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Risk-based warning system design methodology for multimode processes

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Abstract: Complex chemical processes usually operate at multiple operating modes, resulting from various factors, such as changes in market demand, set point modifications, and feedstock changes. It is difficult to monitor a multimode process without generating significant number of false alarms. In this paper, a risk-based alarm system design methodology is proposed to monitor multimode processes. The methodology comprises of three main steps: i) analysis of operating data using Gaussian mixture model, ii) identification of independent operating modes (e.g. set points, virtual transient state), and iii) probabilistic model to assess risk and activation of appropriate warning. A continuous stirred tank reactor with model predictive control system is used to demonstrate the effectiveness of the proposed method.

Keywords: multimode process; Gaussian mixture model; warning system design; alarm management; probability graphical model

1. INTRODUCTION

Over the past decades, more and more attentions have been paid to the process monitoring from both academia and industry because of its indispensable role in guaranteeing safe operation. Complex chemical processes usually operate at multiple operating modes, resulting from various factors, such as changes in market demand, set point modifications, and feedstock changes (Hwang and Han, 1999). The real-time monitoring and warning of danger in multimode processes is a challenging problem, which has drawn increasing attention recently (Zhao et al., 2010).

To resolve the issues associated with monitoring multiple operating modes processes, multivariate statistical process monitoring (MSPM) is becoming popular due to the availability of large sets of data generated by large-scale chemical processes (Ning et al., 2014, Qin, 2012). MSPM techniques, such as partial least-squares (PLS) and principal component analysis (PCA), have been intensively investigated and fruitful of applications have been demonstrated (Wise and Gallagher, 1996). Zhao proposed a method based on multiple partial least-squares models to monitor multimodal process (Zhao et al., 2006). Also, many PCA-based techniques have been reported. Chen and Liu proposed a fault detection method using mixture of PCA models, in which the number of clusters are determined automatically (Chen and Liu, 1999). Ng and Srinivasan proposed an Adjoined PCA approach, where a mixture of PCA models are adjoined (Ng and Srinivasan, 2009). Choi formulated the maximum likelihood principal component analysis (MLPCA) mixture model to monitor process. Feital proposed a multimodal modelling and monitoring approach based on MLPCA analysis and presented an operating modes identification method (Feital et al., 2013). All these PCA-based methods suffer drawbacks of dealing with non-Gaussian distributed operating data in process.

Compared to the PCA-based mixture models, advantages of the Gaussian mixture model (GMM) includes: (1) the model structure is simple so that it is easy to understand and to implement in non-Gaussian process, (2) can be used to monitoring multimode processes, (3) can handle the nonlinear process (Ge et al., 2013). The GMM method can describe complex industrial process dataset by several local linear models. To learn the Gaussian mixture model, the Expectation-Maximization (EM) algorithm is employed to estimate the values of its parameters. GMM is promising method to monitor non-Gaussian, multimode process (Ge et al., 2013, Choi et al., 2004, Yu, 2012, Yu and Qin, 2009, Chen and Zhang, 2010). Ververidis (Ververidis and Kotropoulos, 2008) and Hennig (Hennig, 2010) showed the strong ability of Gaussian mixture model to separate different operating modes in process. Yu and Qin developed a finite Gaussian mixture model (FGMM) and used the Bayesian inference-based probability (BIP) index for process monitoring (Yu and Qin, 2008). The number of modes in a GMM is automatically determined along with its other parameters.

In this paper, a risk-based warning system design method using the GMM is proposed to represent non-Gaussian, multimode operating data and to separate different operational modes. As a result, the process state (including acceptable transient state) can be identified for operating data in real-time, give proper warning message while minimize the false alarms at the same time.

This paper proceeds as follows. First, the proposed methodology is described in Section 2 followed by a case study in Section 3. Finally, discussions and conclusions are presented.

2. METHODOLOGY

The proposed methodology of alarm management in multimode process is shown in Figure 1. The methodology is comprised of three important steps: i) analysis of operating data using Gaussian mixture model, ii) identification of independent operating modes (e.g. set points, virtual transient state), and iii) probabilistic model to assess risk and activation of appropriate warning. The details of the methodology is explained in following subsections.

