let us consider that $\boldsymbol{\Omega}_0$ is the set of instruments which are already installed in the process to fulfill different information requirements. If the detection of the J faults is not satisfied using the measurements contained in that set, new sensors should be located in the process. The minimum-cost set of instruments whose incorporation guarantees the detection of all the process faults using PCA is obtained by solving the following optimization problem

$$\min_{\mathbf{q}} \mathbf{c}^{\mathrm{T}}\mathbf{q}$$
$$\text{s.t.}$$
$$[(D_j(\mathbf{q}) \geq \delta_{D,\alpha}{}^2(\mathbf{q})) \vee (\mathrm{SPE}_j(\mathbf{q}) \geq \delta_{SPE,\alpha}{}^2(\mathbf{q}))]$$
$$j = 1\dots J \tag{22}$$

which involves J nonlinear restrictions and where $\mathbf{c}$ stands for the vector of sensor costs. A zero element of $\mathbf{c}$ is associated with an existing instrument. For the sake of simplicity, the previous formulation does not take into consideration the existence of physical difficulties for the installation of sensors in the plant.

If it is also required to detect a set of KFs even when g_s instruments fail, Problem 22 is reformulated by incorporating the DD constraints represented by eq 20. The resulting upgrade problem is

$$\min_{\mathbf{q}} \mathbf{c}^{\mathrm{T}}\mathbf{q}$$
$$\text{s.t.}$$
$$[(D_j(\mathbf{q}) \geq \delta_{D,\alpha}{}^2(\mathbf{q})) \vee (\mathrm{SPE}_j(\mathbf{q}) \geq \delta_{SPE,\alpha}{}^2(\mathbf{q}))] \quad j = 1\dots J$$
$$\{[D_s^r(\mathbf{q}) \geq (\delta_{D,\alpha}^r(\mathbf{q}))^2] \vee [\mathrm{SPE}_s^r(\mathbf{q}) \geq (\delta_{SPE,\alpha}^r(\mathbf{q}))^2]\} \quad r = 1\dots t_s;$$
$$s = 1\dots S \tag{23}$$

which comprises $(j + \sum_{s=1}^{S} t_s)$ nonlinear restrictions.

Similar instrumentation upgrade formulations can be derived if the constraints are defined in terms of the FMs. In correspondence to Problems 22 and 23, the following upgrade problems are stated

$$\min_{\mathbf{q}} \mathbf{c}^{\mathrm{T}}\mathbf{q}$$
$$\text{s.t.}$$
$$\mathrm{MCFM}_j(\mathbf{q}) \leq f_{\sup_j}(\mathbf{q}) \quad j = 1\dots J \tag{24}$$

$$\min_{\mathbf{q}} \mathbf{c}^{\mathrm{T}}\mathbf{q}$$
$$\text{s.t.}$$
$$\mathrm{MCFM}_j(\mathbf{q}) \leq f_{\sup_j}(\mathbf{q}) \quad j = 1\dots J$$
$$\mathrm{MCFM}_s^r(\mathbf{q}) \leq f_{\sup s}^r(\mathbf{q}) \quad r = 1\dots t_s; \quad s = 1\dots S \tag{25}$$

The solution of Problem 24 satisfies the detection of all the failures when all the measurements are available. This formulation involves J nonlinear constraints defined in terms of the $MCFM_j$ and $f_{\sup_j}$ $(j = 1..J)$. Regarding Problem 25, the incorporation of the DD restrictions, defined by eq 21, to Problem 24 increases the number of nonlinear constraints to $(j + \sum_{s=1}^{S} t_s)$.

With respect to restrictions complexity, it should be noticed that the evaluation of the $MCFM_j$ requires the singular value decomposition of two matrices (see eqs 12 and 13). In contrast, it is necessary to calculate the norm of two vectors to obtain D_j and SPE_j values.

Besides, engineers deal with other instrumentation selection problems. Regarding the design, it can be performed using the methodology presented in this work if a dynamic simulation of the process is available to characterize its dynamic behavior with reasonably good accuracy to study the control and fault diagnosis of the system.[8−10] In this case, all the elements of vector $\mathbf{c}$ are nonzero given that $\boldsymbol{\Omega}_0$ is the null vector.

Another issue of interest is the selection of existing signals to perform PCA monitoring. Let us consider that ES sensors are already installed in the plant. Those measure the I variables involved in the cause−effect matrix $\mathbf{A}$ and another ones. In contrast to the upgrade problem, all the instruments that could be used for the detection of the J faults are already located in the process, and an optimal subset of them should be selected.

In this work, a lexicographic optimization approach is proposed to choose the variables contained in $\mathbf{A}$ which take part of the monitoring procedure; that is, the current solution involves $N(\mathbf{q}) \leq I$ observations. The objective function of Problems 22−25 is modified as follows

