APPLICATION OF MODEL-BASED FAILURE DETECTION AND IDENTIFICATION TO INDUSTRIAL PRODUCTION PROCESSES

Abstract

In this work, new prospects for current process control in the chemical process industry with application of model based predictive methods are presented. The data from a research cooperation work with the Evonik Degussa GmbH at Hanau-Wolfang, Germany let authors work out the models for failure detection and identification besides the basic regulatory control. The data derived from existing controllers, which make use of the predictive functional control method, is an attempt to define lower limits for model quality that is necessary to fulfill the secondary task satisfactory.

Keywords: failure detection and identification, parity equation, parameter estimation, process monitoring, supervision

ZASTOSOWANIE MODELI WYKRywających I IDENTYFIKUJĄCYCH AWARIE W PROCESACH PRODUKCJI PRZEMYSŁOWEJ

Streszczenie

W artykule przedstawiono nowe perspektywy bieżącego sterowania procesami w przemyśle chemicznym z zastosowaniem prognozowania opartego o rozwój precyzyjnych modeli. Wykorzystano dane z instalacji Evonik Degussa GmbH at Hanau-Wolfang, Germany, które pozwoliły, poza usprawnieniem sterowania, na wprowadzenie systemów identyfikacji i wykrywania awarii. Wykorzystując informacje z istniejących czujników sterowania predykyjnego opracowano precyzyjny model jakościowy.

Słowa kluczowe: identyfikacja i wykrywanie awarii, równanie cząstkowe, szacowanie parametrów, monitoring procesu, kontrola

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1. Introduction

1.1. Model-based process control

Through the application of model predictive control (MPC), significant improvements in product quality, energy consumption and overall control performance can be achieved in the chemical processes industry. However, the design stage of such control methods involves a time consuming and thus expensive phase of model development. These process models are mandatory to predict future process behavior. Based on this, decisions can be made about the future manipulation of variables under the explicit consideration of constraints and uncertainties that allow optimum control of the underlying process.

The requirements for the quality of incorporated process models can be reduced with the method of predictive functional control (PFC) introduced by Richalet [1] as a simplified formulation of the MPC algorithm, and thus the development time can be reduced dramatically. Moreover, the lower quality of implemented process models can increase the robustness of the control loops. The robustness connected to the ability to implement a PFC-algorithm directly on a standard commercial distributed control system (DCS) are advantages and make a major contribution to the success of advanced process control (APC) projects in industrial production plants.

For the application of PFC, only discrete, time-invariant linear models are used for prediction with the structure of an nth-order time delay as given in equation (1). For the application in a DCS, discrete process models have to be used. A first order time delay in continuous time (2) can be descretized, which gives the discrete transfer function (3). The same result is obtained if a continuous model as stated in equation (1) would have been transformed using the z-Transformation. The current system’s output, based on past inputs, can then be calculated after backward transformation, using equation (4), using $\alpha = \exp(-\tau_s / \tau)$ with $\tau_s$ being the sample rate

$$G(s) = \frac{b_0 \cdot s^{n-1} + b_2 \cdot s^{n-2} + \ldots + b_n}{a_1 \cdot s^n + a_2 \cdot s^{n-1} + \ldots + a_n \cdot s + a_0}$$  

$(1)$

$$\tau \frac{dy_n(t)}{dt} + y_n(t) = K \cdot MV(t)$$  

$(2)$

$$G(z) = \frac{Y_n(z)}{MV(z)} = \frac{K \cdot (1 - \alpha) \cdot z^{-1}}{1 - \alpha \cdot z^{-1}}$$  

