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Automatic qualitative trend simulation method for diagnosing faults in industrial processes

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ABSTRACT

This work proposes an automatic method of qualitative simulation for industrial processes to predict the steady-state measurement patterns arising from different faults. Due to their characteristics, qualitative simulations tend to generate multiple spurious solutions. The proposed method limits the number of such spurious solutions by automatically generating new qualitative equations from the generic quantitative model (i.e. without the need of knowing the value of its parameters) and using simple qualitative known relations or other readily available information. An algorithm to obtain such solutions from the set of qualitative equations is also presented.

1. Introduction

In the petroleum, chemical and petrochemical industries, abnormal situations or operation faults may occur from sensor drifts, equipment failures, alteration of process parameters, etc. Due to the highly complex and integrated nature of chemical and petrochemical processes and the geographical dispersion of petroleum wells, if a fault is not detected and diagnosed promptly, the system may start producing out of specification and even shut down, leading to heavy economic loss and, more seriously, resulting in dangerous events such as explosion, fire and leak of toxic gases (Gao, Wu, Zhang, & Ma, 2010). Therefore, advanced tools for fault detection and diagnostic have been continuously developed in the last decades and are day by day more frequently applied in industry. Moreover, there are key pieces of equipment in the plant, particularly for continuous production, which have to be specially supervised since their malfunction affects the entire production system, resulting in major economic loss (Liu & Wang, 2009).

Fault diagnosis tools are generally based on quantitative models, qualitative models or on process history data (Chang & Chen, 2011; Venkatasubramanian, Rengaswamy, & Kavuri, 2003a, 2003b). Qualitative physics or common sense reasoning about physical systems has been widely applied in fault diagnosis. The advantage of qualitative simulators is their ability to yield partial conclusions from incomplete and often uncertain knowledge of the process. They start from a description of the physical mechanism, construct a model, and then use an algorithm to determine the system's behavior without precise knowledge of the parameters and functional relationships (Venkatasubramanian et al., 2003b; De Jong, 2004; Maurya, Rengaswamy, & Venkatasubramanian, 2007). A common approach is to derive qualitative equations on the basis of generic engineering principles, like material balances, termed as confluence equations. Rules of qualitative algebra are then used to specify how the qualitative values are combined. Within the qualitative algebra, allowable values for a variable can be a sign, for instance "+", indicating that the variable can take only qualitative high values, i.e. it can only increase. The variable can also decrease or stay constant within certain limits, which is represented as "−" or "0" respectively. It is important to note that a qualitative behavior can be derived even if an accurate mathematical model cannot be developed. Qualitative models do not require detailed information (such as exact expressions and numerical values) about the process; the order of magnitude information about the normal operating values of process parameters and variables is often enough (Venkatasubramanian et al., 2003b).

Qualitative models can be either stationary (Oyeleye & Kramer, 1988) or dynamic (Zhang, Wu, & Wang, 2011, Clancy & Kuipers, 2005, chap. 20). As many faults never reach a stationary state and the most dangerous ones generally occur during the process start-up period, which is intrinsically non stationary, dynamic qualitative

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simulation is often required. However, static qualitative monitoring still offers a good trade-off between performance and simplicity.

Oyeleye and Kramer (1988) proposed a method of qualitative simulation to predict the process variable trends when different process malfunctions occur. Thus, patterns of variable qualitative values corresponding to each process malfunctions can be obtained. These patterns of trends are vectors that represent the direction of deviation of the system variables relative to their nominal steady state values. The qualitative values for each variable are high (+1), low (−1) and normal (0). Their method is based on qualitative process equations and requires no numerical information beyond the signs and relative values of certain groups of parameters. However, qualitative simulation methods usually generate multiple spurious solutions. Oyeleye and Kramer (1988) used different procedures and qualitative constraints to reduce the number of spurious solutions, including those derived from a signed directed graph methodology.

Maurya, Rengaswamy, and Venkatasubramanian (2003a, 2003b);Maurya, Rengaswamy, and Venkatasubramanian (2004) proposed a comprehensive systematic framework for qualitative simulation, with emphasis in the development of signed digraphs models. They also proved the equivalence between signed digraphs and qualitative equations and discussed several methods for reducing spurious solutions through the generation of redundant equations.

In this work, an alternative fully automatic method is proposed to limit the number of spurious solutions using only a generic model of the system, evident qualitative relations and, eventually, easy to obtain quantitative restrictions. The proposed method focuses in the automation of the generation of equations and confluences. It implements two basic strategies to reduce the number of spurious solutions, namely the appropriate algebraic manipulation of the original equations (Maurya et al., 2003b) and the use of eventually available qualitative and/or quantitative information, with the aim of identifying faults without using signed digraphs or heuristic rules.

