

MODEL DECOMPOSITION BASED ABNORMAL PARAMETER ESTIMATION FOR DISTILLATION COLUMN

W.D. TIAN[†] and S.L. SUN[‡]

[†] College of Chemical Engineering, Qingdao University of Science & Technology, Qingdao 266042, China. tianwd@qust.edu.cn

[‡] College of Marine Science and Bioengineering, Qingdao University of Science & Technology, Qingdao 266042, China. qdsunsuli@qust.edu.cn

Abstract— Parameter estimation method can produce useful physical parameters in finding abnormal causes, but nonlinear model makes this method computationally intensive and non-robust for distillation scenario. In this paper, we propose a model decomposition based parameter estimation method for distillation column diagnosis purposes. Nonlinear first principles dynamic model is divided into some disjoint submodels through occurrence matrix analysis. The whole model is used to monitor distillation process and the submodel that gives the highest contribution to the generated residual is selected to perform abnormal parameter estimation. Application results from stripping tower in the popular Tennessee Eastman challenge problem show that the model decomposition based diagnosis scheme is more time-saving and robust than pure nonlinear model based scheme.

Keywords— Model decomposition, Parameter estimation, Fault diagnosis, Distillation.

I. INTRODUCTION

Distillation is an important unit operation in chemical industry. Its minor operational condition change may cause low product quality, high energy consumption, and even catastrophic safety problems. Fault diagnosis technique can timely detect potential degradation trend of operational conditions (Verucchi *et al.*, 2008), so it has become a crucial technique in controlling and preventing distillation accidents. In the literature, several methodologies have been proposed for distillation fault diagnosis (Deshpande and Patwardhan, 2008; Gao *et al.*, 2010; Leung and Romagnoli, 2000; Namdari and Jazayeri-Rad, 2014; Shahabinejad *et al.*, 2014). However, no method can meet all the requirements of a distillation diagnostic system, so hybrid methods that can overcome the limitations of individual solution strategy are more attractive in practice (Venkatasubramanian *et al.*, 2003). In a hybrid system, the parameter estimation method uses input-output, state-space and first principles models to determine process parameters and physically defined process coefficients, thereby allowing for a deeper insight and easier diagnosis than other methods (Isermann, 2005). The main limitation of this method is its complex model which leads to an excessive computation demand in searching fault causes. Accordingly, some improvements have been done to simplify modeling in the last decade. For example, Deshpande and Patwardhan (2008) used a Bayesian approach to identify a combination of several linear perturbation models in different operating regimes for a high-purity binary dis-

tillation column. Their parameter estimation result obtained by a nonlinear generalized likelihood ratio (GLR) method shows a good performance for nonlinear process in a transient state over a wide operating range. Wang and Bai (2013) used some correlation coefficients to depict first principles relationship among distillation variables, and determined the fault location by logic analysis on these coefficients. Tian *et al.* (2013) proposed a two-tier model based fault diagnosis structure where the nonlinear model and its corresponding linear model are used for detection and diagnosis purposes respectively.

Above improved model-based parameter estimation approaches for distillation column have two features. Firstly, model scale is unchanged when equations in the model are simplified, that is, a complete set of equations must be incorporated to perform diagnosis task. Secondly, it is inadequate for robust diagnosis by only replacing nonlinear model with simplified model because it loses a priori knowledge advantage.

In process systems engineering field, decomposition is frequently used to divide complex system into several subsystems which can be treated independently for the purposes of optimization, control and/or design (Himmelblau, 1966). During the past two decades, a number of decomposition applications for large-scale fault diagnosis have been carried out based on qualitative signed digraph model (Ahn *et al.*, 2008; Lee *et al.*, 2004; 2006), qualitative fault-effect tree model (Lee and Yoon, 2001), and quantitative multilinear model (Bhagwat *et al.*, 2003). Model decomposition differs from system decomposition only in objects studied, i.e., the former focuses on equations but the latter focuses on unit modules. Decomposition separates the original large-scale equation set into a series of small-scale sub equation sets which have a high sparse ratio and therefore could be solved efficiently for key variables. Based on our earlier dynamic simulation based distillation fault diagnosis works (Tian *et al.*, 2012; 2013), a model decomposition based abnormal parameter estimation scheme for distillation process is proposed in this paper. The effect of decomposition strategy, submodel algorithm, etc. on performance is discussed.