$(3)$

$$y_n(k) = y_n(k-1) \cdot \alpha + K \cdot (1 - \alpha) \cdot MV(k-1)$$  

$(4)$

With the predictions of the model given in (4), the finite-horizon optimal control can be solved, if the desired dynamics of the control error (5) are defined, e.g. using equation (6) und (7). For the solution of the optimization problem (8), it is assumed that the change in a controlled variable at the end of the prediction horizon $h$ equals the target, given by (6) for a constant set-point (SP) in $h$. It is convenient that the iterative solution of the problem function (8) can be avoided by restricting the possible values for manipulated variables to
one characteristic pattern that uses only a single parameter (e.g. step, ramp). Finally, the
optimal solution is a value for the manipulated variable (MV), which minimizes the
deviation of the change in the control variable (CV) as calculated by the reference
trajectory and the model equation. Since there is only one degree of freedom, the solution
can be explicitly calculated using the using the derivation of the cost function (8)

$$\varepsilon(k) = \text{SP}(k) - \text{CV}(k)$$

$$\varepsilon(k + h) = \varepsilon(k) \cdot \beta^h$$

$$\beta = \exp(-\tau_a / \tau_c)$$

$$\min f = \sum_{i=1}^{n} (\Delta\text{CV}(k+i) - \Delta\text{CV}_a(k+i))^2$$

Besides the application of analytical models for process control, a number of methods
have been developed recently for model-based failure detection and identification (FDI). A
good overview of these methods and applications is given by Chiang et al. [2] and
Isermann [3]. The goal in developing systems for FDI is an accurate, fast, reliable and
comprehensive detection and diagnosis of failures in supervised processes. This includes
inherent process faults, failure of sensors, actuators and assets. But it turns out that
requirements concerning the quality of process models are contradictory to the task of
process control. An accurate model able to describe relevant process variables over a wide
range of operations is necessary to guarantee a robust detection of failures in the early
stages and to provide the operator with a qualified diagnosis. With increasing model
uncertainty the control limits of monitored measures need to be relaxed to avoid a high rate
of false alarms. Furthermore additional efforts have to be made to ensure dependable
diagnoses under the uncertainty in generated symptoms.

For the control task, simplified models with reduced accuracy are preferred. Only most
relevant dynamic properties in process variables are considered to achieve robust control
performance. Furthermore, numerical requirements are lower and reduce computational
costs, which are critical in these kinds of real time applications. The predictions of future
evoulvement of the process are finally robust against changing product properties and
operation between different campaigns, as well as season related variations.

The underlying design problem in the development of process models is explained in
detail and described based on large-scale applications from the chemical industry.

1.2. Contents

In section 2, a systematic approach to the design of systems for automated FDI is
introduced and its key features are described. Then the application of two methods for
model-based FDI is presented in section 3 using two different examples from the chemical
process industry. These examples cover the detection of sensor failures and a typical
process fault. Finally, the results are discussed in terms of evaluation of applicability based
on existing process models from implemented controllers using PFC.
2. Methods for failure detection and identification

2.1. Systematic design approach

The task of detecting faulty states in process operation is mostly assigned to plant operators. The procedure involves mainly unconscious but flexible pattern recognition through the assessment of the plant’s state using available signals of process variables e.g. in a process control room. Drawbacks of this setting are missing or incomplete abilities to formulate quantitative evaluations, the consideration of past incidents as well as theoretical process knowledge.

Current plants in the chemical process industry are affected by continuously improved processes. They are characterized through the occurrence of complex processes and assets, high throughput of material, and long treatment chains. Additionally, the integration of energy and mass through feedback e.g. reflux streams lead to increasingly difficult process dynamics and control structures. Thus, the operator is particularly affected in the execution of supervision and monitoring tasks. Appropriate methods are needed to assist operators in the evaluation of process behavior.