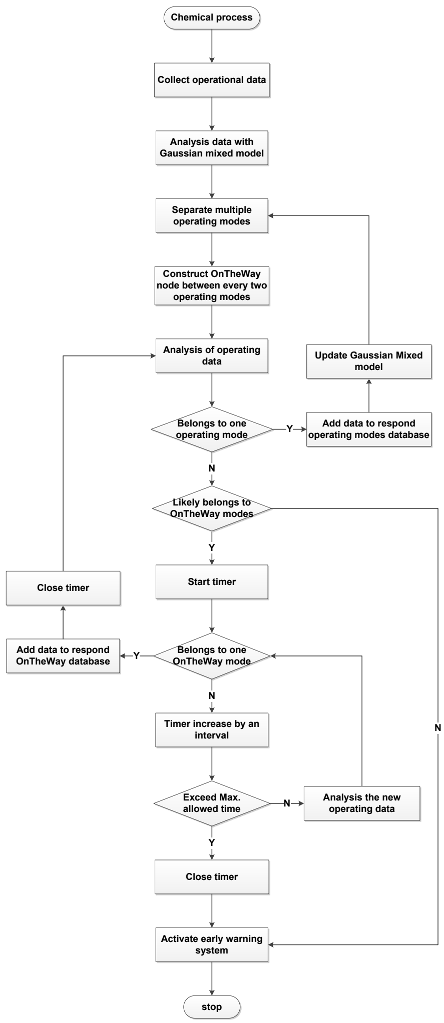


Figure 1. Methodology for alarm management in multimode process

2.1 Gaussian mixture model to represent multimode

Let us consider a simple situation. Suppose data from normal operating situations are represented in Figure 2. All records of operating point values can be represented by Gaussian mixture model, and also can be separated into different operating modes. In this example, there are two different operating modes with set point sp_1 and sp_2.

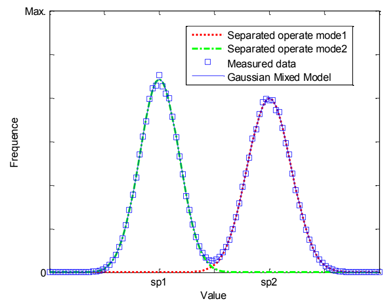


Figure 2. Measured values and separated operation modes

2.2 Identification of operating modes

In this example, there is a variable x, with two possible set point, sp_1, *and sp2*. Also the system may be on the way from sp_1 to sp_2 or vice versa is considered, this is a transient mode. This situation is considered to be a normal situation, not to alarm as a false alarm. So a virtual operating mode is introduced, shown in Figure 3, to help identify the transient mode from operating point sp_1 to sp_2 , or vice versa. In this virtual mode, denoted as the OnTheWay mode, there is a special operating point. All transient operating trajectories frequently pass through it, and it can be a reference location to identify that the operating point is in its transient situation. Because it is a transient state, if all operating data are correctly recorded, this transient mode can be properly separated by the Gaussian mixture model.

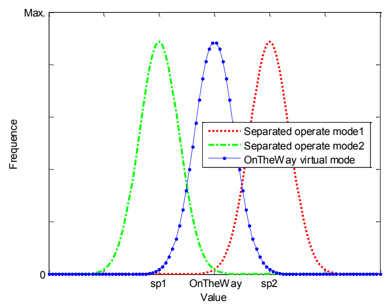


Figure 3. Operating modes and OnTheWay virtual mode

2.3 Risk estimation and activation of alarm

With the OnTheWay virtual mode, process state can be monitored in real time. Fault probability for every operating point can be calculated over time. And then activate different level of early warnings according to the probability and severity. In this method, both severity and probability are represented in terms of distances from the centers. The severity classification schematic is shown in Figure 4. With the probability and severity values, the state of the current operating point can be identified, and give proper warning if it is necessary.

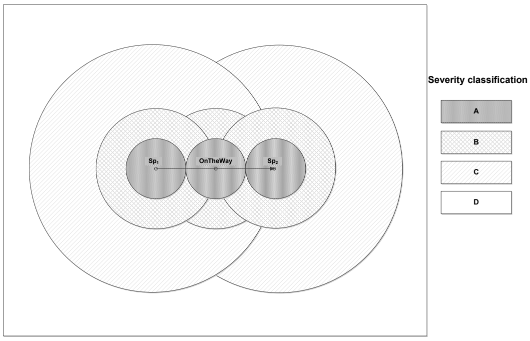


Figure 4. Severity classification schematic, the area A is the normal operation ranges, and area D is a possible fault requiring a warning message.

The severity corresponds to the potential consequence; the values are assigned in Table 1.

Table 1. Severity classification

Classification	Consequence	Meaning
Class A	1	Normal operation
Class B	10	Deviation acceptable
Class C	50	Deviation require attention
Class D	100	Fault require warning message

The consequences in Table 1 denote the relative importance of operating points. These values will be used to calculate the potential risk at an operating point.