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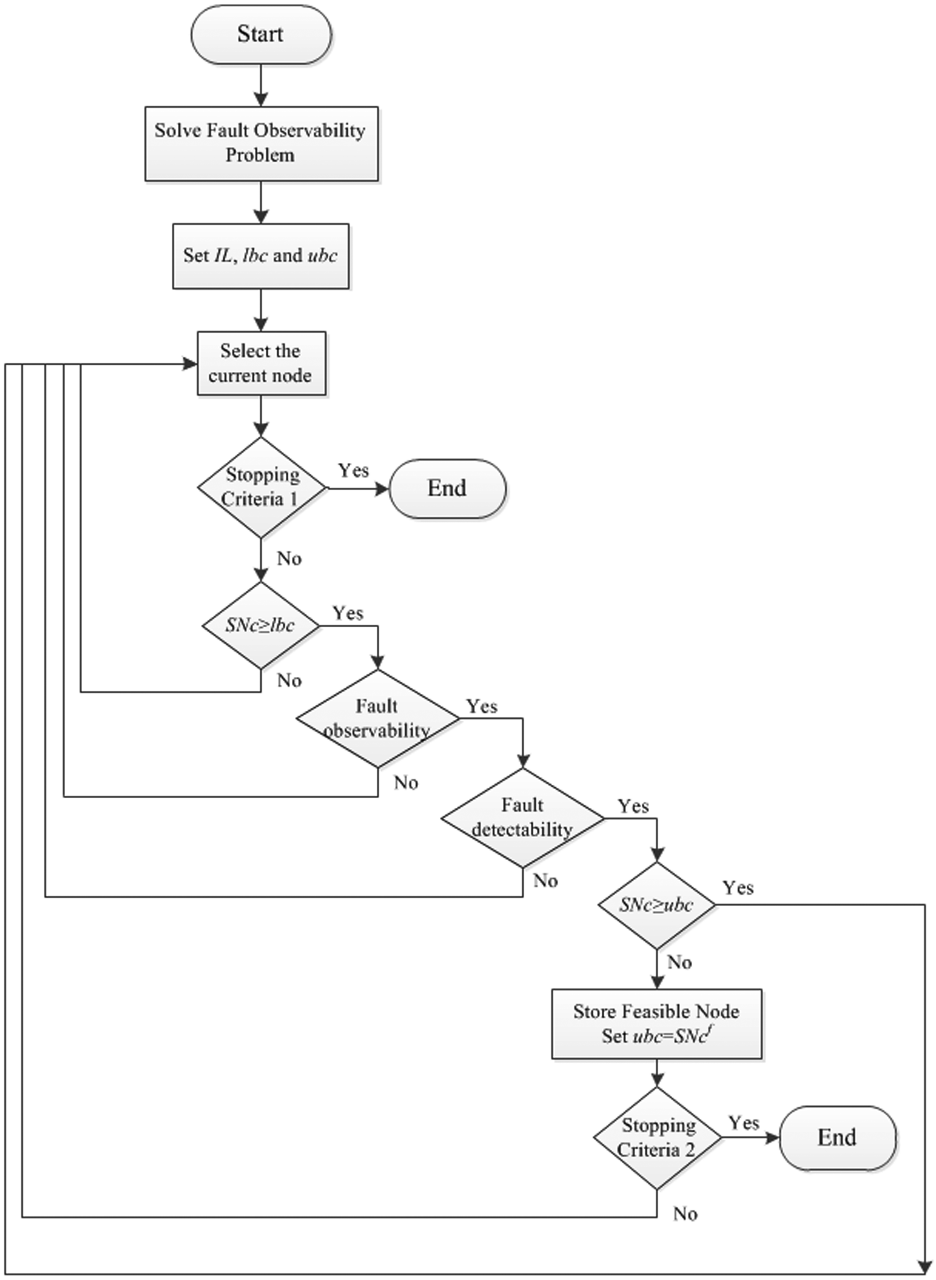

Figure 1. Flowchart of the ad-hoc traversal tree search.

$$\mathrm{OF}_N = [(1 + w_T)N(\mathbf{q}) + \mathbf{w}^\mathrm{T}\mathbf{q}] \tag{26}$$

where $N(\mathbf{q})$ and $\mathbf{w}^\mathrm{T}\mathbf{q}$ are the objectives in decreasing order of preference,[12] $\mathbf{w}^\mathrm{T}$ is the vector of weights assigned to each measured variable, and w_T is the sum of all the individual weights. By minimizing OF_N, the number of signals involved in the PCA-based monitoring is considered as the primary objective and the type of instrument as the secondary one. The weights are assumed by the engineers taking into account their preferences regarding the different kinds of sensors. For example, $\mathbf{w}^\mathrm{T}$ may be the vector of sensor costs, which in some way takes into consideration the advantages and difficulties associated with the measurement of a variable.

4. SOLUTION PROCEDURE

In this work, an ad-hoc traversal tree search is proposed to solve the previously defined sensor upgrade problems. The solution algorithm is based on the Breadth-First/Level Traversal Tree Search with stopping criteria presented by Nguyen and Bagajewicz.[13] It consists of examining the nodes in a tree data structure in level-order. The tree is built using the cheapest candidate (minimum-cost branching criteria), and cost properties of the different nodes of the tree are exploited to efficiently prune nonoptimal nodes.

The procedure[13] is appropriate to solve the proposed optimization problems, but the solution scheme can be improved taking into consideration that the observability (structural determinability) of a fault is a necessary but not a sufficient condition to satisfy its detection when the process is monitored using PCA.[9]

Let us review the fault observability definition. A failure diagnosis system should be able to observe the symptoms of the fault and determine its cause. A fault is categorized as observable if at least one sensor indicates the existence of the

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abnormal event.[1] Given a SN, the observability of the j-th fault can be verified using the operation of conjunction between the fault vector $\mathbf{a_j}$ and the vector $\mathbf{q}$. This failure is observable if the sum of all the elements of the vector $(\mathbf{a_j} \wedge \mathbf{q})$ is greater or equal to 1. Therefore, the observability of all process faults is formulated as follows[6]

$$\sum_{i=1}^{I} (\mathbf{a_j} \wedge \mathbf{q})_i \geq 1 \quad (j = 1, ..., J) \tag{27}$$

where $\mathbf{rv_j} = (\mathbf{a_j} \wedge \mathbf{q})$ is defined as the resolution vector ($\mathbf{rv}$) of the j-th failure, and $rv_j(i) = 1$ indicates that the i-th variable is measured and affected by the occurrence of that fault. It should be noticed that the observability of all the failures can be easily tested using a set of J linear inequalities.

In this work, augmented upgrade problems are solved by incorporating observability restrictions to Problems 22 and 24 to enhance the traversal tree search efficiency. Those are formulated as follows

$$\begin{aligned} &\min_{\mathbf{q}} \mathbf{c^T q} \\ &\text{s.t.} \\ &\sum_{i=1}^{I} (\mathbf{rv_j(q)})_\mathbf{i} \geq 1 \quad j = 1 \ldots J \\ &[(D_j(\mathbf{q}) \geq \delta_{D,\alpha}{}^2(\mathbf{q})) \vee (\mathrm{SPE}_j(\mathbf{q}) \geq \delta_{SPE,\alpha}{}^2(\mathbf{q}))] \\ &\quad j = 1 \ldots J \end{aligned} \tag{28}$$

$$\begin{aligned} &\min_{\mathbf{q}} \mathbf{c^T q} \\ &\text{s.t.} \\ &\sum_{i=1}^{I} (\mathbf{rv_j(q)})_\mathbf{i} \geq 1 \quad j = 1 \ldots J \\ &\mathrm{MCFM}_j(\mathbf{q}) \leq f_{\mathrm{sup}_j}(\mathbf{q}) \quad j = 1 \ldots J \end{aligned} \tag{29}$$

In the Appendix, it is demonstrated that the solutions of Problems 22 and 28 are equal. The same condition is also verified when FM constraints are considered (Problems 24 and 29).