A systematic approach for system design in order to achieve an automated FDI can be described according to Höfling [4] and is schematically depicted in Figure 1. The design of an FDI-system of this type allows the individual assignment of methods. These methods can be selected to match the affordance of a specific monitoring problem and lead to the optimal performance of the single and overall task. In the first step, current measurements of process variables are used to extract significant features from the process. The generated feature space is enriched by a variety of different measures that allow a comprehensive description of the current state. In the second stage, these features are compared to known or assumed values that occur in normal operation conditions (NOC). Then, in the final stage, a decision about the state of the process is formulated using the generated symptom patterns. Consistently, a symptom is generated if a feature exhibits a significant deviation from the reference value for the nominal state, e.g. fault-free state. The underlying assumption is an overall deviation of the process from the NOC state if one or more features generate symptom(s). The reason for this deviation may then be connected to an evolving fault or even an existing failure. The last step finally covers the inference of a single scenario from several possibilities using probabilistic assumptions about the causal relations between symptoms and failures.

Thus, the process of designing a system for FDI involves the selection of methods for the three main tasks of feature extraction, symptom generation and decision making.
Moreover, the definition of reference values for the NOC state using historical process data or simulations and the assembly of a knowledge base for the decision process are crucial elements which determine the final performance of the FDI system. The quality of a designed system can then be described by evaluating the sensitivity, robustness and isolation for different scenarios.

2.2. Methods of model-based FDI

For the purpose of model-based control, the approach is supposed to generate optimized values for manipulated variables based on the predictions of process variables using process models. The idea of adopting process models for monitoring purposes comes from the assumption that a deviation between predicted and measured trajectories must have a reasonable matter. Depending on the quality of process models used for prediction, these differences can be traced back to a small number of possible causes.

A common approach that transfers this reasoning into an algorithm is the use of parity equations as explained by Chow & Willsky [5] or Delmaire et al. [6]. Comparing model output and process measurement generates residuals as a feature that is used to describe the process’ state. The generation of residuals as features is a principle common to all model-based methods for failure detection. Figure 2 describes the procedural setup for the application of different approaches that are mostly relevant. Possible faults may result in the excitation of the system using inputs $u'$ that differ from the assumed $u$ because of attributing effects $\Delta u$ of actuator failure. Another failure mode may be a sensor failure that superimposes the original value $y^o$, e.g. with a steady $\Delta y$, making the recorded measurements $y$ deviate from the true values. Finally any form of failure that has an impact on the process itself besides effects on sensors and actuators need to be considered, too. The fundamental differences between methods from Figure 2 can be described through...
the measures that were incorporated. Since parameter estimation aims at discovering evolutions in certain important model parameters, the target is to detect failures that can be expressed as systematic changes in physical properties of assets or equipment. Similarly, a state observer can be used to explore changes in state variables that are connected to failures. Since parity equations simply evaluate changes in the input-output relation, the applications mainly cover the detection of sensor failures. In the following section, both parity equations and parameter estimation are used to detect different types of failures.

3. Application studies

3.1. Sensor failure detection and identification

Process sensor failures and faults differ in their effects on the recorded process variables. The fault’s characteristic in plant assets usually depends on the state of operation and especially on the system excitation through manipulated variables. Instead, a sensor failure creates a rather constant additional contribution to the recorded signals in most of the times. Then, a residual from a parity equation that is recorded in a fault-free operation exhibits a zero-mean distribution according to Fig. 3 left. The standard deviation of the signal refers to the noise of the measurement. Figure 3 right shows the same distribution of a residual from fault-free operation but with model uncertainty. In this case, the noise of the measurements is superimposed with a dynamic evolution that forces the residual to obtain an estimated mean that is non-zero and time variant.

In case of a failure, e.g. an offset in the measurement, which occurs as a sudden increase of the generated signal without a change in the actual process variable, a possible time series of a residual may look like the plot in Fig. 4 left. The dotted lines mark control limits for the estimated mean value of the residual and its violation will generate a symptom which then infers the cause of that deviation. In Figure 4 left, the upper control
limit is obviously violated at about half of the displayed time interval because of the failure in the measurement. In the case of existing model uncertainties, the decision to raise the alarm is not easy to take. The dynamic behavior from Fig. 3 right (fault-free situation) in fact covers the influence of the failure on the residual as can be seen in Fig. 4 right. A probabilistic decision about the violation of the upper control limit will declare the process as being in normal operation whereas the true state is faulty.