In the following sections, how to decompose the rigorous nonlinear dynamic model is described at first. Then, the proposed model decomposition based abnormal parameter estimation scheme is outlined and its effectiveness is demonstrated through TEP stripper simulator example in comparison with rigorous model based method.

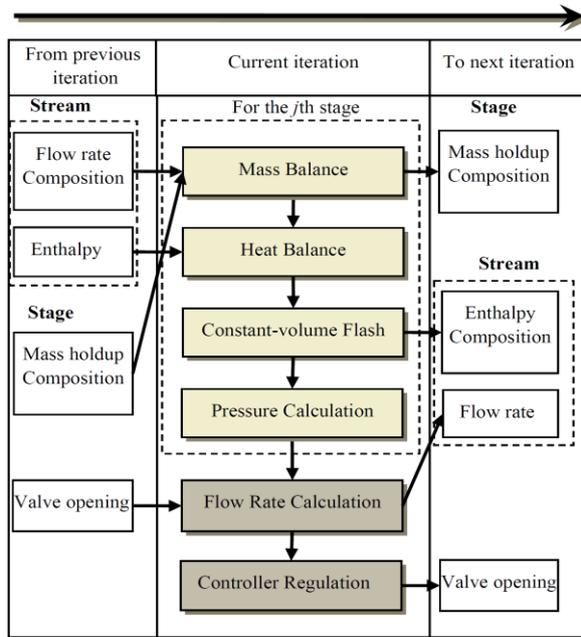


Figure 1. Dynamic model structure of distillation

II. DECOMPOSITION OF NONLINEAR DYNAMIC DISTILLATION MODEL

A. Nonlinear dynamic distillation modeling

This model has been given in our earlier work (Tian *et al.*, 2012). Based on the equilibrium stage assumption, it is composed of mass balance, enthalpy balance and phase equilibrium equations with a lot of abnormal parameters. The main structure of nonlinear dynamic model is depicted in Fig. 1. Explicit Euler method is chosen as the integral algorithm for this dynamic model in consideration of possible operations at each time interval and high calculation speed requirement. In each iteration step, mass and enthalpy balances are conducted with initial stream and stage values from previous iteration and then their integral results becomes initial values of the next iteration.

B. Model decomposition

System decomposition method divides a high-dimension and hereby intractable problem into several low-dimension sub-problems. The latter consists of disjoint subsystems which can be solved easily. Disjoint subsystem is defined as a subsystem that can be separated from original system and can be solved independently to simplify original problem. Under chemical engineering scenarios, process equation set is usually composed of a great number of algebraic and ordinary differential equations (Eqs. 1 and 2). The vectors \mathbf{x} and $\bar{\mathbf{x}}$ in these equations denotes the state variable vector and non-state variables, respectively. Occurrence matrix is used to express dependence relation between equations and variables, as shown in Eq. (3).

$$f(t, \mathbf{x}_t, \bar{\mathbf{x}}_t) = 0, \quad (1)$$

$$\frac{d\bar{\mathbf{x}}_t}{dt} = f(t, \mathbf{x}_t, \bar{\mathbf{x}}_t), \quad (2)$$

$$\mathbf{S} = \begin{matrix} & x_1 & x_2 & \cdots & x_m \\ \begin{matrix} f_1 \\ f_2 \\ \vdots \\ f_m \end{matrix} & \begin{bmatrix} s_{11} & s_{12} & \cdots & s_{1m} \\ s_{21} & s_{22} & \cdots & s_{2m} \\ \vdots & \vdots & \vdots & \vdots \\ s_{m1} & s_{m2} & \cdots & s_{mm} \end{bmatrix} \end{matrix}, \quad (3)$$

where

$$s_{ij} = \begin{cases} 1, & \text{if } x_j \text{ exists in equation } f_i \\ 0, & \text{otherwise} \end{cases}$$