It can be observed that the augmented optimization problems are subject to a set of linear fault observability restrictions and a set of nonlinear failure detectability constraints. A two-step procedure is devised to solve those problems. In Step 1, the minimum-cost SN that satisfies the observability of all the faults is easily obtained using a mixed integer linear optimization code. The solution of Step 1 is used to set: (1) the initial level (IL) of the traversal tree search for solving the augmented problem and (2) a lower limit for the cost (lbc). If all the variables contained in the complement of $\mathbf{\Omega_0}$ are measured, the total cost of the upgrade instrumentation project is ubc. This constitutes an upper bound for the SNc, which is updated when the algorithm finds a feasible node.

In Step 2, the search is initiated by exploring the lower-cost node of the previously fixed IL. The algorithm goes through nodes of incremental SNc until one of the cutting criteria are satisfied.[13]

To evaluate the feasibility of a node, first its SNc is calculated. If it is lower than lbc, the current node is disregarded. If it is not the case, then fault observability restrictions are calculated. If they are unsatisfied, the current node is ignored because failure observability is a necessary condition for FD. In contrast, the computation of detectability constraints continues. In this way, the computational load is reduced because the evaluation of the linear constraints is faster than the computation of the nonlinear ones. If the node satisfies the FD constraints and its SNc is greater than ubc, it is not taken into consideration. On the other hand, it constitutes the current solution and is stored. The ubc is set equal to the cost of that feasible solution, SNc^f. The search continues level by level until one of the stopping criteria is reached.[13]

A flowchart of the solution scheme is shown in Figure 1. In the Appendix, it is also proved that the solutions of the augmented problems are equal to those obtained using the developed procedure.

In summary, the efficiency of the existing traversal tree search with stopping criteria is enhanced using a particular feature of the design problem; that is, fault observability is a necessary condition to satisfy its detection. At first, this is used to determine the search IL of the Step 2, and the lbc. Then, it is applied to perform a fast analysis about the convenience of evaluating the detectability restrictions for a given node.

To consider the possibility of sensor malfunctioning, the observability degree (OD) is defined as follows. A SN has an OD equal to g_s for the s-KF, if this failure remains observable even when g_s observations, contained in the set of measurements affected by the fault occurrence, are not available. In this case, there exist $t_s = (R_s!)/(g_s!(g_s - R_s)!)$ sensor configurations of dimension $(R_s - g_s)$ that are able to observe the s-KF when PCA is applied.

Therefore, t_s conditions for each KF should be satisfied to ensure that the SN is able to cope with the malfunctioning of g_s sensors. This is mathematically formulated as follows

$$\sum_{i=1}^{I} (\mathbf{rv_s^r(q)})_\mathbf{i} \geq 1 \quad r = 1 \ldots t_s; \quad s = 1 \ldots S \tag{30}$$

where $\mathbf{rv_s^r}$ is the resolution vector of the s-KF when g_s observations, affected by the occurrence of this failure, are unavailable.

The OD concept is used to enhance the solution of Problem 23 taking into consideration that the observability of a fault is a necessary condition to satisfy its detection even when one or more observations associated with its $\mathbf{rv}$ are unavailable. Therefore, OD and DD constraints are incorporated as restrictions to Problem 23, and the following augmented optimization problem results

$$\begin{aligned} &\min_{\mathbf{q}} \mathbf{c^T q} \\ &\text{s.t.} \\ &\sum_{i=1}^{I} (\mathbf{rv_j(q)})_\mathbf{i} \geq 1 \quad j = 1 \ldots J \\ &\sum_{i=1}^{I} (\mathbf{rv_s^r(q)})_\mathbf{i} \geq 1 \quad r = 1 \ldots t_s; \quad s = 1 \ldots S \\ &[(D_j(\mathbf{q}) \geq \delta_{D,\alpha}{}^2(\mathbf{q})) \vee (\mathrm{SPE}_j(\mathbf{q}) \geq \delta_{SPE,\alpha}{}^2(\mathbf{q}))] \quad j = 1 \ldots J \\ &\{[D_s^r(\mathbf{q}) \geq (\delta_{D,\alpha}^r(\mathbf{q}))^2] \vee [\mathrm{SPE}_s^r(\mathbf{q}) \geq (\delta_{SPE,\alpha}^r(\mathbf{q}))^2]\} \quad r = 1 \ldots t_s; \\ &\quad s = 1 \ldots S \end{aligned} \tag{31}$$

It comprises $(j + \Sigma_{s=1}^{S} t_s)$ linear constraints that satisfy the observability of all the faults when no instrument fails and the observability of a set of KFs when g_s observations, which belong

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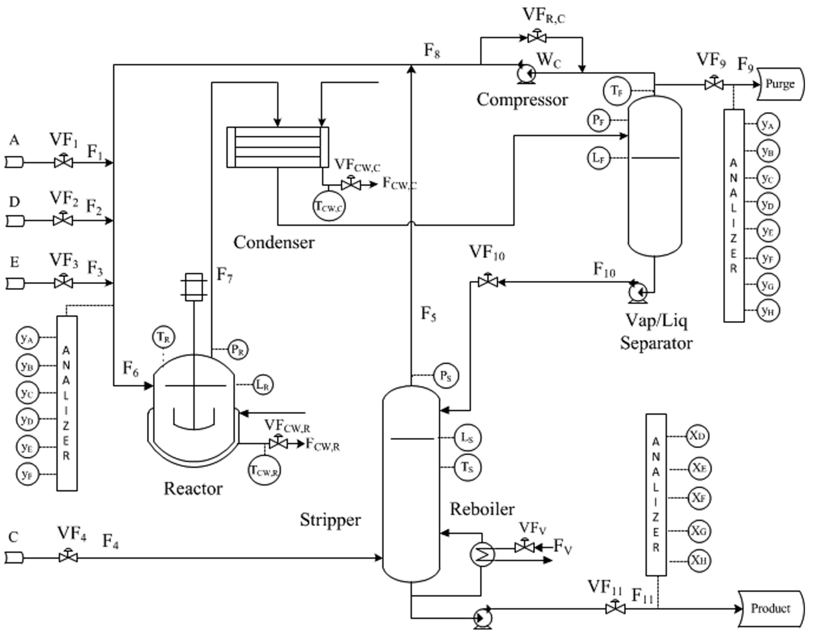