Fig. 4. Faulty residuals from parity equations with and without model uncertainties

Beside these obvious flaws in residual evaluation with model uncertainty, it can be shown that the design of output filters for use in parity equations may become impossible. The former linear state-space process model given with equations (9) and (10) is affected by faults and measurement noise as shown in Fig. 2. As a result, the state equations have to be extended to include these phenomena according to (11), using the shift-operator \( q \) for discretization. The contributions to the current output from modeled process dynamics, considered failures, and measurement noise are given in (12), (13), and (14), respectively. Because we concentrate on additive failures that do not affect the system’s characteristic dynamics, all of these phenomena own the same dynamic and measurement matrices \( A \) and \( C \) in (12)–(14).

\[
\begin{align*}
    \mathbf{x}(k+1) &= \mathbf{A}\mathbf{x}(k) + \mathbf{B}\mathbf{u}(k) \quad (9) \\
    \mathbf{y}(k) &= \mathbf{C}\mathbf{x}(k) + \mathbf{D}\mathbf{u}(k) \quad (10) \\
    \mathbf{y}(q) &= \mathbf{P}(q)\mathbf{u}(k) + \mathbf{P}_f(q)\mathbf{f}(k) + \mathbf{P}_n(q)\mathbf{n}(k) \quad (11) \\
    \mathbf{P}(q) &= \mathbf{C}(q\mathbf{I} - \mathbf{A})^{-1}\mathbf{B} + \mathbf{D} \quad (12) \\
    \mathbf{P}_f(q) &= \mathbf{C}(q\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}_f + \mathbf{D}_f \quad (13) \\
    \mathbf{P}_n(q) &= \mathbf{C}(q\mathbf{I} - \mathbf{A})^{-1}\mathbf{B}_n + \mathbf{D}_n \quad (14)
\end{align*}
\]
The design procedure for applying parity equations relies on the assumption that the residual generator is defined as a filter for input and output variables according to equation (15), which should ideally be equal to zero for the fault-free case (16). This assumption leads to the definition (17). Replacing $V(q)$ in (16) with (17) gives a formulation that reflects the initial idea of comparing measured output and the prediction of the model given by the second term inside the brackets of equation (18). Again, in the case of perfect match of plant and model, the remaining part, after inserting (11) into (18) is given by equation (19), which represents unmodeled and stochastic dynamics. The transfer functions in matrix $W(q)$ can than be designed to amplify failures into desired (different) directions and to dampen measurement noise. Instead, if uncertainty about the process and the model used exists, both $V(q)$ and $W(q)$ in (16) would have to be designed following no descriptive criteria

$$r(k) = V(q)u(k) + W(q)y(k) = 0$$

Consequences of these considerations are that model uncertainties have a direct impact on the detection of failures in sensors using parity equations, since the usual design process can’t be carried out without serious violation of necessary assumptions. Additionally, the control limits for generated residuals have to be relaxed in order to reduce the number of false alarms. Again, this decreases the sensitivity of the FDI systems and leads to an increase in the missed alarm rate which may have even more severe consequences since changes in the final product quality can not possibly be traced back to the root cause and recognized without a large time delay. With the existence of large uncertainties in process models, the analysis of residuals has to be reduced to the dynamic evolution and discarding estimations of absolute mean values.