Himmelblau (1966) proposed the following algorithm to identify the disjoint subsystems for large-scale equation set:

a) Select the k th column that contains most zero elements in $m \times m$ occurrence matrix \mathbf{S} .

b) Reserve rows containing zero elements in the k th column, and combine all rows containing non-zero element by Boolean addition operator into one row and add them at the end of matrix \mathbf{S} . The obtained $j \times m$ matrix is denoted as $\mathbf{S}(0)$.

c) Repeat step b), and get a sequence $\{\mathbf{S}, \mathbf{S}(0), \mathbf{S}(1), \dots, \mathbf{S}(n)\}$.

d) In the finally obtained matrix $\mathbf{S}(n)$ which contains only one non-zero element in each column, each row corresponds to one disjoint subsystem of the original equation set.

The transposed occurrence matrix changes into adjacency matrix after removing all the output variables into diagonal and zeroing them. Reachability matrix is used to identify irreducible subsystems based on an adjacency matrix (Himmelblau, 1966).

The following subsections will highlight the decomposition process for nonlinear distillation model in detail. Only one stage is formulated in this model for simplicity.

(1) Occurrence matrix of nonlinear distillation model

Mass and enthalpy balance of feed and side streams are basic for stage equilibrium calculation. Mass balance of feed streams is given in Eqs. (4) and (5), including $n+1$ equations where n denotes the number of components.

$$x_{F,i} \times F = \sum_{j \in f} (x_{F,j,i} \times F_{0,j}), \quad (4)$$

$$\sum_i x_{F,i} = 1. \quad (5)$$

There is one enthalpy balance equation of feed streams (Eq. 6), liquid side (Eq. 7), and gas side (Eq. 8) respectively.

$$h_F \times F = \sum_{j \in f} (F_{0,j} \times h_{0,j}), \quad (6)$$

$$S = \sum_{j \in s} F_j, \quad (7)$$

$$G = \sum_{j \in g} F_j. \quad (8)$$

Based on above input/output balance, five equations are established for enthalpy balance on stage, including overall enthalpy balance (Eq. 9), jacket heating (Eq. 10), and enthalpy function (Eqs. 11 through 13).

$$h = (fmx_0 \times h_{L0} + fmy_0 \times h_{V0} + stgcp \times t_0) + \quad (9)$$

$$dt \times (F \times f_F - S \times h_{L0} - G \times h_{V0} - Q), \quad (10)$$

$$Q = fop_{stm} \times K \times A \times (T - T_{stm}) \quad (10)$$

$$h = fmx \times h_L + fmy \times h_V + stgcp \times T, \quad (11)$$

$$h_L = \sum_{i=1} [x_i \times (H_{L0,i} + H_{L1,i} \times T)], \quad (12)$$

$$h_V = \sum_{i=1} [y_i \times (H_{V0,i} + H_{V1,i} \times T)]. \quad (13)$$

Overall mass balance on stage includes $n+1$ equations (Eqs. 14 and 15).

$$fmz \times z_i = fmz_0 \times z_{i0} + \quad (14)$$

$$dt \times (F \times x_{F,i} - S \times x_{i0} - G \times y_{i0}), \quad (15)$$

$$\sum_i z_i = 1.$$

Based on above mass and enthalpy balance, the time-consuming equilibrium calculation on stage includes $3n+5$ equations (Eqs. 16 through 23). Vapor ratio e is iteratively solved through these equations based on the equilibrium stage assumption.

$$z_i = y_i \times e + x_i \times (1 - e), \quad (16)$$

$$y_i \times e = ke_i \times x_i, \quad (17)$$

$$\sum_i x_i = 1, \quad (18)$$

$$fmy = fmz \times e, \quad (19)$$

$$fmz = fmx + fmy, \quad (20)$$

$$ke_i = \frac{e^{A_i + \frac{B_i}{t - 273.15 + C_i}} \times ey_i}{1000 \times fmz \times R \times t / Vy}, \quad (21)$$

$$Vx = fmx \times \sum_i (x_i \times Vb_i), \quad (22)$$

$$Vz = Vx + Vy. \quad (23)$$

Two equations are given to calculate pressure and liquid level on stage (Eqs. 24 and 25).

$$p \times Vy = (1 - p01) \times p_0 \times Vy + p01 \times fmy \times R \times T, \quad (24)$$

$$lev = Vx / At. \quad (25)$$

Finally, stream data around column are recalculated, including pressure, composition, temperature, etc.