Figure 2. Tennessee Eastman Process flowsheet.

to their respective **rv**s, are unavailable. Eq 31 also includes $(j + \sum_{s=1}^{S} t_s)$ nonlinear restrictions associated with the FD when all sensors work satisfactorily or not. It is proposed to solve Problem 31 using the two step procedure previously explained. First, the minimum cost SN that satisfies the observability and OD linear restrictions is calculated to set the IL of the traversal search used to solve the augmented problem and the lbc. Then, the solution of Problem 31 is obtained by exploring nodes of incremental cost. When a node is evaluated, the satisfaction of the linear constraints is verified first to reduce the computational load. If they are unfulfilled, the current node is disregarded; if it is not the case, the evaluation of detection and DD constraints is performed.

A similar augmented optimization problem can be formulated to take into account sensor malfunctioning when detectability constraints are expressed in terms of FMs. In this case, Problem 25 is reformulated by incorporating the OD and DD restrictions and the following upgrade problem results

$$\begin{aligned}
&\min_{\mathbf{q}} \mathbf{c}^{\mathbf{T}}\mathbf{q}\\
&\text{s.t.}\\
&\sum_{i=1}^{I} (\mathbf{rv_j}(\mathbf{q}))_{\mathbf{i}} \geq 1 \quad j = 1 \ldots J\\
&\sum_{i=1}^{I} (\mathbf{rv_s^r}(\mathbf{q}))_{\mathbf{i}} \geq 1 \quad r = 1 \ldots t_s; \quad s = 1 \ldots S\\
&\mathrm{MMCF}_j(\mathbf{q}) \leq f_{\sup_j}(\mathbf{q}) \quad j = 1 \ldots J\\
&\mathrm{MMCF}_s^r(\mathbf{q}) \leq f_{\sup s}^r(\mathbf{q}) \quad r = 1 \ldots t_s; \quad s = 1 \ldots S
\end{aligned} \tag{32}$$

5. CASE STUDY

In this paper, the Tennessee Eastman Process (TEP)[14] is used to analyze the solutions provided by the different SN upgrade formulations. The process flowsheet is presented in Figure 2 and comprises five principal units: a jacketed reactor, a condenser, a vapor/liquid separator, a compressor, and a stripper. Simulated data of the normal operation of the process and the dynamic system behavior when certain faults have occurred were reported in ref 15. Those data are used to illustrate the application of the upgrade methodologies proposed in this work. Thus, it is assumed that normal operating data are obtained from an existing plant, whose dynamic behavior is characterized with reasonably good accuracy by means of its dynamic simulation.

The faults associated with this case study are the following[15]

- Fault 1: Step in $y_{A,4}/y_{C,4}$ feed ratio, $y_{B,4}$ constant
- Fault 2: Step in $y_{B,4}$, $y_{A,4}/y_{C,4}$ ratio constant
- Fault 3: Step in $T_{CW,R}$ (inlet)
- Fault 4: Step in $T_{CW,C}$ (inlet)
- Fault 5: Step in F_1
- Fault 6: Step in C header pressure loss, reduced availability (Stream 4)
- Fault 7: Slow drift in reaction kinetics
- Fault 8: Sticking in Reactor CW valve

At first, the maximum deviation of each measurement, md_i, is calculated using normal operating data. Then, a vector $\mathbf{x_j^{PDL}}$ is obtained for each failure considering that PDL(i) = 2md$_i$ (i = 1. . .I). The variables affected by the occurrence of all those faults for the selected PDL values are included in Table 1. It also shows the costs of the available sensors to measure them. In this case study, the purpose of the instrumentation selection problem is to upgrade an existing SN. It is considered that the manipulated variables are measured and their costs are set at zero.

Table 2 shows the signed cause−effect relationship among faults and process variables for the selected PDLs values. Furthermore, the percentage of the total variance reconstructed by the latent variable model is fixed at 80%.

For this case study, different types of instrumentation upgrade problems are solved. One class takes into account only observability and detection restrictions (O+D) (Problems 28 and 29). The other type also includes observability and detection degree (ODD) constraints (Problems 31 and 32). An

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Table 1. Process Variables

process variables	notation	cost
reactor pressure	P_R	100
stripper pressure	P_S	100
flash pressure	P_F	100
A Feed (Stream 1)	F_1	300
D Feed (Stream 2)	F_2	300
E Feed (Stream 3)	F_3	300
total feed (Stream 4)	F_4	300
reactor feed rate (Stream 6)	F_6	300
purge rate (Stream 9)	F_9	300
compressor work	W_C	400
A Feed Flow, manipulated variable (Stream 1)	VF_1	0
D Feed Flow, manipulated variable (Stream 2)	VF_2	0
E Feed Flow, manipulated variable (Stream 3)	VF_3	0
total feed flow, manipulated variable (Stream 4)	VF_4	0
purge valve, manipulated variable (Stream 9)	VF_9	0
compressor recycle valve, manipulated variable	$VF_{R,C}$	0
reactor cooling water flow, manipulated variable	$VF_{CW,R}$	0
reactor temperature	T_R	500
flash temperature	T_F	500
reactor cooling water outlet temperature	$T_{CW,R}$	500
condenser cooling water outlet temperature	$T_{CW,C}$	500
molar fraction of E in Stream 11	$x_{E,11}$	700
molar fraction of H in Stream 11	$x_{H,11}$	700
molar fraction of A in Stream 6	$y_{A,6}$	800
molar fraction of B in Stream 6	$y_{B,6}$	800
molar fraction of C in Stream 6	$y_{C,6}$	800
molar fraction of D in Stream 6	$y_{D,6}$	800
molar fraction of A in Stream 9	$y_{A,9}$	800
molar fraction of B in Stream 9	$y_{B,9}$	800
molar fraction of C in Stream 9	$y_{C,9}$	800
molar fraction of D in Stream 9	$y_{D,9}$	800
molar fraction of E in Stream 9	$y_{E,9}$	800
molar fraction of G in Stream 9	$y_{G,9}$	800
molar fraction of H in Stream 9	$y_{H,9}$	800

