On-line Dynamic Model Correction Based Fault Diagnosis in Chemical Processes

TIAN Wen-de(田文德)[1], SUN Su-li(孙素莉)[2]

(*1. College of Chemical Engineering, Qingdao University of Science & Technology, Qingdao, Shandong 266042, China;*
2. School of Polymer Science and Engineering, Qingdao University of Science & Technology, Qingdao, Shandong 266042, China)

Abstract: A novel fault detection and diagnosis method was proposed, using dynamic simulation to monitor chemical process and identify faults when large tracking deviations occur. It aims at parameter failures, and the parameters are updated *via* on-line correction. As it can predict the trend of process and determine the existence of malfunctions simultaneously, this method does not need to design problem-specific observer to estimate unmeasured state variables. Application of the proposed method is presented on one water tank and one aromatization reactor, and the results are compared with those from the traditional method.

Key words: fault diagnosis; chemical process; dynamic simulation; parameter estimation

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1 INTRODUCTION

Chemical industry generally employs a great deal of combustible, explosive and toxic chemicals under the high temperature and pressure or low temperature and vacuum operating conditions, so there exist inevitable hidden fire, explosion and poisoned hazard within its equipment[1]. Consequently the fault diagnosis technique has attracted more and more attentions recently, and become the key to assist in solving process reliability and safety problems.

Fault diagnosis method can be classified into three categories: model-based method, knowledge-based method, and process history based method. In practice, the structure and fault of chemical process are complicated by its large scale, continuity and high speed production, so the majority of present diagnosis methods are focused on the latter two methods, including fault tree, directed graph, knowledge base, and neural network[2−4]. These qualitative methods emphasize mostly on the analysis of target attributes, with such advantages as quickness and simplicity, but such disadvantages as limited analytical depth and accuracy as well. To overcome these weaknesses, model-based method supplies one dynamic mechanism model about internal relationships within a system, and then extracts abnormal deviations through state identification, parameter estimation, parity relations, etc. Because it can produce meaningful result and demonstrate the deduction procedure, more and more fault diagnosis research is concerned with such a quantitative model based method[2].

Grantham et al.[5], for example, presented a prototype first-principles based trouble shooting system. It reasons with an understanding of physical and chemical phenomena, and allows analysis and explanation at a more fundamental level. Watanabe et al.[6] proposed a two-level strategy for fault detection and diagnosis by examining the detection of instrument faults in nonlinear time-varying process using state estimation filters. Gertler et al.[7] presented a design procedure to generate isolable parity equation based on sensitivities, and illustrated the application of the technique on a distillation column. Huang et al.[8] applied the extended Kalman filter (EKF) to the fluidized catalytic cracking unit (FCCU), and proposed a dynamic optimization based control redesign scheme using the results from fault diagnosis. Recently, Prakash et al.[9] integrated fault diagnosis with model predictive control (MPC) to eliminate offset between the true values and set points of controlled variables in the presence of a variety of faults.

Most approaches mentioned above contain the following three features. Firstly, the fact that different steps during fault diagnosis are clearly separated: detection, isolation and estimation of the magnitude of a fault bring some troubles in process model selection and calculation. Secondly, the measured data are usually incomplete and inaccurate, so it needs to design some

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Biography: TIAN Wen-de (1973−), male, native of Heze City, Shandong Province, Ph.D., associate professor, majoring in process systems engineering, Tel: 0532-84022026, E-mail: tianwd@qust.edu.cn.

specific observers to deduce the values of unmeasured variables, thus leading to a weak generalization property for the chosen model. Finally, dynamic model adopted is limited to residual evaluation use only.

In addition, a number of applications of dynamic simulation have appeared in recent years for analyzing dynamic features, directing start-up and shut-down, and designing advanced control systems[10,11]. And steady state model based real-time optimization, in which on-line model correction plays an important role, has been used in many industrial processes. Motivated by these efforts, in this work, a dynamic simulation based fault detection and diagnosis system is proposed, in which dynamic simulation continues comparing its output with measured value to determine whether to execute fault diagnosis, and then fault parameters are calculated via model correction when faults take place. Differing from those methods mentioned above, such a fault accommodation system integrates separate steps closely on the same dynamic model, and deduces incomplete measurements from this model itself but not observers.

