Multiple Filter Methods for Detection of Hazardous States in an Industrial Plant

Model-based detection systems are presented and classified according to their complexity. The main emphasis is put on multiple Kalman filters. A two-stage approach including Bayes formula and inhomogeneous Markovian processes is suggested to achieve a fault discrimination. Methods are presented to use the information of nondisjunctive models in this context. To show the proper working of the detection algorithms simulation studies and on-line laboratory experiments with runaway reactions are considered first. A report on an implementation at a large-scale industrial process unit concludes the discussion.

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Introduction

Due to the highly nonlinear and parameter-sensitive dependence of chemical plant behavior on the process state, even slight changes in process parameters can result in severe implications. This can happen when the substances handled or produced are thermally unstable or toxic. The difficulties will be enhanced when, due to higher demands on quality and productivity, multiple material and energy couplings between process units are introduced.

The control and monitoring of a plant is usually done by means of easily accessible measurements, such as temperature. Therefore it is necessary to ask whether the monitoring system is able to detect hazardous states using only this information. Furthermore, it is important to know what happens if sensors partly or completely fail.

The early detection of hazardous states in chemical systems can be a difficult task. The reasons are:

1. A chemical process can only be described by a high number of state variables, such as temperature, pressure, concentrations, and so on. Only part of this process state $x(t)$ can be measured on-line with an acceptable time delay
2. The processes are very complex and strongly nonlinear
3. The safety assessment must be based on the history of the process as well as on the actual measurements. That means a simple yes/no decision based only on the measurements at a certain time—as used in some expert systems—is insufficient.

This paper will show that the use of model-based measuring techniques, including pattern recognition, will help to overcome these characteristic problems of chemical engineering.

Detection of hazardous states with model-based techniques has been proposed for a variety of processes (Willsky, 1976; Frank, 1986; Himmelblau, 1986). Most of the work has been concerned with systems described by linear state equations. Only very few detection systems have been proposed for problems in chemical engineering. The first applications in chemical engineering dealt with simulation studies (Himmelblau, 1978). Park and Himmelblau (1983) considered two different possible faults. In their simulation, parameters indicating a fault were estimated with a fully measured state vector. Watanabe and Himmelblau (1983) based their detection system on a very special form of the simulation model, estimating fault parameters as well. However, Gilles and Schuler (1981) and Schuler (1982) showed for the first time the way in which all the information given by a Kalman filter can be used in a detection system. They evaluated, for a simple simulation model, state-dependent criteria characterizing dangerous behavior. Furthermore, they predicted the future development of a process and distinguished between a normal operation mode and a fault mode. The first experimental results based on these methods were reported by King and Gilles (1984). These methods were extended to consider multiple faults by King (1986).

This article summarizes the principal methods and reports on an industrial application. It should be pointed out that the problems considered here are not mainly concerned with easily detectable failures or degradations of process units. Problems such as the early detection of a runaway reaction when the measurements do not differ significantly from the normal values at the beginning are of principal concern. Such early detection is very important because a runaway reaction is characterized by a self-accelerating, very fast increase in temperature and hence in pressure.

Another difficult example is illustrated by a large-scale industrial semibatch reactor in which a critical sulfonation reaction takes place. Temperature readings are shown in Figure

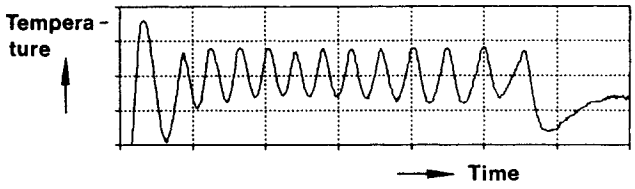

Figure 1. Temperature reading of an industrial semibatch reactor.

1. In this case the onset of a runaway reaction would be concealed by a distinct oscillation that is a result of a discontinuous cooling strategy. Again, we try to detect hazardous states and distinguish between different faults. Only the temperature measurement and information about control inputs are used for this purpose. Examples of possible faults are the onset of a runaway reaction, the presence of catalytical substances, degradation of the cooling capacity, and others.