Table 2. Signed Cause−Effect Relationship

variables	F1	F2	F3	F4	F5	F6	F7	F8
P_R	1	0	0	0	0	0	−1	0
P_S	1	0	0	0	0	−1	−1	0
P_F	1	0	0	0	0	0	−1	0
F_1	1	0	0	0	−1	0	0	0
F_2	0	0	0	0	0	0	−1	0
F_3	0	0	0	0	0	0	1	0
F_4	0	0	0	0	0	−1	0	0
F_6	0	0	0	0	0	−1	0	0
F_9	0	1	0	0	0	0	1	0
W_C	−1	0	0	0	0	0	0	0
VF_1	1	0	0	0	1	0	0	0
VF_2	0	0	0	0	0	0	−1	0
VF_3	0	0	0	0	0	0	1	0
VF_4	0	0	0	0	0	1	0	0
VF_9	0	1	0	0	0	0	1	0
$VF_{R,C}$	−1	0	0	0	0	0	0	0
$VF_{CW,R}$	0	0	1	0	0	−1	0	1
T_R	0	0	1	0	0	−1	0	1
T_F	0	0	0	1	0	0	1	0
$T_{CW,R}$	1	0	0	−1	1	1	0	0
$T_{CW,C}$	0	0	0	1	0	−1	1	0
$x_{E,11}$	0	0	0	0	0	0	−1	0
$x_{G,11}$	0	0	0	0	0	0	−1	0
$y_{A,6}$	−1	0	0	0	0	0	0	0
$y_{B,6}$	0	1	0	0	0	0	0	0
$y_{C,6}$	1	0	0	0	0	0	0	0
$y_{D,6}$	1	0	0	0	0	0	0	0
$y_{A,9}$	−1	0	0	0	0	0	0	0
$y_{B,9}$	0	1	0	0	0	0	0	0
$y_{C,9}$	1	0	0	0	0	0	0	0
$y_{D,9}$	0	0	0	0	0	0	1	0
$y_{E,9}$	0	0	0	0	0	0	−1	0
$y_{G,9}$	0	0	0	0	0	0	1	0
$y_{H,9}$	0	0	0	0	0	0	1	0

ad-hoc level traversal search algorithm programmed in Matlab code is applied to solve the optimization problems. Their solutions are reported in Tables 3 and 4 for α = 0.05 and 0.03, respectively. It is interesting to note the following issues:

- The overall result analysis indicates that the maximum ODD for faults 3 and 8 is equal to 1, while ODD ≤ 2 for the rest of the failures.
- The total number of binary variables is 34. The total number of constraints for upgrade problems that involve (O+D) restrictions is 16 (8 for observability and 8 for FD). That number increases when ODD constraints should be also fulfilled. In this sense, the optimization problems that satisfy the set of conditions closed into brackets [O+D+ODD_3 = 1; O+D+ODD_8 = 1], [O+D+ODD_4 = 1; O+D+ODD_4 = 2; O+D+ODD_5 = 1; O+D+ODD_5 = 2], [O+D+ODD_2 = 1], [O+D+ODD_2 = 2], [O+D+ODD_6 = 1], [O+D+ODD_6 = 2], [O+D+ODD_1 = 1], [O+D+ODD_1 = 2], [O+D+ODD_7 = 1], [O+D+ODD_7 = 2] comprise 20, 22, 24, 28, 32, 72, 42, 94, 50, and 152 restrictions, respectively.
- The computational time increases with the number of constraints. It also depends on the approach used to evaluate the fault detection capability of the network. Lower computational times are required when the restrictions proposed in this work are used. For this example, the achieved reduction factor is 4.3 for problems subject to (O+D) constraints, and that factor is 4.6 for the upgrade problem that fulfills (O+D+ODD_7 = 2) restrictions.
- In general, the solutions depend on the α values. Higher-cost SNs are obtained when α decreases for the same set of restrictions. For example, when the constraints are (O+D+ODD_1 = 1) and α = 0.05 for the statistic-based approach, the solution set is (P_R VF_9 $VF_{CW,R}$ $T_{CW,R}$), but it is (P_R F_1 VF_9 $VF_{CW,R}$ $T_{CW,R}$) for α = 0.03.
- Higher-cost SNs are also obtained when FM-based constraints are applied. This technique assumes that $\|\mathbf{D}_\lambda^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x}_0\| = \delta_{D,\alpha}$ when in fact $0 \leq \|\mathbf{D}_\lambda^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x}_0\| \leq \delta_{D,\alpha}$. Therefore, the solutions which verify the inequality $\|\mathbf{D}_\lambda^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x}_0\| < \delta_{D,\alpha}$ are discarded. In contrast, those are considered feasible SNs when statistic-based restrictions are considered. For example, the SN that fulfills (O+D) constraints for α = 0.05 (VF_9 $VF_{CW,R}$ $T_{CW,R}$) can not detect the fault 6 when FM-based restrictions are evaluated.
- For a given fault, the solution cost increases with the increment of the ODD requirements. For example, the SN that satisfies (O+D+ODD_2 = 1) restrictions for α = 0.05 when statistic-based constraints are used has four instruments (F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$) and its cost is 800,