2.4 *The probability graphical model for warning system*

The probability graphical model is shown in Figure 5.

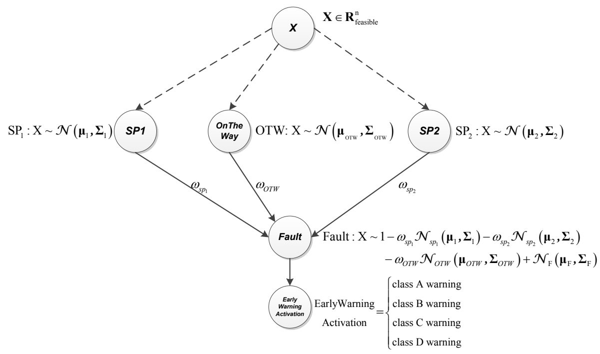


Figure 5. Probability graphical model for warning system.

Here, the variable **x** is the value of operating point in feasible spaces, the node SP1 is a multivariate normal distribution to describe the probability of current operating point **x** belongs to the operating mode SP1, the mean is $\boldsymbol{\mu}_1$, which is an operating set point, and the variance is $\boldsymbol{\Sigma}_1$. The same situation can be found to node SP2. The node OnTheWay is a node for virtual operating mode, together with SP1 and SP2, the fault distribution can be calculated in Fault node, based on the probability of fault and the possible consequence loss. The state of current operating point can be correctly identified, and the risk is estimated. Finally, different warnings according the calculation result are activated.

3. CASE STUDY

A continuous stirred tank reactor (CSTR) with model predictive control system is used to demonstrate the effectiveness of the proposed method.

3.1 *CSTR process description*

The schematic of the CSTR process (Seborg et al., 2010) is shown in Figure 6.

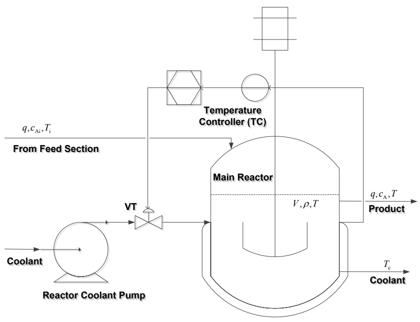


Figure 6. Schematic of CSTR with temperature controller

A liquid phase, irreversible chemical reaction takes place in the reactor where chemical species A reacts to form species B. The rate of reaction is first order with respect to component A,

$$r = kc_{\mathrm{A}}$$

Where r is the rate of reaction of A per unit volume, k is the reaction rate constant, and c_{A} is the molar concentration of species A.

$$k = k_0 e^{-\frac{E}{RT}}$$

The inlet stream consists of pure component A with molar concentration, c_{Ai}. A cooling jacket is used to maintain the reaction mixture at the desired operating temperature.

A perfect mixing condition is assumed. The mass densities of reactant and product are assumed to be the same. The liquid volume of the reactor is kept constant. The dynamic model of the CSTR is as follow.

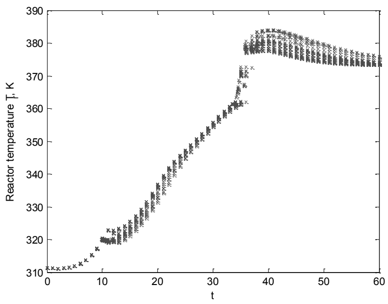
$$V\frac{\mathrm{d}c_A}{\mathrm{d}t} = q(c_{\mathrm{Ai}} - c_{\mathrm{A}}) - Vkc_{\mathrm{A}}$$

$$V\rho C_{\mathrm{p}}\frac{\mathrm{d}T}{\mathrm{d}t} = wC_{\mathrm{p}}(T_{\mathrm{i}} - T) + (-\Delta H_{\mathrm{R}})Vkc_{\mathrm{A}} + UA(T_{\mathrm{c}} - T)$$

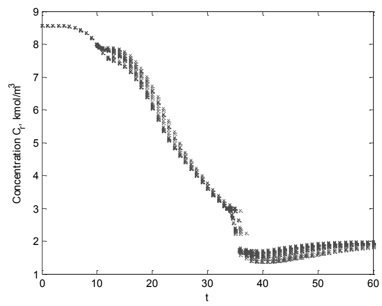
The CSTR is under a model predictive controller (MPC). A Simulink model is developed to simulate the dynamic process.