2 FAULT DESCRIPTIONS

Fault is a general term used to describe a departure from an acceptable range of an observed variable that degrades process performance[12]. Fault diagnosis is normally defined as the problem of real-time identification of the root reason of malfunctions from current sensor data and some *a priori* knowledge about the process behavior under abnormal situations. The source of fault can be classified into three categories: gross parameter changes, structural changes and malfunctioning sensors and actuators. To find the particular fault source in chemical processes, it frequently needs to identify the unknown process parameters since the degradation of process performance mostly takes place as parameters change[6,13]. Consequently, this work aims at the faults that correspond merely to the model parameters. These faults can be further divided into three types according to the basic principles of transport phenomenon and reaction engineering.

2.1 Pipeline Fault

The pipeline fault arises from abnormal variation in flow rate, mainly caused by measurement deviation, valve stuck, property change of inlet fluid in composition, temperature and pressure, and broken pipe. The first two reasons can be indicated by the calculated flow rate multiplying correction coefficient; the third one can be formulated with mass and energy balance, the last one can be considered through the complex flow rate calculation in branch pipes, and will be mainly explained in detail in this section. Occurrence of fluid leakage will reduce the flow rate entering equipments, but not the flow rate leaving these equipments, as shown in Fig.1. It should be noted that leakage on pipeline 1–2–3 is simplified as a branch pipeline 2–4.

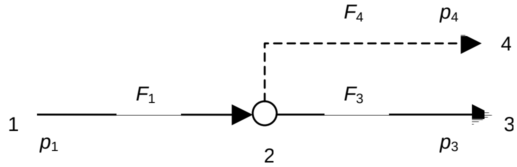

Fig.1 Schematic diagram of leaking pipe

Without leakage (no branch 2–4), the volumetric flow rate in pipeline 1–2–3 can be expressed as a function of pressure drop according to mechanical energy balance principle, ignoring the potential energy change between the inlet and outlet.

$$\frac{-\Delta p}{\rho}=\frac{p_1-p_3}{\rho}=\lambda\frac{l}{d}\frac{u^2}{2}, \tag{1}$$

$$F=\frac{\pi d^2}{4}u=\frac{\pi d^2}{4}\sqrt{\frac{2d(-\Delta p)}{\rho\lambda l}}. \tag{2}$$

In the case of leakage, the flow rate in pipeline 1–2 equals the flow rate sum of pipeline 2–3 and 2–4, and mechanical energy at point 3 and 4 both equals the one at point 2. This implies that the flow rate in pipeline 1–2 is proportional to the one in pipeline 2–4 if their pressure change is negligible.

$$\frac{F_4}{F_1}=\sqrt{\frac{\lambda_1 l_1/d+1}{\lambda_4 l_4/d+1}}. \tag{3}$$

So the flow rate of 2–3 can be thought as a function of the flow rate of 1–2 as

$$F_3=\left(1-\sqrt{\frac{\lambda_1 l_1/d+1}{\lambda_4 l_4/d+1}}\right)F_1. \tag{4}$$

Combining with Eq.(2), Eq.(4) is changed into

$$F_3=\left(1-\sqrt{\frac{\lambda_1 l_1/d+1}{\lambda_4 l_4/d+1}}\right)\frac{\pi d^2}{4}\sqrt{\frac{2d(-\Delta p)}{\rho\lambda l}}=C_{\mathrm{Q}}\sqrt{\frac{p_1-p_3}{\rho}}. \tag{5}$$

It can be seen from Eq.(5) that C_{Q} decreases gradually with decreasing of λ_4 and l_4, which means that fluid leakage occurs. Given fixed pressure drop p_1–p_3, the outlet flow rate F_3 will drop correspondingly. Eq.(5) also shows that such a causal transformation procedure is not convenient to use in practice because of its nonlinearity. Nevertheless, since only the final result of this transformation is needed in fault diagnosis, C_Q is ultimately chosen as the internal parameter to express the leaking pipeline situation in this research.

2.2 Heat Transfer Fault

The wall-type heat exchange procedure is performed in heat exchangers and jacketed reactors, formulated as Eqs.(6) and (7) where the overall heat transfer coefficient K consists of convection heat transfer resistance in both sides of fluid, fouling resistance and wall resistance.

$$Q=KS\Delta T_m, \tag{6}$$

$$\frac{1}{K}=\frac{1}{\alpha_i}\frac{d_o}{d_i}+R_{S,i}\frac{d_o}{d_i}+\frac{b}{\lambda}\frac{d_o}{d_i}+R_{S,o}+\frac{1}{\alpha_o}. \tag{7}$$