Only extended Kalman filters are used for estimating unmeasured state variables, because most of the detection systems described below use statistical information. However, for highly nonlinear systems an extended Kalman filter will give only a rough approximation of the probability distribution of the state vector. Simulation studies and laboratory experiments must show the correct working of the model-based detection algorithms. The general structure of the considered models is given with Eq. 1, where Θ is a vector of parameters

$$\Lambda: \begin{cases} \dot{x}(t) = f[x(t), u(t), \Theta, t] + G[x(t), \Theta, t] \cdot w(t) \\ y(t_k) = h[x(t_k), \Theta, t_k] + v_k \end{cases} \tag{1}$$

Model-Based Detection Systems

Model-based detection systems can be classified according to their complexity.

Innovation-based methods

A chemical plant shall be described by Eq. 1. This model includes all effects of the nominal nonfaulty behavior. The dynamical consequences of a fault or failure are not included in this mathematical description. For a nondisturbed linear plant with white, Gaussian noises $w(t)$ and y_k, the innovation

$$\gamma(t) = y(t_k) - \hat{y}(t_k) \tag{2}$$

where $\hat{y}(t_k)$ denotes the estimated measurement of a Kalman filter, should be a random variable with zero mean and covariance matrix

$$S_k = H_k \cdot P_k \cdot H_k^T + R_k \tag{3}$$

For a nonlinear system this statement holds true only approximately. However, an approximation of S_k can be obtained with an extended Kalman filter (Gelb, 1974). Hence, to supervise a plant the mean, covariance, and correlation function of the innovation sequence are determined statistically. In hypotheses testing, Figure 2a, significantly different values of the statistical guesses compared with theoretical values show possible malfunction of the plant (Mehra and Peschon, 1971).

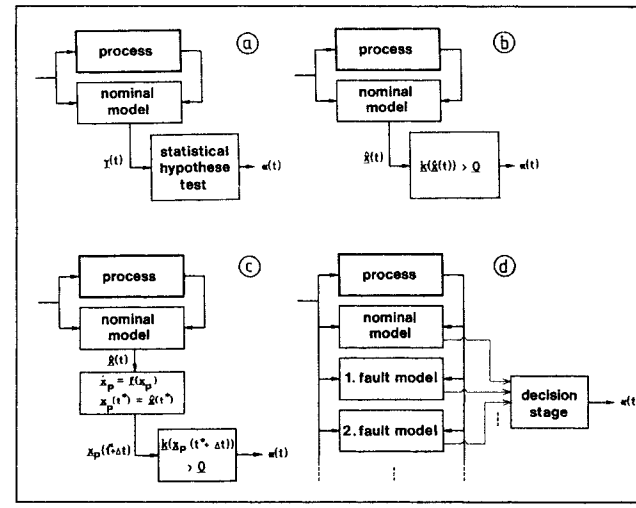

Figure 2. Model-based detection systems.

State-based methods

If safe operation of a process can be characterized by state-dependent criteria

$$k[x(t)] > 0 \tag{4}$$

$\hat{x}(t)$ can be used to evaluate Eq. 4, Figure 2b. Examples are the supervision of unmeasured concentrations and trends of concentrations, as well as the estimation of parameters, for instance, heat transfer coefficients. A well-known criterion states a chemical reaction system to be critical if

$$\frac{d[T^{(L)} - T^{(C)}]}{dt} > 0 \quad \text{and} \quad \frac{d^2T^{(L)}}{dt^2} > 0 \tag{5}$$

hold true, where $T^{(L)}$ and $T^{(C)}$ are reactor and cooling temperature, respectively. Since differentiation of a temperature measurement will greatly enhance every noise in the signal, Schuler (1982) proposed calculation of the first derivative by means of the balance of enthalpy, which is a function of all state variables, for example:

$$\frac{dT^{(L)}}{dt} = f_1[T^{(L)}(t), n_1^{(L)}(t), \ldots, n_\nu^{(L)}(t)] \tag{6}$$

The second derivative

$$\frac{d^2T^{(L)}}{dt^2} = f_2[T^{(L)}(t), n_1^{(L)}(t), \ldots, n_\nu^{(L)}(t)] \tag{7}$$

can be obtained analytically from Eq. 6 by replacing the time derivative of molar amounts $dn_i^{(L)}/dt$ by the appropriate material balances. If $n_i^{(L)}(t)$ is not known, it is replaced by its estimate. One can show that evaluation of Eqs. 6 and 7 gives a much better signal to noise ratio, compared to a numerical differentiation of the temperature measurement or of the temperature estimate.