The proposed method is restricted to stationary cases and it is particularly aimed to be applied to limited systems with low level of instrumentation. Multivariate statistical monitoring tools that typically rely on correlation among measured process variables are poorly suited for these installations. Examples of such systems are lube oil circuits of centrifugal compressors and many oil production wells. In this second case, the geographical dispersion of the wells increases the communication costs and the depth of the wells increases the cost of placing downhole instruments. With steady state qualitative simulation monitoring tools, a certain degree of discrimination among different faults can still be achieved using the existing instrumentation.

We also propose in this work an algorithm to obtain qualitative solutions given the initial system of qualitative equations. This is a step toward increasing the application of qualitative simulation methodology in industrial environments, particularly to those systems with low level of instrumentation that are ill suited to be monitored with commercial software based on multivariate statistical analysis.

2. Methodology

The proposed method aims to find the sign pattern that represents the steady state attained by the system after a certain failure occurs. It starts formulating a set of independent equations from first principles describing the unperturbed system.

$$f_i(x_1, \ldots, x_n, p_1^*, \ldots, p_m^*) = 0; \quad i = 1, \ldots, n; \quad n, m \in N \tag{1}$$

where x_i are the variables and p_i^* are parameters required for the equations, n is the number of variables, m is the number of parameters and N is the set of natural numbers.

It is worthwhile mentioning that, as shown by Oyeleye and Kramer (1988), even if a quantitative equation is unknown, a qualitative equation can be derived as shown in Eq. (5) of the cited work. Therefore, apart from the standard mass, heat and momentum balances, which can always be used, one can include in the quantitative model, equations expressing a positive or negative dependence without knowing the exact functional relation.

To consider a fault, one or more of these equations are modified to reflect the perturbation on the variables or parameters. A new variable R_s, which accounts for the perturbation, is conveniently included where it corresponds, depending on the simulated fault, as expressed by Eq. (2).

$$f_i^{new}(x_1, \ldots, x_n, R_s, p_1^*, \ldots, p_m^*) = 0; \quad i = 1, \ldots, n; \quad n, m \in N \tag{2}$$

Afterwards, following the method proposed by Oyeleye and Kramer (1988), a set of algebraic equations that provide qualitative constraints on the ultimate direction of change of the system variables, termed confluences, are obtained. These qualitative confluences are used to determine the sign of each perturbed variable in steady state. Although the original set of equations (Eq. (2)) could be enough for determining the steady state solution of the system, it generates a set of qualitative confluences that is generally not enough to determine the sign of each perturbed variable. To solve this problem, new equations/qualitative confluences should be generated from the initial set. Oyeleye and Kramer (1988) suggested different ways to get these new equations. They generally require expert knowledge and cannot be automated, discouraging their application in real industrial environments. Maurya et al. (2003a) have also suggested several ways of generating new qualitative equations to reduce the number of spurious solutions obtained through signed digraph for chemical processes.

In the present method, the qualitative confluences are obtained automatically as schematized in Fig. 1 and described below.

The first step to obtain the confluences involves deriving the set of equations expressed by Eq. (2) with respect to each variable. In this work, these new equations are termed quantitative confluences.

$$g_i = \frac{\partial f_i}{\partial x_1} \cdot dx_1 + \frac{\partial f_i}{\partial x_2} \cdot dx_2 + \cdots + \frac{\partial f_i}{\partial x_n} \cdot dx_n + \frac{\partial f_i}{\partial R_s} \cdot dR_s; \qquad g_i = 0; \quad i = 1, \ldots, n \tag{3}$$

Qualitative confluences are then obtained from the quantitative confluences (Eq. (3)) by determining the sign of the derivatives.

$$h_i = \left[\frac{\partial f_i}{\partial x_1}\right] \cdot [dx_1] + \left[\frac{\partial f_i}{\partial x_2}\right] \cdot [dx_2] + \cdots + \left[\frac{\partial f_i}{\partial x_n}\right] \cdot [dx_n] + \left[\frac{\partial f_i}{\partial R_s}\right] \cdot [dR_s]; \quad h_i = 0; \quad i = 1, \ldots, n \tag{4}$$

The square brackets represent the qualitative value (sign) of the argument. Evaluation of these confluences requires operations of symbolic algebra as indicated by Oyeleye and Kramer (1988). In this work, the sign of the derivatives is determined automatically by a symbolic manipulator software using only evident qualitative relations, no detailed quantitative information is required.