There are twelve equations for flow rate relevant calculation (Eqs. 26 through 28), where subscript 1 through 4 denotes reflux, top vapor, feed, and bottom liquid stream respectively.

$$mw_{str,1} = \sum_i (x_{1,i} \times mw_i), \quad (26a)$$

$$mw_{str,2} = \sum_i (y_i \times mw_i), \quad (26b)$$

$$mw_{str,3} = \sum_i (x_{3,i} \times mw_i), \quad (26c)$$

$$mw_{str,4} = \sum_i (x_i \times mw_i), \quad (26d)$$

$$\rho_1 \times \sum_i (x_{1,i} \times vb_i) = mw_{str,1}, \quad (27a)$$

$$\rho_2 \times R \times T = p \times mw_{s,2}, \quad (27b)$$

$$\rho_3 \times R \times T_{str,3} = pfr_3 \times mw_{s,3}, \quad (27c)$$

Table 1. Variables in nonlinear distillation model

No.	Name	Number	No.	Name	Number
1	$x_{F,i}$	n	14	y_i	n
2	F	1	15	fmz	1
3	h_F	1	16	z_i	n
4	S	1	17	e	1
5	G	1	18	ke_i	n
6	h	1	19	Vy	1
7	Q	1	20	Vx	1
8	T	1	21	p	1
9	fmx	1	22	lev	1
10	h_L	1	23	$mw_{s,j}$	4
11	fmy	1	24	ρ_j	4
12	h_V	1	25	fm_i	4
13	x_i	n	26	fop_4	1
Total number		$5n+30$			

$$\rho_4 \times \sum_i (x_i \times vb_i) = mw_{str,4}, \quad (27d)$$

$$fm_1 \times mw_{s,1} = \frac{fop_1}{kvr_1} \times \sqrt{\rho_1 \times (pfr_1 - pto_1 + adp_1)}, \quad (28a)$$

$$fm_2 \times mw_{s,2} = \frac{fop_2}{kvr_2} \times \sqrt{\rho_2 \times (p - pto_2 + adp_2)}, \quad (28b)$$

$$fm_3 \times mw_{s,3} = \frac{fop_3}{kvr_3} \times \sqrt{\rho_3 \times (pfr_3 - pto_3 + adp_3)}, \quad (28c)$$

$$fm_4 \times mw_{s,4} = \frac{fop_4}{kvr_4} \times \sqrt{\rho_4 \times (pfr_4 - pto_4 + adp_4)}. \quad (28d)$$

Control loops are prerequisite for stable process controllability. Especially, bottom liquid level is controlled in an allowable scope by manipulating bottom production flow rate (Eq. 29).

$$fop_4 = fop_{0,4} + kp \times \left[\left(50 - \frac{lev}{wh} \times 100 \right) \times \left(1 + \frac{dt}{t_i} \right) - err_0 \right]. \quad (29)$$

In all, the nonlinear distillation model is composed of $5n+30$ equations. There are $5n+30$ variables in these equations, as listed in Table 1. So variable number is equal to that of equation, meaning model can be solved definitely.

Based on above equations and variables, the corresponding occurrence matrix of nonlinear distillation model is obtained, as shown in Table 2.

(2) Disjoint subsystems

Above occurrence matrix is finally transformed with Himmelblau algorithm into a matrix, as shown in Table 3. It indicates three disjoint equation sets, denoted by I, II, and III, respectively. They represent top feed (I), bottom feed (II) and rest part (III) in distillation model according to related variables.