In such heat-exchange equipment, $R_{S,i}$ and $R_{S,o}$ in the right hand side of Eq.(7) always change due to heat transfer wall deposit or operation error, resulting in the decrease of K and heat transfer efficiency thereby. So, to represent the heat transfer fault, these two variables are combined into an inner model coefficient R_S as

$$R_S=R_{S,i}\frac{d_o}{d_i}+R_{S,o}. \tag{8}$$

2.3 Reaction Fault

Reaction fault in real chemical processes is commonly encountered when the fractional conversion for reactants decreases owing to degraded catalyst. In a reaction model, catalyst influences the reaction rate via the reaction rate constant k in Eq.(9). K furthermore is a function of pre-exponential factor k_0 and activation energy E according to the Arrhenius equation. The decrease of k_0 means physical degradation of the catalyst whereas the decrease of E means chemical degradation. The difficulty in estimating k_0 and E simultaneously due to their nonlinear relationship is often alleviated by some specified transformation. If the fact that temperature T is generally kept constant in a real process is taken into consideration, it is however more difficult to obtain these two parameters separately. Therefore, only the coefficient k_0 is used as model parameter to represent reaction fault in this paper.

$$r_i=k\prod C_i^{\nu_i}=k_0 e^{-\frac{E}{RT}}\prod C_i^{\nu_i}. \tag{9}$$

3 FAULT DIAGNOSIS

3.1 Dynamic Simulation

Having given the corresponding model parameters for chemical process faults, the dynamic model can be formulated on the basis of mass and heat balance as Eqs.(10) and (11). It should be noted that after integrating Eq.(10) for all components, an overall material balance can be deduced, reflecting the fluctuation of liquid level in equipment. These two equations express how reactor liquid level h, component x and temperature T change with time, and why such a relationship is a function of the fault parameters given in Section 2.

$$A\rho\frac{d(hx_i)}{dt}=\sum_j F_{i,j}x_{i,i,j}-\sum_j F_{V,j}x_i-\sum_j F_{L,j}y_i+AhM\sum_j r_{j,i}, \tag{10}$$

$$A\rho C_p\frac{d(hT)}{dt}=\sum_j F_{i,j}C_{p,i,j}T_{i,j}-C_{p,V}T\sum_j F_{V,j}-C_{p,L}T\sum_j F_{L,j}+Ah\sum_j\left(-\Delta H_{R,j}\right)r_j+KS(T_0-T). \tag{11}$$

Dynamic simulation can be conducted based on the model built above plus appropriate ordinary differential equations (ODEs) numerical algorithm. Frequently used ODEs algorithms are Runge–Kutta method and Euler method presently. The former has higher integration accuracy but a lower speed and requires the derivatives to be continuous in addition. Because of operating actions that may be performed during each time interval in chemical process and the high calculation speed requirement for fault diagnosis, the Euler method is frequently chosen as the dynamic simulation algorithm in practice.

3.2 Fault Diagnosis Procedure

Figure 2 depicts the fault diagnosis procedure on the basis of the dynamic simulation system introduced in the previous section. The fault detection step is carried out at first, in which dynamic simulation output is compared with the local history data collection to decide whether the running state of the real process complies with its theoretical prediction. If yes, it indicates that the real process is normal and thus only inspection is needed in the next cycle; otherwise, it indicates that the real process is out of work and trouble shooting is needed in the next step. Because the external faults result from abnormal changes of internal model parameters, fault diagnosis will proceed with on-line correction of these parameters. The trajectory of obtained parameters is analyzed to retrieve the basic causes under current faults. Finally, operation staff will make corresponding decisions in light of these underlying reasons, while the process is still under the supervision of the fault detection and diagnosis system.

3.3 Fault Detection

The existence of faults is determined according to

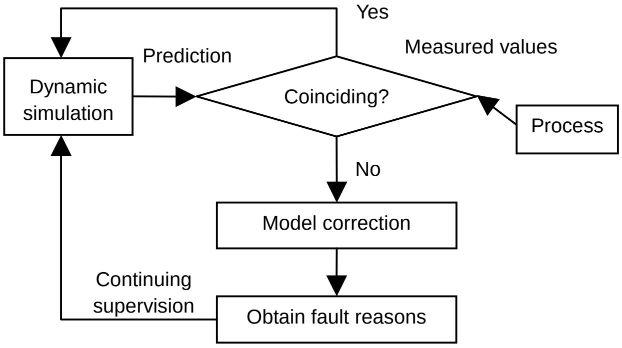

Fig.2 Steps involved in fault diagnosis

the residual between measured value and simulated one. To eliminate the determination error caused by the small measured value, the coinciding criterion in Fig.2 is given as