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Table 3. Results for α = 0.05

constraints	statistic-based solution	cost	FM-based solution	cost
O+D	VF_9 $VF_{CW,R}$ $T_{CW,R}$	500	F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$	800
O+D+ODD_1 = 1	P_R VF_9 $VF_{CW,R}$ $T_{CW,R}$	600	P_R F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$	900
O+D+ODD_1 = 2	P_R P_S VF_9 $VF_{CW,R}$ $T_{CW,R}$	700	P_R F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1400
O+D+ODD_2 = 1	F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$	800	F_6 F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$	1100
O+D+ODD_2 = 2	F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$ $y_{B,9}$	1600	F_6 F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$ $y_{B,6}$	1900
O+D+ODD_3 = 1	F_1 VF_9 $VF_{CW,R}$ T_R T_F	1300	F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$ T_R	1300
O+D+ODD_4 = 1	F_6 VF_9 $VF_{CW,R}$ T_F	800	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_4 = 2	VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$ $T_{CW,C}$	1500	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$ $T_{CW,C}$	1800
O+D+ODD_5 = 1	F_1 F_2 VF_9 $VF_{CW,R}$ $T_{CW,R}$	1100	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_5 = 2	F_1 F_2 VF_9 $VF_1VF_{CW,R}$ $T_{CW,R}$	1100	F_1 F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1600
O+D+ODD_6 = 1	VF_9 $VF_{CW,R}$ $T_{CW,R}$	500	F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$	800
O+D+ODD_6 = 2	P_S VF_9 $VF_{CW,R}$ $T_{CW,R}$	600	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_7 = 1	P_R VF_9 $VF_{CW,R}$ $T_{CW,R}$	600	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_7 = 2	P_R P_S VF_9 $VF_{CW,R}$ $T_{CW,R}$	700	P_R F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1400
O+D+ODD_8 = 1	F_1 VF_9 $VF_{CW,R}$ T_R T_F	1300	F_6 VF_9 $VF_{CW,R}$ T_R $T_{CW,R}$	1300

Table 4. Results for α = 0.03

constraints	statistic-based solution	cost	FM-based solution	cost
O+D	VF_9 $VF_{CW,R}$ $T_{CW,R}$	500	F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$	800
O+D+ODD_1 = 1	P_R F_1 VF_9 $VF_{CW,R}$ $T_{CW,R}$	900	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_1 = 2	P_R P_S F_1 VF_9 $VF_{CW,R}$ $T_{CW,R}$	1000	P_R F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1400
O+D+ODD_2 = 1	F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$	800	F_6 F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$	1100
O+D+ODD_2 = 2	F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$ $y_{B,9}$	1600	F_6 F_9 VF_9 $VF_{CW,R}$ $T_{CW,R}$ $y_{B,6}$	1900
O+D+ODD_3 = 1	F_1 VF_9 $VF_{CW,R}$ T_R T_F	1300	F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$ T_R	1300
O+D+ODD_4 = 1	F_6 VF_9 $VF_{CW,R}$ T_F	800	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_4 = 2	F_6 VF_9 $VF_{R,C}$ T_F $T_{CW,R}$ $T_{CW,C}$	1800	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$ $T_{CW,C}$	1800
O+D+ODD_5 = 1	F_1 VF_9 T_R $T_{CW,R}$	1300	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_5 = 2	F_1 VF_9 VF_1 T_R $T_{CW,R}$	1300	F_1 F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1600
O+D+ODD_6 = 1	VF_9 $VF_{CW,R}$ $T_{CW,R}$	500	VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1000
O+D+ODD_6 = 2	P_S VF_9 $VF_{CW,R}$ $T_{CW,R}$	600	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_7 = 1	F_2 VF_9 $VF_{CW,R}$ $T_{CW,R}$	800	F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1300
O+D+ODD_7 = 2	P_R F_2 VF_9 $VF_{CW,R}$ $T_{CW,R}$	900	P_R F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$	1400
O+D+ODD_8 = 1	F_1 VF_9 $VF_{CW,R}$ T_R T_F	1300	F_6 VF_9 $VF_{CW,R}$ T_R $T_{CW,R}$	1300

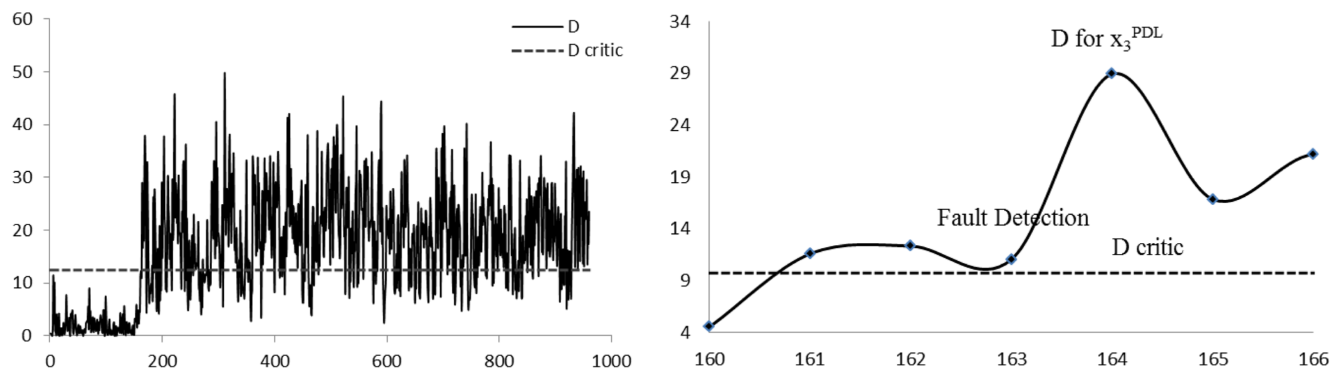

Figure 3. *D* chart for fault 3 (set SN1).

while if (O+D+ODD_2 = 2) restrictions are imposed, the solution comprises an additional instrument, $y_{B,9}$. The solutions obtained for the FM-based approach also show the same behavior.

- The solutions only guarantee KFs detectability when sensors fail. For example, the SN that satisfies (O+D+ODD_6 = 1) statistic-based constraints for α = 0.05 and α = 0.03 (VF_9 $VF_{CW,R}$ $T_{CW,R}$) can not detect the non-key faults 4 and 5 if the $T_{CW,R}$ sensor is unavailable. Moreover, the SN that fulfills (O+D+ODD_6 = 1) FM-based restrictions for α = 0.05 (F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$) is unable to detect the failures 3 and 8 if the $VF_{CW,R}$ sensor fails.