3.2 Gaussian mixture model

Using the CSTR model, 1461 operating points are generated in simulation. Among all variables, the two key state variables, reactor temperature and concentration are shown in Figure 7.



(a)



(b)

Figure 7. Reactor temperature and concentration change with time, (a) temperature, (b) concentration

The correlation between temperature and concentration are shown in 8.

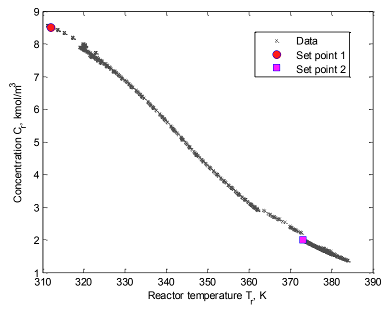


Figure 8. Concentration and temperature

There are two operating modes, and the set point values are listed in Table 2.

From Figure 7 and Figure 8, it can be seen there is a transient between these two set points. With data in Figure 8, the Gaussian mixed model is established to represent the distribution of these operating data, details can be found in Figure 9.

$$X = \omega_1 \mathcal{N}(\boldsymbol{\mu}_1, \boldsymbol{\Sigma}_1) + \omega_2 \mathcal{N}(\boldsymbol{\mu}_2, \boldsymbol{\Sigma}_2) + \omega_3 \mathcal{N}(\boldsymbol{\mu}_3, \boldsymbol{\Sigma}_3)$$

Table 2. Set points for the CSTR process

	set point 1, sp_1	set point 2, sp_2	units
Temperature, T_r	311.0	373.0	K
Concentration, C_r	8.5	2.0	kmol/m^3

These data can be well represented by three bivariate normal distributions, corresponding to two set points and an OnTheWay virtual state. The details of these three components of Gaussian mixture model are in Table 3.

Table 3. Components in the Gaussian mixture model

	Component 1	Component 2	Component 3
Name	Set point 1	Set point 2	OnTheWay
Means	$\boldsymbol{\mu}_1 = \begin{pmatrix} 317.3 \\ 8.1 \end{pmatrix}$	$\boldsymbol{\mu}_2 = \begin{pmatrix} 376.8 \\ 1.8 \end{pmatrix}$	$\boldsymbol{\mu}_{\text{OTW}} = \begin{pmatrix} 348.4 \\ 4.6 \end{pmatrix}$
Variances	$\boldsymbol{\Sigma}_1 = \begin{pmatrix} 20.9 & -1.7 \\ -1.7 & 0.1 \end{pmatrix}$	$\boldsymbol{\Sigma}_2 = \begin{pmatrix} 12.5 & -0.9 \\ -0.9 & 0.1 \end{pmatrix}$	$\boldsymbol{\Sigma}_{\text{OTW}} = \begin{pmatrix} 127.0 & -15.8 \\ -15.8 & 2.0 \end{pmatrix}$
Weights	0.30	0.40	0.30

The weights of these components are: 0.30, 0.40 and 0.30. The total 1461 operating points can be well represented by mixing these three bivariate normal distributions with the mentioned weights.

From Gaussian mixture model, these operating components are separated, including the mode around set points and the virtual OnTheWay mode. In practice even if the actual set points and the virtual modes are unknown, the GMM can separate them correctly with proper data. Next, a probability graphical model for warning system is developed.

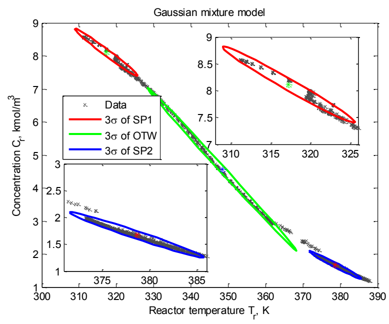


Figure 9. Gaussian mixture model of operating data

3.3 Warning (alarm) system model

The probability graphical model of the CSTR for warning system is shown in Figure 10. According to this model, every operating point can be evaluated by all operating modes, that is, calculate probabilities of operating point that belongs to these operating modes (including virtual operating modes). With these probabilities, the probability of fault is calculated. Based on this probability and the consequence severity values, the risk can be estimated and then different warning will be activated accordingly.