$$\left|\frac{y-\hat{y}}{\hat{y}}\right|<\varepsilon, \tag{12}$$

where ε denotes the threshold value of the residual. In practice, gradual change in normal parameters and abrupt change in fault parameters often coexist, so disparate thresholds should be given accordingly. But in consideration of the fact that the former will turn into a fault state once it exceeds certain value, they are under supervision with the same Eq.(12). Besides, a large ε can lead to low fault sensitivity and a high fault miss ratio upon gradually changing faults, whereas a small ε can lead to a high false retrieval ratio due to the existence of random disturbances. Based on the above consideration, the value of ε is given using the statistic deviation of measured data plus certain allowance in this paper.

When faults are correlated to the change of unmeasured state variables, it is conventional to design some specific observers to estimate these variables following system redesign according to the input–output relationship[14]. Such a redesign procedure, mostly performed with Luenberger or Kalman filter methods, needs to specify the relative observer coefficients based on the stability, sensibility and robust requirements. Because this method requires different observers for different faults, it has some disadvantages like complex deduction process, low generalization performance and ambiguous physical meaning. But in practice, at least measured variables will change when faults occur, so the faults can be detected through the residuals between the measured and predicted value of these variables according to Eq.(12). Consequently, fault detection in this work is done with the real time simulation results of all measured process variables using the dynamic model given in Section 3.1. In this way, the dynamic simulation based fault detection system showed in Fig.2 needs no observer any longer, with the calculation process simplified and the application scope widened.

3.4 Model Correction for Fault Diagnosis

Because the fault diagnosis makes use of a mechanism model about state space in chemical process, the meaningful state changes will facilitate the isolation and estimation of fault once the residual is over this threshold value. As time lapses, deviations of the situation in plant from its ordinary designed value occur due to a couple of reasons like catalyst degradation, load change in heat exchanger, and existence of impurity. These reasons can be described with the fault parameters in Section 2. So, only through continuous model correction using real-time data collection can the coincidence be guaranteed for the response characteristic between model and plant. Such an updating process is implemented *via* parameter estimation. As Section 3.3 shows, a generalized process model in terms of parameters, as a modified version of the model in Section 3.1, is given as follows to facilitate parameter estimation.

$$\frac{\mathrm{d}z}{\mathrm{d}t}=az(t)+bu(t)+f(t)+s(t)p. \tag{13}$$

Since the Euler method is adopted in the dynamic model in Section 3.1, the differential calculation in the left hand side of Eq.(13) can be approximated by difference to perform fault detection and diagnosis on the same model. So Eq.(13) can be rewritten as

$$c(t)=s(t)p, \tag{14}$$

where

$$c(t)=\frac{z(t+1)-z(t)}{\Delta t}-az(t)-bu(t)-f(t). \tag{15}$$

After estimating the parameter vector p with linear least square method, the following formula is obtained.

$$\hat{p}=\left[\hat{s}(t)^T\hat{s}(t)\right]^{-1}\hat{s}(t)^T\hat{c}(t). \tag{16}$$

4 CASE STUDIES

The proposed dynamic simulation based fault detection and diagnosis method is applied to a water tank and a chemical reactor respectively, in order to test its feasibility under a case of multiple faults.

4.1 Water Tank

This is a problem about input–output material balance in a water tank[14], displayed in Fig.3. Water enters the tank with a flow rate of F_i, and then leaves it with F_L. Because the source pressure of F_L is affected by tank level h, F_L increases gradually as h increases until equilibrium in the tank is achieved when F_L is equal to F_i.

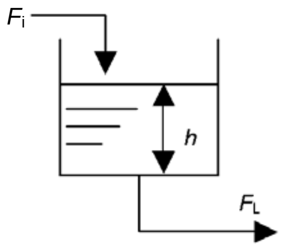

Fig.3 Water tank system

Because water temperature is constant in this process, mass balance can be changed into water volume balance, and heat balance is not considered here. Thus Eq.(10) is simplified as:

$$A\frac{dh}{dt}=F_i-F_L, \tag{17}$$

where

$$F_i=C_i\sqrt{\frac{p_i-p_0}{\rho}}, \tag{18}$$

$$F_L=C_o\sqrt{gh}. \tag{19}$$

Equation (19) takes into consideration the effect of water level on source pressure for exit flow.