This set of qualitative equations given by Eq. (4) has multiple solutions, the majority of which are spurious. Only one of them represents the final perturbed steady state of the system. To reduce the number of spurious solutions, new qualitative confluences are required. Even if new qualitative confluences could be obtained by linear combination of the original ones, Alfíe et al. (2010)

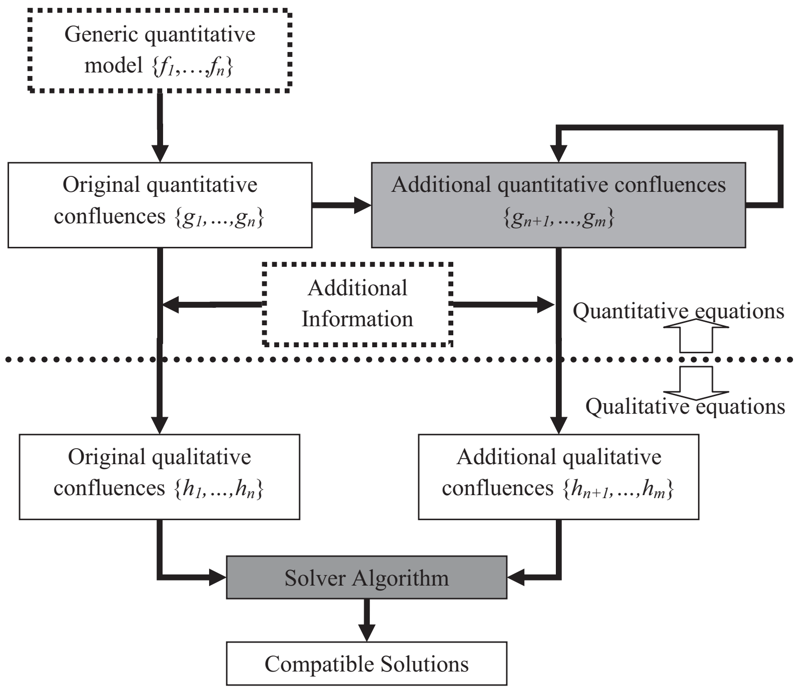

Fig. 1. Schematics of the proposed method to get the patterns of variable trends. Dashed boxes represent information input, continuous boxes represent automatic steps and gray boxes indicate important steps.

demonstrated that they are generally not useful for reducing the number of spurious solutions. Alfíe et al. (2010) also suggested that conveniently defined quantitative confluences can lead to qualitative ones capable of reducing spurious solutions.

Once the new quantitative confluences are obtained, the corresponding qualitative ones introduce further constraints to limit the number of possible solutions. These additional quantitative confluences are obtained as linear combinations of the ones given by Eq. (3), by eliminating one variable defining an appropriate constant lambda according to Eq. (5). This approach would be similar to the strategy of algebraic manipulation proposed by Maurya et al. (2003a). The automatic method proposed in this work generates the new equations in an iterative way. The first iteration takes the set of original equations and performs all the linear combinations given by Eq. (5), thus obtaining a new set of equations. This new set, in its turn, can be used as the starting point of a new iteration, and so on.

$$g_l = g_i - \lambda(i, j, x_k) \cdot g_j, \tag{5}$$

Additional information like, for instance, qualitative equations built by adding original equations of the same magnitude (e.g. material balances), known qualitative relations between variables and parameters and quantitative values of certain variables which could be easily measured in the field can be added to help the software run smoothly (i.e. to readily determine the coefficients signs in the quantitative confluences, and construct the qualitative confluences). The developed software is provided as supplementary material to this work.

Once the set of qualitative confluences has been obtained, the solutions are found using the automatic procedure detailed in Table 1.

It is important to remark that steps 4, 7 and 8 should be performed efficiently, given the high number of potential possible solutions. The strategy followed in the present work was based on representing multiple solutions in a succinct manner. For instance, Eq. (6) described below has 27 compatible solutions. Those solutions can be represented as shown in Table 2, where '*' denotes any value (i.e. −1, 0 or 1).

$$h([dx_1], [dx_2], [dx_3], [dx_4]) = [dx_1] + [dx_2] = 0 \tag{6}$$

In step 8 of the algorithm, the solutions obtained for one set of equations are compared against the solutions obtained for the new equation. This step is simplified by using the succinct representation of multiple solutions

For example, given the Eqs. (7a) and (7b)

$$[dx_1] + [dx_2] = 0 \tag{7a}$$

$$[dx_2] - [dx_3] = 0 \tag{7b}$$

There are 9 possible solutions for each one, and the 9 solutions can be represented using 3 expressions, as shown in Tables 3a and 3b, where * denotes any value (i.e. −1, 0 or 1).

Table 1
Solver algorithm.

(1)	Sort the qualitative equations according to increasing number of nonzero values
(2)	Let r = number of qualitative equations
(3)	Let k = 1
(4)	Compute the set S of the solutions compatible with Eq. (1)
(5)	If k = r then finish, else go to step 6
(6)	Let k = k + 1
(7)	Compute the set P of the compatible solutions with equation k
(8)	Remove from set S all the solutions that are not compatible with those in set P
(9)	Go to step 5

Table 2
Solutions representation.

$[dx_1]$	$[dx_2]$	$[dx_3]$	$[dx_4]$
1	−1	*	*
0	0	*	*
−1	1	*	*

Table 3a
Solutions of Eq. (7a).

	$[dx_1]$	$[dx_2]$	$[dx_3]$
(1)	1	−1	*
(2)	0	0	*
(3)	−1	1	*

Table 3b
Solutions of Eq. (7b).