Next, the fault detection capabilities of both upgrade approaches are illustrated for some failures in terms of the time evolution of *D*. Let us remember that, when the PCA monitoring technique is used, it is a common practice to declare the fault state if *D*, *SPE*, or both of them exceed their critical values during three consecutive time intervals.[16] For the analyzed examples, *SPE* detects the failure after that *D* exceeds its critical value; therefore, only the *D* charts are presented.

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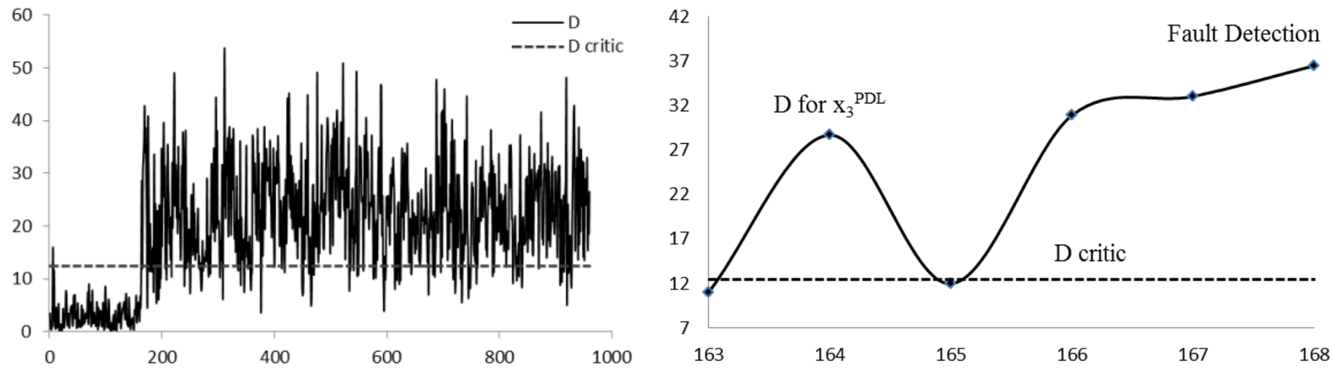

Figure 4. *D* chart for fault 3 (set SN2).

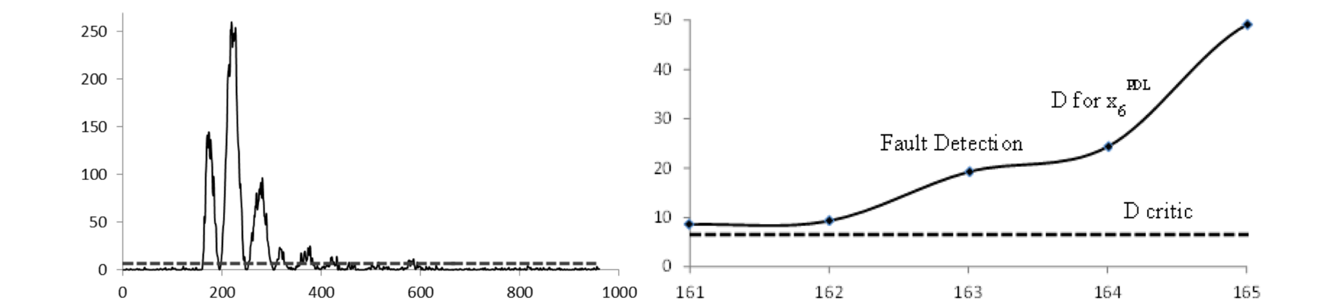

Figure 5. *D* chart for fault 6 (set SN3).

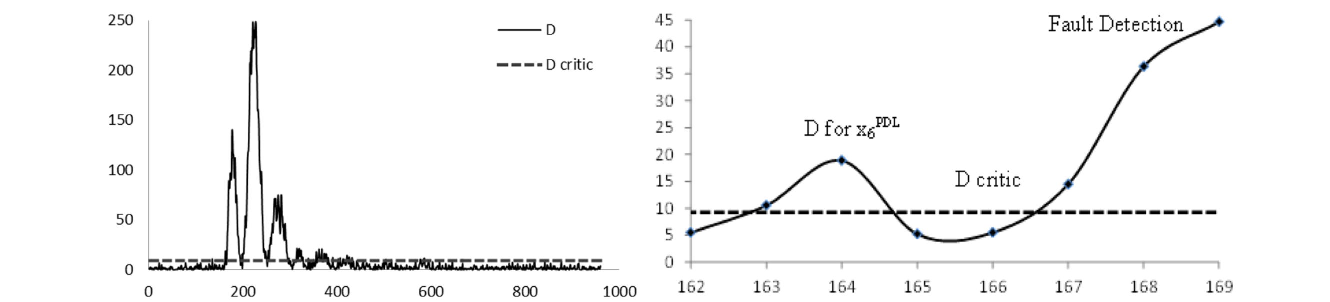

Figure 6. *D* chart for fault 6 (set SN4).

Regarding the upgrade problem for O+D constraints (α = 0.03), *D* values when fault 3 occurs are shown on the left-hand side of Figure 3. Those are obtained when the SN is constituted by the set of instruments VF_9 $VF_{CW,R}$ $T_{CW,R}$, called set SN1, which is the solution provided by the statistical-based approach. A zoom of the previous figure around the fault-detection time interval is displayed on the right-hand side of that picture. It is observed that SN1 allows the detection of the fault before the PDLs are reached. The same information is contained in Figure 4 for the SN formed by the instruments F_6 VF_9 $VF_{CW,R}$ $T_{CW,R}$, called set SN2, which is the solution obtained by the FM-based approach. Even though SN2 allows the detection of fault 3, its cost is higher than the corresponding one to SN1 and the failure is detected after the PDLs are exceeded. Thus, the installation of the sensor F_6 increases the cost of the upgrade project and no improvement on this fault detection is achieved.