The leakage in the inlet pipeline, represented by the decrease of C_i in Eq.(18) from 1.0 to 0.7 at 15 h, is set as the single fault in this tank. In fault diagnosis procedure, the variables in Eq.(16) are given as

$$\hat{p}=C_i, \tag{20}$$

$$\hat{s}(t)=\sqrt{gh}, \tag{21}$$

$$\hat{c}(t)=A\frac{h(t+1)-h(t)}{\Delta t}+C_o\sqrt{\frac{p_i-p_0}{\rho}}. \tag{22}$$

Table 1 provides the process parameters appearing in Eqs.(17)~(22).

Table 1 Parameters for water tank example

Parameter	Value
Floor area, A (m^2)	1.0
Flow rate coefficient for leaving pipe, C_o (m^2)	0.08
Water density, ρ (kg/m^3)	1000
Sampling interval, Δt (h)	0.5
Initial flow rate coefficient for entering pipe, C_i (m^2)	1.0
Ambient pressure, p_0 (Pa)	1.010×10^5
Source pressure for inlet flow, p_1 (Pa)	1.011×10^5

The measurement of h is realized through dynamic simulation with Eq.(17) solved by fourth order Runge–Kutta algorithm. The simulation time period is 50 h. The noise of h is added using normal distribution where mean and stand deviations equal 0 and 0.02 respectively.

Leakage fault can result in decrease of the measurement of h, and Fig.4 illustrates the procedure in which the proposed fault diagnosis system tracks this variation. It can be seen that the retrieved parameter C_i reflects the real leaking situation correctly.

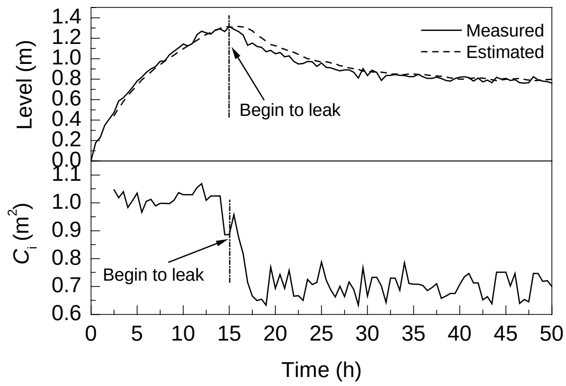

Fig.4 Fault detection and diagnosis procedure in water tank system

Figure 5 shows how the magnitude of ε in Eq.(12) affects the curve shape of obtained parameter. With the increase of ε, there appear more horizontal lines for C_i. This indicates that enhancing detection deviation threshold can markedly reduce fault diagnosis frequency. However, this increment also generates some response delays to the fault despite small fluctuation of C_i.

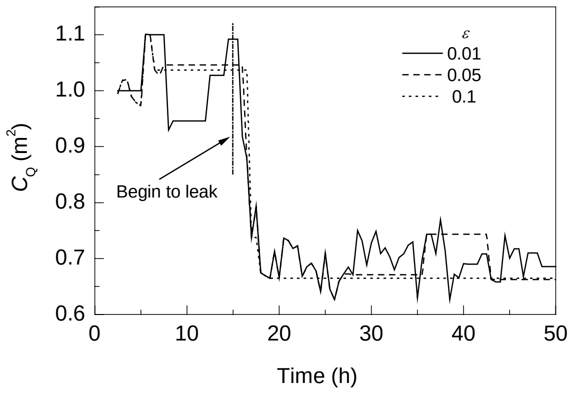

Fig.5 Variation of fault parameter with fault detection threshold

4.2 Aromatization Reactor

Heptane is transformed into toluene and hydrogen *via* a catalyst in the reactor[15] showed in Fig.6. The involved reaction is

$$C_7H_{16}(A)\rightarrow C_7H_8(B)+4H_2(C). \tag{23}$$

This is a first order reaction, heated by steam in the jacket. Different from the previous example, both mass