III. FAULT DETECTION AND DIAGNOSIS SCHEME WITH DISJOINT SUBSYSTEMS

Because each disjoint subsystem only corresponds to partial measurement, principle component analysis (PCA) is used to activate them in this paper. As one widely used process analysis and inspection method, PCA extracts relativity information through low-dimension modeling based on statistics principle (Ge et

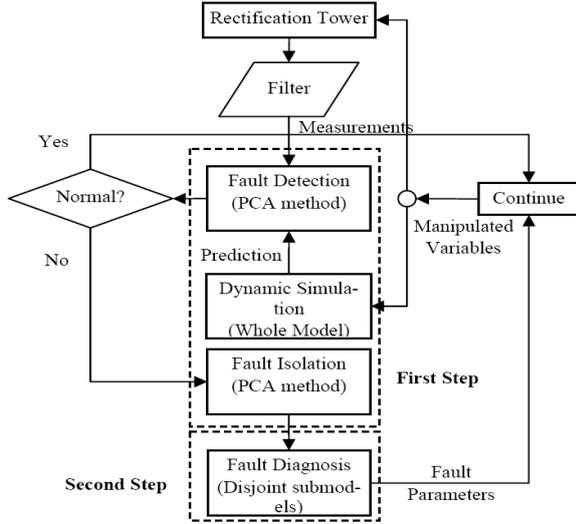


Figure 2. Two-step framework of fault diagnosis

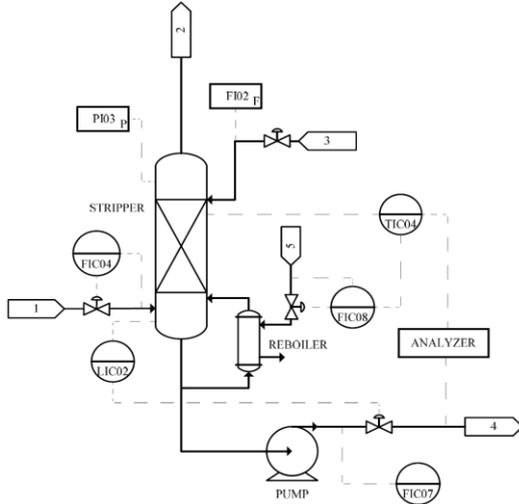


Figure 3. Overview of TEP stripper case study

ture steam (Stream 5) provides the necessary heat for stripping operation. Gaseous reactants and liquid products leave stripper from top (Stream 2) and bottom (Stream 4) respectively. There are 4 input manipulated variables and 12 output measurable variables in the stripper simulator. Five abnormal scenarios exist for this stripper consisting of composition, temperature and pressure variation in Stream 1. Abnormal data set given by stripper simulator includes 500 training data points and 960 testing data points with 3 minutes as sampling period. The two-step fault diagnosis system is coded with Matlab language, and its model parameters can be found in our earlier paper (Tian *et al.*, 2012).

Fault No. 7 is selected as an example to compare model decomposition based diagnosis method with whole model based one. This fault, arising from the step decrease of source pressure in Stream 1 at 8h, reduces flow rate of Stream 1 and thereafter stripping effect greatly. Pressure loss coefficient ε_1 is added into Eq. (28a) to quantify fault No. 7 as follows:

$$fm_1 \times mw_{s,1} = \frac{fop_1}{kvr_1} \times \sqrt{\rho_1 \times \varepsilon_1 \times (pfr_1 - pto_1 + adp_1)}. \quad (30)$$

Figure 4 shows change of pressure loss coefficient obtained by the fault diagnosis algorithm based on whole distillation model (Tian *et al.*, 2012). It can be seen that coefficient curve waves greatly because of control loops and measurement noise. As this violent wave hampers clarifying root abnormal causes during diagnosis, it is necessary to limit submodel scope to decrease effect of external disturb on inferred fault parameters.