To compensate for this loss of information, signal-based measures can be added to the feature space of the FDI-system. Through this approach, supplemental process knowledge can be integrated. As an example Fig. 5 left shows a static characteristic curve created in the design stage of a control structure from a polymerization batch-process. Several measurements from different batch runs, which were extracted from NOC process data, are plotted in this diagram. During process transitions, e. g. startup phase or reaction phase, several measurements deviate from the static relationship of temperature and pressure. However, for the stationary phase, after the major part of the chemical reaction has taken place, the process’ state settles at the static relation somewhere at 95% of the temperature depending on the operating point of the batch run considered. With this NOC process data, the static relation can be extended through upper and lower control limit curves, as depicted in Fig. 5 right. This procedure turns the application of a measurement upon the diagram into a feature and a violation of one of the curves into a symptomatic behavior.
Fig. 5. Faulty residuals from parity equations with and without model uncertainties

Rys. 5. Niewyrównane sygnały z instalacji; z i bez wykorzystania równania cząstkowego

Combining the above mentioned features to a finite set with corresponding symptoms enables the final decision about the process state using an online knowledge base that covers the causal relationships between symptoms and failures. One very simple approach which is powerful and easily extended is to develop a symptom-failure-tree-model (SFTM) either from expert knowledge, historical process data, process simulation or a combination of these. Before an application of the developed SFTM, a training phase has to take place. Recorded process data is being processed by the FDI-system and the decisions of the diagnosis module using the SFTM are analyzed. Thus, if in any case more than one possibility of a failure cause is computed, the SFTM can be extended to a weighted symptom-tree-model (WSTM). This approach incorporates probabilistic information about the true cause of a failure in a multiple candidate situation. An arbitrary example of a WSTM is displayed in Fig. 6. The situation of simultaneous raising of symptoms S2 and S3 gives the candidates F2 and F3 as possible causes. In weighting the relations using $W_{22}$, $W_{32}$, $W_{23}$ and $W_{33}$, the most probable cause can be diagnosed even if the complete symptom pattern, e.g. for failure cause F2, would require symptom S1 to be active, too.

Fig. 6. Weighted symptom tree model

Rys. 6. Ważony graf modelu
3.2. Detection of process faults

As mentioned before, process faults exhibit a different characteristic influence on process variables. Therefore the approach uses the methods of parameter estimation to detect a typical process fault in a polymerization batch-process. The underlying assumption is that a process fault must involve the degradation of one or more physical property of the assets that can be expressed in a set of process parameters $\mathbf{p}$. Moreover, these parameters have a strong relation to the coefficients $\Theta$ used in the process model as described in (20).

The reason to apply parameter estimation in the FDI-system is given in (21) for the assumption of a backward transformation of model parameters into physical process parameters. This can be illustrated by consideration of the heat transfer coefficient that has an impact on the time constant for a linear approximation of the dynamic behavior of a heat exchanger. Thus, if a significant increase in the time constant of the process model can be estimated, one reason may be increased fouling effects through long operation time of the heat exchanger without maintenance.

\[
\Theta = f(\mathbf{p}) \quad (20)
\]

\[
\mathbf{p} = f^{-1}(\Theta) \quad (21)
\]

In comparison to sensor malfunctions, these types of failures and their corresponding effects increase very slowly and are extremely difficult for an operator to perceive by judging signals. Using parameter estimation in a moving time horizon can capture changing process parameters efficiently even for very complex estimation problems as demonstrated in Arellano-Garcia et al. [7].

For a demonstration, we assume that the transfer function of a second order time delay is used in a PFC-controller to describe the transmission of a valve in order to conduct cooling water into the batch reactor jacket (22). The reactor temperature is measured by a sensor that points into the liquid holdup of the reactor. After a batch-run is finished and the product is discharged, a small amount of product remains on the surface of the sensor. After several runs of successful production, the layer of old product slowly increases and changes the dynamic behavior of the sensor. The transfer function of a second order time delay consists of three parameters (23). This set of parameters can be estimated using measurements of valve position and reactor temperature. Additionally, the estimated parameters can be plotted in a three-dimensional diagram. If each parameter is chosen as coordinate, the spanned space is described as parameter space (PS)

\[
G(s) = \frac{T_v(s)}{U_v(s)} = \frac{K}{(T_v s + 1)(T_i s + 1)} \quad (22)
\]

\[
\Theta = f(\mathbf{p}) = [K, T_i, T_v] \quad (23)
\]

Figure 7 shows some estimation results in the PS. After a batch-run finished, the complete trajectories of the relevant process variables were used to identify the dynamic behavior using the model parameters as independent variables. First, all results settle somewhere in a small space surrounding parameter values that may be useful to describe
conditions with thin product layer on the sensor. But, with an increasing number of batch-runs without cleaning the sensor, the estimates deviate from the close space of NOC-parameters.