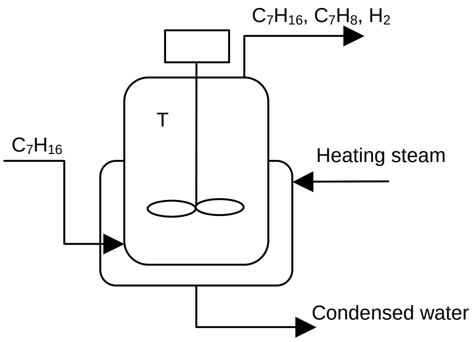

Fig.6 Aromatization reactor for transformation of heptane to toluene

and energy balances are necessary here. For convenience, mass concentration and flow rate in Eqs.(10) and (11) change to mole per volume concentration and volumetric flow rate respectively. Besides, a hypothesis is given that volumetric flow rates for input and output flow are kept constant because fractional conversion is not large in this reactor. This reactor is supposed as a continuous stirring reactor (CSTR). Then Eqs.(10) and (11) are simplified as

$$V\frac{\mathrm{d}C_{\mathrm{A}}}{\mathrm{d}t}=FC_{\mathrm{i,A}}-FC_{\mathrm{A}}-VkC_{\mathrm{A}}, \tag{24}$$

$$V\frac{\mathrm{d}C_{\mathrm{B}}}{\mathrm{d}t}=-FC_{\mathrm{B}}+VkC_{\mathrm{A}}, \tag{25}$$

$$V\frac{\mathrm{d}C_{\mathrm{C}}}{\mathrm{d}t}=-FC_{\mathrm{C}}-VkC_{\mathrm{A}}, \tag{26}$$

$$V\rho C_{\mathrm{p}}\frac{\mathrm{d}T}{\mathrm{d}t}=F\rho C_{\mathrm{p}}\left(T_{\mathrm{i}}-T\right)-V\Delta H_{\mathrm{R}}kC_{\mathrm{A}}+KS\left(T_0-T\right). \tag{27}$$

There are two types of fault in such a reactor system. The first one is a gradual decrease of fouling resistance R_{S} in Eq.(8) from 10 h due to the fouling of heat exchange surface. R_{S} changes with time through the following linear function:

$$R_{\mathrm{S}}=9.53\times10^{-8}t-9.53\times10^{-7}. \tag{28}$$

Because R_{S} is nonlinear with Q and K is linear with Q in Eq.(7), R_{S} is determined with K as intermediate variables in fault diagnosis. Overriding the wall resistance and diameter correction term in Eq.(7), the transformation between K and R_{S} is given as

$$\frac{1}{K}=\frac{1}{\alpha_{\mathrm{i}}}+R_{\mathrm{S}}+\frac{1}{\alpha_{\mathrm{o}}}. \tag{29}$$

The second fault is the decrease of k_0 in Eq.(9) from 5.01×10^{8} to 4.01×10^{8} h^{-1} at 20 h due to the deterioration of catalyst performance, when impurity enters the feed.

In fault diagnosis procedure, the variables in Eq.(16) are given as

$$\hat{p}=[K\ k_0]. \tag{30}$$

$$\hat{s}(t)=\begin{bmatrix}\dfrac{A(T_0-T)}{\rho C_{\mathrm{p}}V} & -\dfrac{\Delta H_{\mathrm{R}}\mathrm{e}^{-\frac{E}{RT}}C_{\mathrm{A}}}{\rho C_{\mathrm{p}}}\\ 0 & -\mathrm{e}^{-\frac{E}{RT}}C_{\mathrm{A}}\\ 0 & \mathrm{e}^{-\frac{E}{RT}}C_{\mathrm{A}}\\ 0 & 4\mathrm{e}^{-\frac{E}{RT}}C_{\mathrm{A}}\end{bmatrix}, \tag{31}$$

$$\hat{c}(t)=\begin{bmatrix}\dfrac{\Delta T}{\Delta t}-\dfrac{F\left(T_{\mathrm{i}}-T\right)}{V}\\ \dfrac{\Delta C_{\mathrm{A}}}{\Delta t}+\dfrac{F\left(C_{\mathrm{A}}-C_{\mathrm{i,A}}\right)}{V}\\ \dfrac{\Delta C_{\mathrm{B}}}{\Delta t}+\dfrac{FC_{\mathrm{B}}}{V}\\ \dfrac{\Delta C_{\mathrm{C}}}{\Delta t}+\dfrac{FC_{\mathrm{C}}}{V}\end{bmatrix}. \tag{32}$$

Table 2 lists all the constants in Eqs.(24)~(32) for this case. Specifically, the reaction heat is expressed as a polynomial of temperature T:

$$\Delta H_{\mathrm{R}}=2.2026\times10^{5}T+62.0244T-5.536\times10^{-2}T^2-1.15\times10^{-6}T^3+3.1496\times10^{-7}T^4\ \ (\mathrm{J/mol}). \tag{33}$$