	$[dx_1]$	$[dx_2]$	$[dx_3]$
(a)	*	1	1
(b)	*	0	0
(c)	*	−1	−1

Table 3c
System solutions.

	$[dx_1]$	$[dx_2]$	$[dx_3]$
(1,c)	1	−1	−1
(2,b)	0	0	0
(3,a)	−1	1	1

To remove from the set S (i.e. the solutions of Eq. (7a)) the solutions that are not compatible with those in set P, a Cartesian product is performed between all pairs of representations. In this case, there are 9 possible combinations: (1,a); (1,b); (1,c); (2,a); (2,b); (2,c); (3,a); (3,b); (3,c). The next step is removing those pairs with conflicting values in one or more variables. In this cases, only the pairs (1,c), (2,b), and (3,a) are compatible. All other pairs have conflicting values for variable $[dx_2]$. Thus, the result of combining the solutions yields the result shown in Table 3c

When the number of solutions in S can be easily handled, the procedure of computing the set P and removing the incompatible solutions can be replaced by representing explicitly all the solutions in S and directly testing whether they fulfill the remaining equations.

3. Case studies

In this section three examples are presented, aimed at clarifying the methodology and illustrating an industrial application.

3.1. Toy example

In this first example aimed at deeply illustrating the methodology, a linear system is considered for the sake of simplicity.

$$f_1 = 2x_1 + x_2 + 2x_3 \tag{8a}$$

$$f_2 = -1x_1 - 3x_2 - R_s \tag{8b}$$

$$f_3 = 4x_1 + 4x_2 \tag{8c}$$

where $f_i = 0\ \forall i$

The initial quantitative confluences g_i are obtained by determining the first derivatives of the functions given in Eqs. (8). These quantitative confluences are expressed in Eqs. (9)

$$g_1 = 2dx_1 + dx_2 + 2dx_3 \tag{9a}$$

$$g_2 = -1dx_1 - 3dx_2 - dR_s \tag{9b}$$

$$g_3 = 4dx_1 + 4dx_2 \tag{9c}$$

where $g_i = 0\ \forall i$

The steady state solution of the system with a perturbation is represented by Eq. (10)

Assuming $dR_s = 1$, the quantitative solution of Eqs. (9a)–(9c) is:

$$\begin{cases} dx_1 = \dfrac{1}{2} \\ dx_2 = -\dfrac{1}{2} \\ dx_3 = -\dfrac{1}{4} \\ dR_s = 1 \end{cases}, \quad \text{or equivalently} \quad \mathbf{dx} = \begin{pmatrix} \frac{1}{2} & -\frac{1}{2} & -\frac{1}{4} & 1 \end{pmatrix}^T \tag{10}$$

It should be noted that in general, the equations g_i are not completely known and it will not be possible to directly compute the solution **dx**.

The proposed method circumvents this limitation by computing additional quantitative confluences as linear combinations of the original ones. For example, Eqs. (11a)–(11c) give a few of the new confluences created following the procedure indicated in Eq. (5).

$$g_4 = g_1 - \lambda(1, 2, x_1) \cdot g_2 = g_1 + 2g_2 = -5dx_2 + 2dx_3 - 2dR_s \tag{11a}$$

$$g_5 = g_1 - \lambda(1, 3, x_1) \cdot g_3 = g_1 - \frac{1}{2}g_3 = -dx_2 + 2dx_3 \tag{11b}$$

$$g_6 = g_2 - \lambda(2, 3, x_1) \cdot g_3 = g_2 + \frac{1}{4}g_3 = -2dx_2 - dR_s \tag{11c}$$

Then, the qualitative confluences are computed (Eqs. (12)). In this example, this step is represented by determining the sign of every term in Eqs. (9) and (11).

$$h_1 = [dx_1] + [dx_2] + [dx_3] \tag{12a}$$

$$h_2 = -[dx_1] - [dx_2] - [dR_s] \tag{12b}$$

$$h_3 = [dx_1] + [dx_2] \tag{12c}$$

$$h_4 = -[dx_2] + [dx_3] - [dR_s] \tag{12d}$$

$$h_5 = -[dx_2] + [dx_3] \tag{12e}$$

$$h_6 = -[dx_2] - [dR_s] \tag{12f}$$

where $h_l = 0\ \forall l$.