System decomposition strategy is then applied to diagnosis process. In Section II, the whole distillation model is decomposed using Himmelblau algorithm into three submodels, that is, top feed part (I), bottom feed part (II) and remaining part (III). Fault No. 7 appears in Stream 1, so submodel II is exclusively needed during diagnosis and fault parameter computation process is thus simplified and accelerated. Figure 4 also gives diagnosis result with submodel about fault No. 7. It shows a clearer curve shape of fault parameter than whole model based method. In view of computation speed, the latter consumes 30 seconds while the former consumes 704 seconds for fault No. 7. So decomposition strategy is very effective in speeding up time-consuming nonlinear model based fault diagnosis process.

Median filter and lifting wavelet analysis method are used to remove measurement noise for sampling data and enhance diagnosis robustness. Figure 5 gives the diagnosis result after using data filter. It shows that curve shape of pressure loss coefficient basically keeps unchanged for whole model based method, although filter removes almost all the random noise from inferred parameter. This figure also gives a much more clear and legible change curve of fault parameter than Fig. 4 with submodel based method, benefiting identification of base abnormal reasons. Consequently, decomposition strategy should be combined with filter to expect greatly improved fault diagnosis result.

Above marked improvement of computational efficiency results from small scale of submodel II. For another fault No. 10, i.e. random variation of temperature in Stream 1 (embedded in $h_{0,j}$ in Eq. 6), its computational efficiency cannot be expected to enhance greatly because it lies in large scale submodel III. Consequently, in consideration of modeling complexity and computational efficiency, this decomposition based approach is still limited to unit models with a high sparse

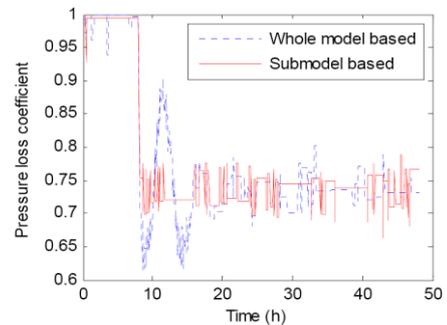


Figure 4. Diagnosis result for fault No. 7 without data filter

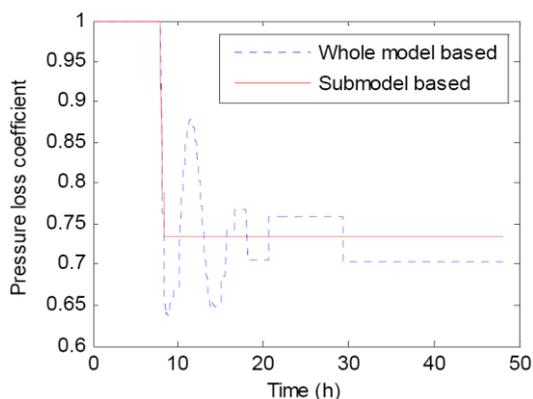


Figure 5. Diagnosis result for fault No. 7 with data filter

ratio. Otherwise, overly tight connections between variables will neutralize computing benefit from decomposition strategy greatly. So, future research should focus on the partial decomposition strategy for non-sparse models.

V. CONCLUSIONS

A two-step model decomposition based diagnosis framework has been implemented for distillation process. The whole nonlinear distillation model was divided into three disjoint parts with the aid of Himmelblau algorithm. After identifying fault type with PCA method, fault diagnosis work employs different disjoint submodels to cut down computation time and weaken effect of fault propagation on result. Moreover, median filter and lifting wavelet analysis method are used to remove gross noise and white noise from measured data to enhance diagnosis robustness. The proposed method was applied to the stripper example in TEP simulator. Result shows that two-step diagnosis framework facilitates obtaining faster and clearer fault parameter trend than whole nonlinear model based scheme as it reduces model scale undertaken. Future work will be focused on irreducible submodel by tearing variable loops to obtain complex fault parameters.

ACKNOWLEDGEMENTS

This work is supported by the National Natural Science Foundation of China (No. 21576143).