If the initial parameters were defined to be reference values according to the systematic approach, a feature which can be generated from the estimated parameters is the distance in the PS of Fig. 7 to the nominal values as stated in equation (24). Again, the basis for this approach is that model parameters deviate from nominal values, if and only if the underlying physical properties change according to (25). The result of a feature extraction in such a manner and the evolution over a reasonable large number of batch runs is shown in Fig. 8. A remarkable deviation from the space of normal operation can be recognized. In these observations, the failure causing product layer on the temperature sensor has been removed after the 32nd batch run through scheduled maintenance. It is remarkable, that the estimated parameters finally recover to a close space around nominal values again.

\[ r = \Delta \Theta = \dot{\Theta} - \Theta_e \]  \hspace{1cm} (24)

\[ \dot{\Theta} = \Theta_e + \Delta \Theta = f(p_e + \Delta p) \]  \hspace{1cm} (25)
4. Discussion

In this work, simplified process models from existing PFC-controllers are integrated into systems for failure detection and identification. Thus, the value creation chain initiated in the design stage of the MPC-application can be extended without the requirement of creating new process models for monitoring purpose.

However, the crucial factor for the design of an FDI-system is the available model quality especially concerning the influences of model uncertainties on the generated residuals. If residuals tend to show permanent deviation from a constant mean, only dynamic aspects of these measures can be analyzed. Additionally, the feature space of the FDI-system is an essential part determining the final quality of the system and the dimension gets reduced with increasing model uncertainty. Thus, enriching the feature space with signal-based features can help to reestablish the quality of the developed FDI-system especially with regard to robustness of alarms and diagnosis.

The need to carefully select methods for residual generation has been demonstrated using examples from the chemical process industry. Moreover, parameter estimation demonstrates to be able to successfully detect degradation in batch performance that would remain unobserved otherwise. Based on the developed measure of fault magnitude, the required maintenance procedures can be assigned precisely by taking the current development of the emerging failure into account.
Symbols

CV – controlled variable
MV – manipulated variable
SP – setpoint
A – process dynamics matrix
B – process input matrix
B_f – process input matrix (faults)
B_n – process input matrix (noise)
C – process measurement matrix
D – process reach-through matrix
D_f – process reach-through matrix (faults)
D_n – process reach-through matrix (noise)
G – transfer function
K – gain [K/%]
P – matrix of discrete transfer functions
P_f – matrix of discrete transfer functions (faults)
P_n – matrix of discrete transfer functions (noise)
T_x – reactor temperature
T_1 – time delay [s]
T_2 – time delay [s]
U_r – valve input
V – parity equations design matrix
W – parity equations design matrix
a_i – model parameter
b_i – model parameter
f – objective function
f – vector of functions
f – fault process input
h – prediction horizon length
k – sample interval
n – noise process input
p – physical process parameters
p_0 – nominal physical process parameters
q – shift-operator
r – model based residuals
s – Laplace-variable
u – nominal process inputs
u' – true process inputs
Δu – actuator failure contribution
x – process state vector
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$y$ – process output
$y$ – process measurements
$y^0$ – true process value
$\Delta y$ – sensor failure contribution
$z$ – discrete variable
$\alpha$ – time constant
$\beta$ – reference trajectory dynamics
$\varepsilon$ – control error
$\tau$ – time delay
$\tau_d$ – sample interval length [s]
$\tau_{ref}$ – time delay of reference trajectory [s]
$\Theta$ – model parameters
$\hat{\Theta}$ – estimates of model parameters
$
\Theta_0$ – nominal model parameters

References


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