Regarding the upgrade solutions for O+D+ODD$_6$ = 2 constraints when α = 0.03, the set of instruments P_S VF_9 $VF_{CW,R}$ $T_{CW,R}$ satisfies the detection of all the faults when no sensor fails and also fault 6 detection when two of those measurements are unavailable. That sensor set is obtained by applying the statistic-based approach. Figure 5 presents the *D* chart when fault 6 occurs, and the available measurements are only P_S VF_9, called set SN3. It can be seen that the fault is detected before the PDLs are exceeded. In contrast, Figure 6 shows that if two measurements of the set F_6 VF_9 $VF_{CW,R}$ T_F $T_{CW,R}$, which is the solution of the same upgrade problem provided by the FM-based technique, are unavailable, then the fault 6 is detected after the PDLs are surpassed. In that picture, the set of working sensors is made up of F_6 VF_9 T_F, called set SN4.

For the analyzed examples, figures show that the sensor configurations obtained using both methodologies satisfy the fault's detection, both when O+D and O+D+ODD$_i$ restrictions are imposed. This condition has been validated for all the solutions contained in Tables 3 and 4. Also, it is observed from Figures 4 and 6 that the sensor networks provided by the FM-based approach could perform the detection after the fault magnitudes reach the PDLs. Furthermore, that approach gives high-cost solutions in general (see Tables 3 and 4).

6. CONCLUSIONS

In this work, the upgrade of minimum cost SNs that fulfill the detection of a given set of faults when the process is monitored using PCA is addressed. The technique guarantees that the

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faults are detected before their magnitudes exceed a given threshold. With this purpose, a new fault detection constraint is straightaway formulated in terms of the PCA's statistics. It is also discussed how that restriction can be used when other statistical monitoring techniques are applied.

Moreover, the fault DD concept is defined in this work, and the conditions that satisfy the detectability requirements of a set of KFs in the presence of malfunctioning sensors are stated and included as constraints of the SN upgrade problems. These are subject to nonlinear restrictions (fault detection and DD), and their solutions can be obtained using a level traversal search with cutting criteria or stochastic procedures.

Taking into account that the observability of a fault is a necessary condition for its detection, the efficiency of the algorithms used to solve the aforementioned optimization problems can be enhanced by incorporating the observability and OD constraints to their formulations. In this work, a level traversal search with cutting criteria is implemented to get the solution of those augmented problems.

The initial level of the search and a lower bound for the cost are quickly determined solving the upgrade problem subject only to a set of linear inequalities constraints, which takes into account the faults observability and OD requirements. Moreover, the solution of this linear optimization problem provides other advantages. When the feasibility of a node is examined during the solution of the augmented problem, many unfeasible nodes can be easily discarded if linear constraints are examined at first. This reduces the computational load of the solution scheme.

Different upgrade problems are formulated using both statistic- and FM-based restrictions. From the analysis of the obtained results, it can be observed that the first approach finds feasible solutions that the second one discards. For this reason, the methodology that uses statistic-based constraints provides lower-cost solutions. Moreover, the results indicate that the SN cost increases when the requirements on the ODD increase.

■ APPENDIX

At first it is demonstrated that FD is a sufficient condition to satisfy failure observability.

Let us consider a SN represented by a vector $\mathbf{q}$, which comprises N measured variables. The j-th fault is detectable by the PCA monitoring method if eq 19 is satisfied: $[(D_j(\mathbf{q}) \geq \delta_{D,\alpha}{}^2(\mathbf{q})) \vee (SPE_j(\mathbf{q}) \geq \delta_{SPE,\alpha}{}^2(\mathbf{q}))]$ $j = 1...J$, where $D_j(\mathbf{q}) = \|\mathbf{\Lambda}^{-1/2}\mathbf{P}^{\mathrm{T}}\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}*}\|^2$ and $SPE_j(\mathbf{q}) = \|(\mathbf{I} - \mathbf{PP}^{\mathrm{T}})\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}*}\|^2$. Therefore, at least one variable, i.e., the n-th variable, is affected by the j-th fault occurrence, and the inequality $x_j^{PDL}*(n) \geq 3 > x_0(n)$ is satisfied. If the n-th element of $\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}*}$ corresponds to the i-th element of $\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}}$ ($x_j^{PDL}(i) = x_j^{PDL}*(n)$), the equality $a_{ij} = 1$ is true, and the fault observability condition $\Sigma_{i=1}^{I} (\mathbf{a}_{\mathbf{j}} \wedge \mathbf{q})_i \geq 1$ is also verified. Consequently, if a SN satisfies FD restrictions, it also fulfills observability constraints, and Problems 22 and 28 are equivalent. Then, it is demonstrated that fault observability is a necessary condition for failure detection.

On the contrary, let us assume that the j-th fault is not observable but can be detected. If that failure is unobservable, then $\Sigma_{i=1}^{I} (\mathbf{a}_{\mathbf{j}} \wedge \mathbf{q})_i \geq 1$; that is, the positions where the elements of both vectors are equal to 1 are not coincident, i.e., for the i-th measured variable, $q(i) = 1$ and $a_j(i) = 0$.

Because the i-th measured variable is not affected by the occurrence of the failure ($a_j(i) = 0$), then $3 > x_j^{PDL}(i) > x_0(i)$. If the i-th element of the vector $\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}}$ corresponds to the n-th element of $\mathbf{x}_{\mathbf{j}}^{\mathbf{PDL}*}$, $x_j^{PDL}(i) = x_j^{PDL}*(n)$, the values of both statistics are lower than their respective critical limits $\delta_{D,\alpha}{}^2$ and $\delta_{SPE,\alpha}{}^2$; that is, $[(D_j(\mathbf{q}) < \delta_{D,\alpha}{}^2(\mathbf{q})) \wedge (SPE_j(\mathbf{q}) < \delta_{SPE,\alpha}{}^2(\mathbf{q}))]$. Therefore, eq 19 is not satisfied, and the failure can not be detected. This refutes the initial assumption. Given that fault observability is a necessary condition for failure detection, the minimum cost solution that satisfies the linear observability constrains (solution of Step 1) sets the initial level of the traversal tree search used to solve Problem 29.

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Notes

The authors declare no competing financial interest.

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