Table 2　Parameters for reactor example

Parameter	Value
Sampling interval, Δt (h)	0.4
Input/output volumetric flow rate, F ($\mathrm{m^3/h}$)	3.0
Reactor volume, V ($\mathrm{m^3}$)	30.0
Fluid specific heat capacity, C_{p} [J/(mol·K)]	490.7
Fluid density, ρ ($\mathrm{mol/m^3}$)	593.0
Heat transfer area, S ($\mathrm{m^2}$)	10.0
Temperature of input flow, T_{i} (K)	600.0
Concentration of C_7H_{16} for input flow, $C_{\mathrm{i,A}}$ ($\mathrm{mol/m^3}$)	1000.0
Steam temperature, T_0 (K)	850.0
Activation energy, E (J/mol)	1.369×10^{5}
Pre-exponential factor, k_0 ($\mathrm{h^{-1}}$)	5.01×10^{8}
Reactant-side convection heat transfer coefficient, α_{i} [$\mathrm{J/(m^2\cdot h\cdot K)}$]	6.54×10^{5}
Steam-side convection transfer coefficient, α_{o} [$\mathrm{J/(m^2\cdot h\cdot K)}$]	8.37×10^{6}

The reaction temperature and toluene concentration in exit flow are measured in this system through dynamic simulation using Eqs.(24)~(27). Because of small scale for this problem, the fourth order Runge−Kutta method is adopted as solving algorithm. The above measurements are tracked by the proposed diagnosis system, as shown in Fig.7. For the unmeasured variables C_{A} and C_{C} in Eq.(31), they are estimated through specific observer traditionally. Because their design pattern affects the diagnosis precision greatly, the observer-based method can not be generalized normally. In this study, these variables are the output of the dynamic model adopted during fault diagnosis, so the proposed method does not need observer any longer and can be applied more widely.

Figure 8 highlights the parameter changes obtained from this tracking process, and indicates that R_S increases gradually from 10 h and k_0 decreases at 20 h respectively. The slight decrease of k_0 at about 10 h results from the change of R_S and the measurement of noise. Consequently, a conclusion can be drawn that the proposed fault diagnosis method can simultaneously identify multi-faults as well.

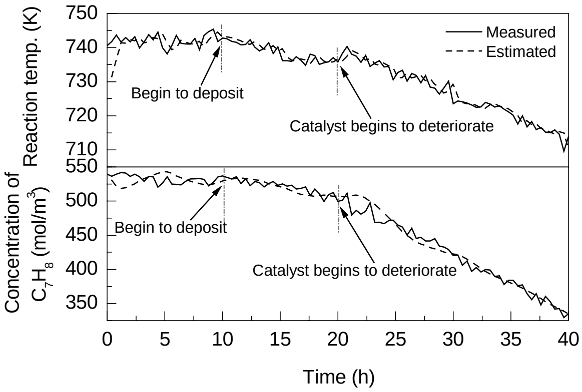

Fig.7 Trajectories of reactor changes tracked by fault diagnosis

Figure 8 also provides the diagnosis results with the conventional observer-based method, which estimates the measured values of C_A and C_C using the following equations[15]:

$$\frac{dz_A}{dt} = -\frac{F}{V}\left(-z_A + C_{A0}\right), \tag{34}$$

$$\frac{dz_C}{dt} = -\frac{F}{V} z_C, \tag{35}$$

$$C_{Aest} = z_A - C_B, \tag{36}$$

$$C_{Cest} = z_C + 4C_B. \tag{37}$$

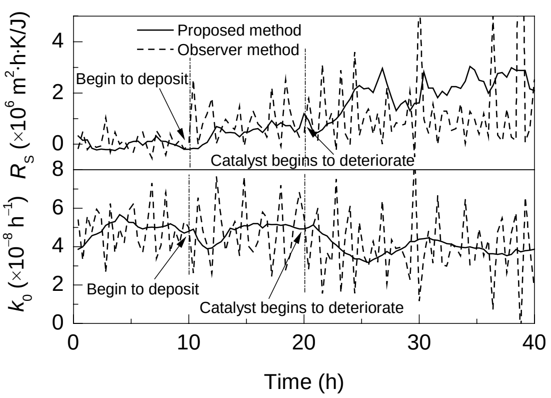

Fig.8 Trajectories of identified fault parameters in reactor

For the proposed method, these two output values are obtained through Eqs.(24) and (26). It can be seen that the produced fault parameters fluctuate so much that the real change is almost concealed. In contrast, the parameters achieved with the proposed method change gradually and clearly. Such a difference arises from the fact that the proposed method, built on rigorous dynamic model, makes an indirect use of measured values during on-line model correction. So the proposed method presents a more distinct diagnosis result in trouble shooting than the conventional one.