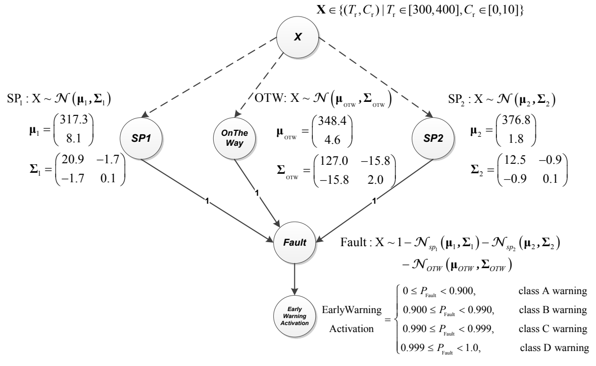
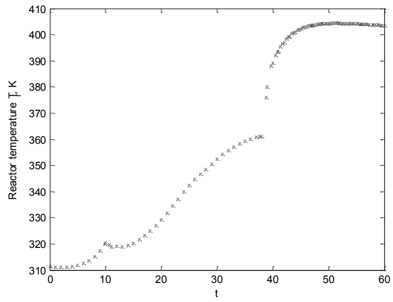


Figure 10. Probability graphical model of CSTR for warning system.

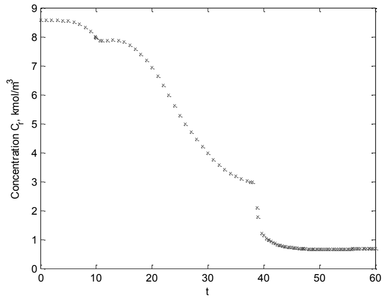
Parameter values in this probability model will be continuously updated with increasing dataset and feedbacks.

3.4 Risk-based warning (alarm) system

With probability graphical model, the operating data sequences can be analyzed and identified dynamically over time. Figure 11 shows the recorded data in CSTR with a runaway situation.



(a)



(b)

Figure 11. Simulation with temperature and concentration run away

There are totally 122 operational data here to simulate with temperature and concentration run away, and these data in sequence can be classified into different severity classes. The consequence value to every probability are considered to calculate the dynamic risk of the process, the result is shown in Figure 12.

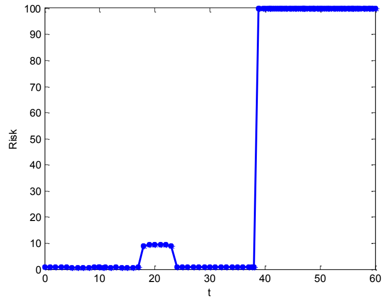


Figure 12. Dynamic risk in CSTR process

From Figure 12 the different level of risk can be identified and the corresponding early warning is given accordingly. When the calculated risk value is greater than 50, it indicates that there is an unacceptable deviation from any operating mode (including the transient mode).

3.5 Identify run away operating points

Here 800 operating point data are generated for testing, some of them with very large deviation from neither the set points operating modes nor the OnTheWay mode. These operating points are shown in Figure 13.

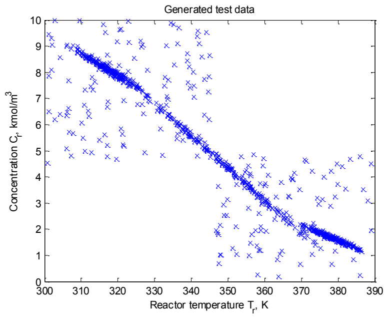


Figure 13. Generated data for testing

With the established probability graphical model, the state of every operating point can be identified, and the proper early warning of different classes is issued.

With the same threshold, these testing operating point data can be classified into different classes with/without virtual mode, details as follow in Table 4:

Table 4. Comparison between with/without OnTheWay mode in testing data classification

Type	With OnTheWay mode	Without OnTheWay mode
Class A	479	350
Class B	115	52
Class C	20	12
Class D	186	386

It can be seen from Table 4, with the OnTheWay virtual mode which determined by the proposed methodology, the transient states can be identified, and the false alarm of the fault (e.g. the class D) is reduced significantly; 200 false alarms are avoided (from 386 to 186 in Class D). The virtual mode is separated by GMM-based methodology, in this way, the number of false alarm is reduced greatly.

4. CONCLUSION

Multiple operating modes should be considered carefully in daily operation. The Gaussian mixture model can represent data set of operating points involving different operating modes, Furthermore, it can separate the operating modes, together with on the way virtual mode, as independent components. With these multiple components, the probability graphical model for warning system can be established to analyze the operating data and give proper warning at different safety levels. Furthermore, with the increasing number of operating data, the parameters of Gaussian mixture model and the probability graphical model can be updated, and the performance of the methodology can be improved continuously. As a result, the false alarms can be reduced greatly and the different early warning messages can be properly passed to operators based on the dynamic risk in multimode process.

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