REFERENCES

- Ahn, S.J., C.J. Lee, Y. Jung, C. Han, E.S. Yoon and G. Lee, "Fault diagnosis of the multi-stage flash desalination process based on signed digraph and dynamic partial least square," *Desalination*, **228**, 68-83 (2008).
- Bhagwat, A., R. Srinivasan and P. R. Krishnaswamy, "Multi-linear model-based fault detection during process transitions," *Chemical Engineering Science*, **58**, 1649-1670 (2003).
- Deshpande, A.P. and S.C. Patwardhan, "Online fault diagnosis in nonlinear systems using the multiple operating regime approach," *Industrial & Engineering Chemistry Research*, **47**, 6711-6726 (2008).
- Gao, D., C. Wu, B. Zhang and X. Ma, "Signed directed graph and qualitative trend analysis based fault diagnosis in chemical industry," *Chinese Journal of Chemical Engineering*, **18**, 265-276 (2010).
- Ge, Z., L. Xie, U. Kruger and Z. Song, "Local ica for multivariate statistical fault diagnosis in systems with unknown signal and error distributions," *AIChE Journal*, **58**, 2357-2372 (2012).
- Himmelblau, D.M., "Decomposition of large scale systems—i. Systems composed of lumped parameter elements," *Chemical Engineering Science*, **21**, 425-438 (1966).
- Isermann, R., "Model-based fault-detection and diagnosis – status and applications," *Annual Reviews in Control*, **29**, 71-85 (2005).
- Lee, G. and E.S. Yoon, "A process decomposition strategy for qualitative fault diagnosis of large-scale processes," *Industrial & Engineering Chemistry Research*, **40**, 2474-2484 (2001).
- Lee, G., C.H. And and E.S. Yoon, "Multiple-fault diagnosis of the tennessee eastman process based on system decomposition and dynamic pls," *Ind. Eng. Chem.*, **43**, 8037-8048 (2004).
- Lee, C.J., G. Lee, C. Han and E.S. Yoon, "A hybrid model for fault diagnosis using model based approaches and support vector machine," *Journal of Chemical Engineering of Japan*, **39**, 1085-1095 (2006).
- Leung, D. and J. Romagnoli, "Dynamic probabilistic model-based expert system for fault diagnosis," *Computers & Chemical Engineering*, **24**, 2473-2492 (2000).
- Ms, L.H.C., E.L. Russell and R.D. Braatz, *Fault detection and diagnosis in industrial systems*, Springer, London (2001).
- Namdari, M. and H. Jazayeri-Rad, "Incipient fault diagnosis using support vector machines based on monitoring continuous decision functions," *Engineering Applications of Artificial Intelligence*, **28**, 22-35 (2014).
- Shahabinejad, H., S.A.H. Feghhi and M. Khorsandi, "Structural inspection and troubleshooting analysis of a lab-scale distillation column using gamma scanning technique in comparison with monte carlo simulations," *Measurement*, **55**, 375-381 (2014).
- Tian, W., Q. Guo and S. Sun, "Dynamic simulation based fault detection and diagnosis for distillation column," *Korean Journal of Chemical Engineering*, **29**, 9-17 (2012).
- Tian, W., S. Sun and Q. Guo, "Fault detection and diagnosis for distillation column using two-tier model," *The Canadian Journal of Chemical Engineering*, **91**(10), 1671-1685 (2013).
- Venkatasubramanian, V., R. Rengaswamy, S.N. Kavuri and K. Yin, "A review of process fault detection and diagnosis: Part iii: Process history based methods," *Computers & Chemical Engineering*, **27**, 327-346 (2003).
- Verucchi, C.J., G.G. Acosta and F.A. Bengier, "A review on fault diagnosis of induction machines," *Latin American Applied Research*, **38**, 113-121 (2008).

Wang, Z. and H. Bai, "Process system fault detection and diagnosis based on correlation," *CIESC Journal*, **64**, 4621-4627 (2013).

Received: April 11, 2017.

Sent to Subject Editor: April 27, 2017.

Accepted: February 1, 2018.

Recommended by Subject Editor:

Marcelo Martins Seckler