From the above two examples, it can be found that one of the major advantages of dynamic model based approach is that a user can gain an insight into the behavior of the results. However, several factors such as system complexity, high dimensionality, and process nonlinearity often render it very difficult to execute on-line. So the future work for this study will concentrate on construction of a hybrid fault diagnosis system with the main body of dynamic simulation based method, combining knowledge and history based methods.

5 CONCLUSIONS

This study has presented a method for the dynamic simulation based fault diagnosis in chemical processes. This method adopts rigorous mechanism model to simulate the process change with the time when faults occur, so it simultaneously realizes model updating and fault diagnosis without any need of observers. Case studies conducted on water tank and aromatization reactor show that this method is not only valid for single and multiple faults, but also superior to the existing observer-based method. In order to accommodate faults in a large scale process, further investigation on equipment modeling and parameter estimation algorithm is needed.

NOMENCLATURE:

a	Dynamic model coefficient matrix
A	Equipment floor area (m^2)
b	Model coefficient matrix in Eqs.(13), (15) and pipeline thickness in Eq.(7) (m)
c	Vector for fault parameter determination
C_{Aest}	Estimated concentration of C_7H_{16} using observer (mol/m^3)
C_{Cest}	Estimated concentration of H_2 using observer (mol/m^3)
C_i	Concentration of input feed (mol/m^3)
C_i	Concentration of component i in Eq.(9) (mol/m^3)
C_i	Leakage parameter for feed pipeline in Eq.(18) (m^2)
$C_{i,A}$	Concentration of A component in input feed (mol/m^3)
C_o	Leakage parameter for discharge pipeline (m^2)
C_p	Specific heat capacity [J/(mol·K)]
C_Q	Leakage fault parameter (m^2)
d	Pipeline diameter (m)
E	Activation energy (J/mol)
F	Volumetric flow rate (m^3/s)
$F_{i,j}$	The jth feed volumetric flow rate (m^3/s)
$F_{V,j}$	The jth vapor discharge volumetric flow rate (m^3/s)

$F_{L,j}$	The jth liquid discharge volumetric flow rate (m^3/s)
f	Nonlinear function in model
h	Liquid level (m)
$\Delta H_{R,j}$	Reaction heat (J/mol)
k	Reaction rate constant (h^{-1})
k_0	Pre-exponential factor (h^{-1})
K	Overall heat transfer coefficient [J/(m^2·h·K)]
l	Valid pipeline length (m)
M	Molecular weight (kg/kmol)
p	Pressure in Eq.(1) (Pa) and fault parameter vector in Eq.(13)
p_0	Environment pressure (Pa)
p_1	Inlet pressure (Pa)
p_3	Outlet pressure (Pa)
Δp	Pressure drop (Pa)
Q	Heat transfer rate (J/h)
$r_{j,i}$	Reaction rate for the ith component in the jth reaction [mol/(m^3·s)]
R	Gas constant [8.314 J/(mol·K)]
R_S	Fouling resistance (m^2·h·K/J)
S	Heat transfer area (m^2)
s	Linear transformation matrix for p in Eq.(13)
ΔT_m	Mean temperature difference (K)
t	Time (h)
Δt	Sampling interval (h)
T	Reaction temperature (K)
T_0	Steam temperature (K)
T_i	Temperature of input feed (K)
u	Velocity (m/h)
V	Reactor volume (m^3)
$x_{i,j,i}$	Molar fraction of component i in the jth feed
x_i	Liquid molar fraction of component i in reactor
y	Measured variable vector
y_i	Vapor molar fraction of component i in reactor
z, u	State and control variable vector
α_i	Interior convection heat transfer coefficient [J/(m^2·h·K)]
α_o	Outer convection heat transfer coefficient [J/(m^2·h·K)]
λ	Friction factor (dimensionless) in Eq.(1) and thermal conductivity [J/(m·h·K)]
ν_i	Reaction measured coefficient
ρ	Density (kg/m^3)

Subscript

A, B, C	Reactants in Eq.(23): A. heptane, B. toluene, C. hydrogen		
1, 2, 3, 4	Positions in Fig.1: 1. inlet, 2. leakage, 3. outlet, 4. environment		
o	Output feed	i	Component index
i	Input feed	j	Feed or reaction index
V	Gas	L	Liquid

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