These quantitative and qualitative equations in matrix form are written, respectively, as indicated in Eqs. (13) and (14).

$$\mathbf{G}\ \ \mathbf{dx} = 0 \tag{13}$$

$$\mathbf{G} = \begin{pmatrix} 2 & 1 & 2 & 0 \\ -1 & -3 & 0 & -1 \\ 4 & 4 & 0 & 0 \\ 0 & -5 & 2 & -2 \\ 0 & -1 & 2 & 0 \\ 0 & -2 & 0 & -1 \end{pmatrix} \quad \text{and} \quad \mathbf{dx} = \begin{pmatrix} dx_1 \\ dx_2 \\ dx_3 \\ dR_s \end{pmatrix}$$

$$\mathbf{H}[\mathbf{dx}] = 0 \tag{14}$$

$$\mathbf{H} = \begin{pmatrix} 1 & 1 & 1 & 0 \\ -1 & -1 & 0 & -1 \\ 1 & 1 & 0 & 0 \\ 0 & -1 & 1 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & -1 \end{pmatrix} \quad \text{and} \quad [\mathbf{dx}] = \begin{pmatrix} [dx_1] \\ [dx_2] \\ [dx_3] \\ [dR_s] \end{pmatrix}$$

Applying the solver algorithm described in Table 1, using only the confluences obtained from the three initial equations, six different solutions or sign patterns are obtained, which are shown in the first column of Table 4.

Applying the complete automated algorithm as schematized in Fig. 1, the number of solutions is reduced as new confluences are

Table 4
Solutions for different set of confluences.

Sign patterns [**dx**]	Solution of $\{h_1, h_2, h_3\}$	Solution of $\{h_1, \ldots, h_4\}$	Solution of $\{h_1, \ldots, h_5\}$	Solution of $\{h_1, \ldots, h_6\}$
$(-1, 1, -1, 1)^T$	√	×	×	×
$(-1, 1, 0, 1)^T$	√	×	×	×
$(-1, 1, 1, 1)^T$	√	√	√	×
$(1, -1, -1, 1)^T$	√	√	√	√
$(1, -1, 0, 1)^T$	√	√	×	×
$(1, -1, 1, 1)^T$	√	√	×	×

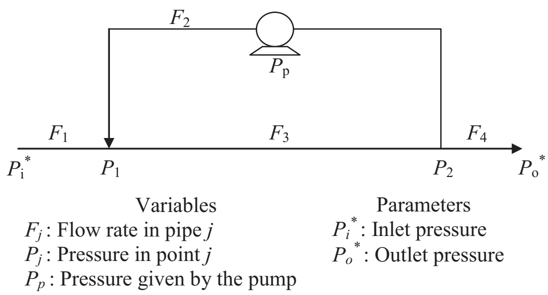

Fig. 2. Recycle loop example used by Oyeleye and Kramer (1988).

added. This is also shown in Table 4, indicating the sign patterns that remain being solution after adding each new confluence. It can be seen that, in this case, after adding only 3 equations, a single solution is found. Eq. (15) shows the obtained solution. Comparing with Eq. (10), it is observed that the sign pattern is the same in the quantitative and qualitative solutions.

$$[\mathbf{dx}] = \begin{pmatrix} 1 & -1 & -1 & 1 \end{pmatrix}^T \tag{15}$$

For this simple case, the algorithm proposed in the present paper finds a unique solution in a fully automated way.

3.2. Recycle loop

The second example is a simple recycle loop with fixed boundary pressures as illustrated in Fig. 2. This example was originally proposed by Oyeleye and Kramer (1988) to describe their method.

The quantitative equations which describe the unperturbed system are given by Eqs. (16). Variables and parameters are indicated in Fig. 2.

$$P_i^* - P_1 - K_1^* F_1^2 = 0 \tag{16a}$$

$$P_2 + P_p - P_1 - K_2^* F_2^2 = 0 \tag{16b}$$

$$P_1 - P_2 - K_3^* F_3^2 = 0 \tag{16c}$$

$$P_2 - P_o^* - K_4^* F_4^2 = 0 \tag{16d}$$

$$F_1 + F_2 - F_3 = 0 \tag{16e}$$

$$F_2 - F_3 + F_4 = 0 \tag{16f}$$

$$P_p - P_{p0}^* + C_{cp}^* F_2^2 = 0 \tag{16g}$$

where K_i^*, P_{p0}^* and C_{cp}^* are design parameters.

To simulate the fault proposed by Oyeleye and Kramer, an increase in pressure drop in line 1, Eq. (16a) is modified, leading to the set of equations that describes the perturbed system, which contains Eqs. (16b)–(16h).

$$P_i^* - P_1 - R_s - K_1^* F_1^2 = 0 \tag{16h}$$

Using the seven confluences obtained from Eqs. (16b)–(16h), Oyeleye and Kramer (1988) find eleven compatible solutions. They further reduced the set of solutions by introducing two additional latent confluences.

Following the method proposed in this work, quantitative confluences arising from Eqs. (16b)–(16h) are given in Eqs. (17a)–(17g) and the first four new quantitative confluences obtained through the procedure described in Eq. (5) are given in Eqs. (17h)–(17k).

$$g_1 = -2K_1^* F_1 \cdot dF_1 - dP_1 - dR_s \tag{17a}$$

$$g_2 = -2K_2^* F_2 \cdot dF_2 - dP_1 + dP_2 + dP_p \tag{17b}$$

$$g_3 = -2K_3^* F_3 \cdot dF_3 + dP_1 - dP_2 \tag{17c}$$

$$g_4 = -2K_4^* F_4 \cdot dF_4 + dP_2 \tag{17d}$$

$$g_5 = dF_1 + dF_2 - dF_3 \tag{17e}$$

$$g_6 = dF_2 - dF_3 + dF_4 \tag{17f}$$

$$g_7 = 2C_{cp}^* F_2 \cdot dF_2 + dP_p \tag{17g}$$

$$\begin{aligned} g_8 &= g_1 - \lambda(1, 2, P_1) \cdot g_2 = g_1 - g_2 \\ &= -2K_1^* F_1 \cdot dF_1 + 2K_2^* F_2 \cdot dF_2 - dP_2 - dP_p - dR_s \end{aligned} \tag{17h}$$

$$\begin{aligned} g_9 &= g_1 - \lambda(1, 3, P_1) \cdot g_3 = g_1 + g_3 \\ &= -2K_1^* F_1 \cdot dF_1 - 2K_3^* F_3 \cdot dF_3 - dP_2 - dR_s \end{aligned} \tag{17i}$$

$$\begin{aligned} g_{10} &= g_1 - \lambda(1, 5, F_1) \cdot g_5 = g_1 + 2K_1^* F_1 \cdot g_5 \\ &= 2K_1^* F_1 \cdot dF_2 - 2K_1^* F_1 \cdot dF_3 - dP_1 - dR_s \end{aligned} \tag{17j}$$

$$\begin{aligned} g_{11} &= g_2 - \lambda(2, 3, P_1) \cdot g_3 = g_2 + g_3 \\ &= -2K_2^* F_2 \cdot dF_2 - 2K_3^* F_3 \cdot dF_3 + dP_p \end{aligned} \tag{17k}$$

where $g_l = 0 \; \forall \, l$.

Qualitative confluences corresponding to the quantitative confluences (Eqs. (17)) are shown in Eqs. (18).

$$h_1 = -[dF_1] - [dP_1] - [dR_s] \tag{18a}$$

$$h_2 = -[dF_2] - [dP_1] + [dP_2] + [dP_p] \tag{18b}$$

$$h_3 = -[dF_3] + [dP_1] - [dP_2] \tag{18c}$$

$$h_4 = -[dF_4] + [dP_2] \tag{18d}$$

$$h_5 = [dF_1] + [dF_2] - [dF_3] \tag{18e}$$

$$h_6 = [dF_2] - [dF_3] + [dF_4] \tag{18f}$$

$$h_7 = [dF_2] + [dP_p] \tag{18g}$$

$$h_8 = -[dF_1] + [dF_2] - [dP_2] - [dP_p] - [dR_s] \tag{18h}$$

$$h_9 = -[dF_1] + [dF_3] - [dP_2] - [dR_s] \tag{18i}$$

$$h_{10} = [dF_2] - [dF_3] - [dP_1] - [dR_s] \tag{18j}$$

$$h_{11} = -[dF_2] - [dF_3] + [dP_p] \tag{18k}$$

where $h_l = 0 \; \forall \, l$

Table 5
Solutions of Eqs. (18a)–(18g) and final (*) solution of Eqs. (18a)–(18k).

Solution	F_1	F_2	F_3	F_4	P_1	P_2	P_p	R_s
1	−1	−1	−1	−1	−1	−1	1	1
2	0	−1	−1	−1	−1	−1	1	1
3	1	−1	−1	−1	−1	−1	1	1
4	−1	0	−1	−1	−1	−1	0	1
(*) 5	−1	1	−1	−1	−1	−1	−1	1
6	−1	1	0	−1	−1	−1	−1	1
7	−1	1	1	−1	−1	−1	−1	1
8	0	1	1	−1	−1	−1	−1	1
9	1	1	1	−1	−1	−1	−1	1
10	−1	−1	−1	1	1	1	1	1
11	−1	1	1	1	1	1	−1	1

Finally, the set of solutions of Eqs. (18a)–(18g) and the unique final solution of Eqs. (18a)–(18k), marked with an (*) are shown in Table 5.

Using the method proposed in the present work, the correct solution is found directly from the equations (16b-h) with the only assumption of positive variables and parameters.

3.3. *Lubrication system of a centrifugal compressor*

As an example of a real industrial application, the lube oil system of a centrifugal compressor installed in a methanol plant is considered. This type of systems are generally not enough instrumented to be monitored using classic methods like Principal Component Analysis (PCA). In this case, qualitative simulation methods have been suggested to perform better than quantitative methods (Zhang et al., 2011). In addition, their smooth operation is crucial for the plant since a malfunction can lead to a shutdown. A simplified scheme of a typical lube oil system of centrifugal compressors can be found in Bloch (2006) and it is schematized in Fig. 3.

The compressor lubrication system is described by Eqs. (19a)–(19o), considering the 14 variables indicated in Fig. 3 and the compressor velocity, which is a key variable to control proper operation in this case.

$$F_1 - F_2 - F_3 = 0 \tag{19a}$$

$$F_1 - F_4 - F_5 = 0 \tag{19b}$$

$$P_p - P_{p0}^* + C_{cp}^* F_1^2 = 0 \tag{19c}$$

$$P_0^* - P_1 + P_p - K_p^* F_1^2 = 0 \tag{19d}$$

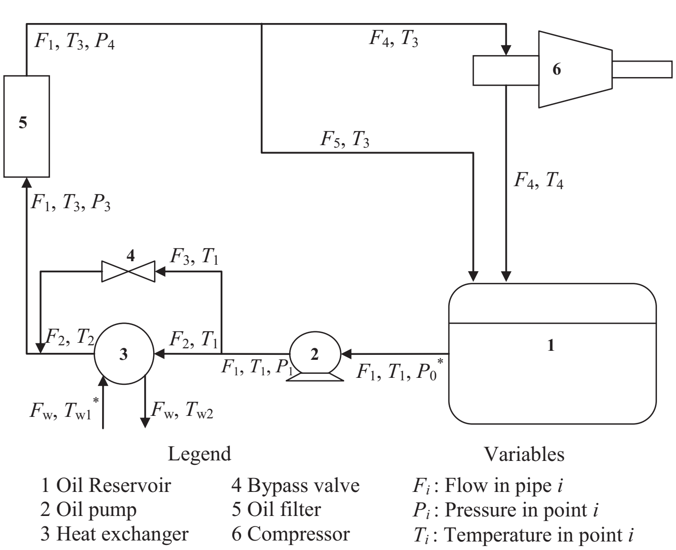

Fig. 3. Schematics of a typical lube oil system of a centrifugal compressor.

$$T_2F_2 + T_1F_3 - T_3F_1 = 0 \tag{19e}$$

$$-C_p^*(T_2 - T_1)F_2 - k_{UA}^* F_2^{1/2} \frac{(T_1 - T_{w2}) - (T_2 - T_{w1}^*)}{\ln((T_1 - T_{w2})/(T_2 - T_{w1}^*))} = 0 \tag{19f}$$

$$C_{pw}^*(T_{w2} - T_{w1}^*)F_w^* - k_{UA}^* F_2^{1/2} \frac{(T_1 - T_{w2}) - (T_2 - T_{w1}^*)}{\ln((T_1 - T_{w2})/(T_2 - T_{w1}^*))} = 0 \tag{19g}$$

$$P_2 - P_3 - K_1^* F_1^2 = 0 \tag{19h}$$

$$F_4 C_p^*(T_4 - T_3) - K_r^* rpm = 0 \tag{19i}$$

$$F_4T_4 + F_5T_3 - F_1T_1 = 0 \tag{19j}$$

$$P_3 - P_0^* - K_4^* F_4^2 = 0 \tag{19k}$$

$$P_3 - P_0^* - K_5^* F_5^2 = 0 \tag{19l}$$

$$P_1 - P_2 - K_3^* F_3^2 = 0 \tag{19m}$$

$$P_1 - P_2 - K_2^* F_2^2 = 0 \tag{19n}$$

$$-C_p^*(T_2 - T_1)F_2 - K_r^* rpm = 0 \tag{19o}$$

where C_{cp}^*, C_p^*, C_{pw}^*, F_w^*, K_1^*, K_2^*, K_3^*, K_4^*, K_5^*, K_p^*, K_r^*, K_{UA}^*, P_o^*, P_{p0}^*, T_{w1}^* are design parameters and *rpm* is the compressor velocity.

The proposed equations arise from formulating mass, heat and momentum balances taking into account design equations; in addition, some equations are incorporated expressing relations between variables without knowing the exact functionality (e.g., the proportionality between the generated heat and the compressor velocity given in Eqs. (19i) and (19o), for which the exact functionality is unknown).

In real plants, only a limited number of the included variables are actually measured.

Seven faults are considered for this system:

1. Clogged oil filter.
2. Increased lubricant temperature due to bearing malfunction.
3. Unexpected change in the heat exchanger bypass valve aperture.
4. Decrease in heat exchanger efficiency.
5. Increased pressure drop in the branch F4.
6. Pipe leak at the pump discharge.
7. Faulty rpm control.

Given that *rpm* is externally controlled, this variable was assumed constant in every fault except in fault #7. To represent each fault, a positive perturbation was added to one or more equations. The perturbations are always positive and their values are considered to be less than the value of the perturbed variable or parameter.

As an example, modifications in the equations required to represent fault 1 are described in more detail.

Fault 1 involves the oil filter clogging; then Eq. (19h) must be replaced by Eq. (19p), indicating an increase in the pressure drop through the filter.

$$P_2 - P_3 - (K_1^* + R_s)F_1^2 = 0 \tag{19p}$$

Additional information considered for this case includes the following restrictions:

- all variables are positive
- all parameters are positive
- The following expected qualitative relations:
- $P_{p0}^* > P_1 > P_2 > P_3 > P_0^*$
- $F_w^* > F_1 > \{F_2; F_3; F_4; F_5\}$; $F_2 > \{F_3; F_5\}$; $F_4 > \{F_3; F_5\}$
- $T_4 > T_1 > T_3 > T_2 > T_{w2} > T_{w1}^*$
- $P_{p0}^* > K_3 > \{P_2 > P_3 > P_0^*\}$; $K_3^* > \{K_1^*; K_2^*; K_4^*\}$; $K_5^* > \{K_1^*; K_2^*; K_4^*\}$
- $C_{cp}^* > K_p^*$; $C_{pw}^* > C_p^*$

Table 6
Compatible solutions for fault #1, including the expected one.

Solution	F_1	F_2	F_3	F_4	F_5	P_p	P_1	P_2	P_3	T_1	T_2	T_3	T_4	T_{w2}	*rpm*	R_s
1	−1	−1	−1	−1	−1	1	1	1	−1	1	1	−1	−1	0	0	1
2	−1	−1	−1	−1	−1	1	1	1	−1	1	1	−1	0	0	0	1
3	−1	−1	−1	−1	−1	1	1	1	−1	1	1	−1	1	0	0	1
4	−1	−1	−1	−1	−1	1	1	1	−1	1	1	0	1	0	0	1
5	−1	−1	−1	−1	−1	1	1	1	−1	1	1	1	1	0	0	1

Table 7
Number of compatible solutions for each fault.

	Fault 1	Fault 2	Fault 3	Fault 4	Fault 5	Fault 6	Fault 7
# Solutions	5	1	3	3	3	4	8

When the exact functionality of an equation is unknown, there is scarce chance of assuming additional information considering the related parameters. For instance, in this case, as the exact dependence of *rpm* with the generated heat (Eqs. (19i) and (19o)) is unknown, no additional information can be given for the involved parameter (K_r).

To simplify the implementation of the proposed method in a qualitative unit simulation software that would encourage the use of qualitative simulation in industrial application, a modular approach was selected. As was previously mentioned by Oyeleye and Kramer (1988), there is a trade-off between modularity and solution multiplicity. Taking this into account, three extra equations, obtained by summing up original equations of the same magnitude (mass balances, enthalpy balances and momentum balances), have been considered.

$$\text{Eq. (19g)} - \text{Eq. (19f)} = 0 \tag{20a}$$

$$\text{Eq. (19c)} + \text{Eq. (19d)} + \text{Eq. (19h)} + \text{Eq. (19k)} + \text{Eq. (19l)} + \text{Eq. (19m)} + \text{Eq. (19n)} = 0 \tag{20b}$$

$$\text{Eq. (20a)} + \text{Cp} * \text{Eq. (19e)} + \text{Eq. (19f)} + \text{Eq. (19g)} + \text{Eq. (19i)} + \text{Cp} * \text{Eq. (19j)} + \text{Eq. (19o)} = 0 \tag{20c}$$

Finally, a set of approximate skin tube temperatures measured in the plant with an infrared thermometer are also given as extra information.

To make the solver run smoothly and faster, other expected qualitative relations between certain variables arising from Eqs. (19), could be imposed. No additional information is given at this stage.

It should be noted that this information is far less than the necessary to simulate the system in a quantitative manner. Yet, it is sufficient to predict the sign patterns corresponding to each fault and therefore allows diagnosing those faults. The procedure described by Eq. (5) to generate more quantitative confluences can be applied iteratively including as original confluences all the quantitative ones generated in the previous iteration. The number of solutions can be further reduced by providing additional information. Applying the proposed method to Eqs. (19) and performing two iterations, five compatible solutions are obtained. The solutions are shown in Table 6; the set of solutions includes the expected one (Solution #5).

Table 7 shows the total number of solutions obtained for each fault. Even if more than one solution is obtained for each fault, in all cases, the expected one is included among the obtained solutions and there is no overlap for different faults.

Given that more than one solution was obtained for each fault, the method's ability to identify each fault is guaranteed a priori only when no overlapping between solutions of different faults occurs, as was obtained in this case.

4. Conclusions

An automatic method to generate steady state measurement patterns for fault identification is proposed and tested. It offers the advantage of requiring a minimum set of system equations and general qualitative relations between variables and parameters arising from basic process knowledge. The proposed method has the advantage of being simple and low demanding, thus it is appropriate for an eventual industrial application. Although the proposed method does not lead to a unique pattern of ultimate direction of change of the system variables, it is able to significatively reduce the number of compatible patterns. This reduction allowed a complete discrimination among the proposed faults.

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Appendix A. Supplementary data

Supplementary material related to this article can be found, in the online version, at http://dx.doi.org/10.1016/j.compchemeng.2014.01.007.

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