Prediction methods

If the estimate $\hat{x}(t)$ is known at time $t = t^*$, a fast simulation can predict the future development of the process based on this actual estimate, Figure 2c. Therefore, some of the possible criteria of the type of Eq. 4 can be estimated at time $t = t^* + \Delta t$:

$$k[x(t^* + \Delta t)] > 0 \tag{8}$$

It should be emphasized that prediction is very sensitive to unknown future disturbances and to model uncertainties. Therefore, prediction should be used, only if another detection algorithm has created an alarm, to estimate the remaining time in which countermeasures can be applied.

Discrimination methods

If different fault modes must be considered, multiple filter methods, Figure 2d, can be used to distinguish between nominal operation and fault modes. To do this, a probability for every model representing normal operation or a specific fault is calculated. The structure of the model with the highest model probability will then best represent the actual structure of the process. Hence, a fault discrimination is achieved. The following sections show how these probabilities can be calculated and how such a system can be used for detection of hazardous states.

Multiple-Filter Methods

We consider a process, Eq. 1, that can change in structure $f(\cdot)$ or in parameters Θ over time to represent the nominal and all fault modes. To distinguish between different modes of operation a multiple-filter method is used in which different models M^i

$$M^i: \begin{cases} \dot{x}^i(t) = f^i[x^i(t), u(t), \Theta^i, t] + G^i[x^i(t), \Theta^i, t] \cdot w^i(t) \\ y^i(t_k) = h^i[x^i(t_k), \Theta^i, t_k] + v_k^i \end{cases} \tag{9}$$

are implemented. We now choose a model M^i out of a model library $\{M^0, M^1, \ldots, M^N\}$ in such a way that with the knowledge of all manipulated variables $u_i = u(t = t_i); i = 1, \ldots, k$:

$$U_k = (u_k, u_{k-1}, \ldots, u_1) \tag{10}$$

the sequence of measurements $y_i = y(t = t_i); i = 1, \ldots, k$:

$$Y_k = (y_k, y_{k-1}, \ldots, y_1) \tag{11}$$

can best be explained. In other words, we look for the conditional probability of model M^i given the sequences U_k and Y_k

$$p(M^i|Y_k, U_k) = p(M = M^i|Y_k, U_k) \tag{12}$$

Given all conditional probabilities, we determine the model with the highest probability to conclude model discrimination. Control inputs u_k are usually calculated by a deterministic law, for example:

$$u_k = g(y_k, y_{k-1}, \ldots, y_1) \tag{13}$$

Therefore, Eq. 12 can be replaced by

$$p(M^i|Y_k) = p(M = M^i|Y_k, U_k) \tag{14}$$

Another problem formulation might ask for a history of fault models $M^{j_k} = \{M^{j_k}, M^{j_{k-1}}, \ldots, M^{j_1}\}, j_i \in \{0, 1, \ldots, N\}$ where i is a time index. However, this formulation is not adequate for the problems considered in this paper. If a fault is detected, immediate countermeasures are to be applied.

To calculate the conditional model probabilities we propose a two-stage approach.

Stage 1. With measurements y_k at time $t = t_k$, model probabilities are updated with the Bayes rule (Peterka, 1981)

$$p(M^i|Y_k) = \frac{p(y_k|M^i, Y_{k-1}) \cdot p(M^i|Y_{k-1})}{\sum_j p(y_k|M^j, Y_{k-1}) \cdot p(M^j|Y_{k-1})} \tag{15}$$

The denominator need not be calculated, for the sum of all model probabilities equals 1:

$$\sum_{j=0}^{N} p(M^j|Y_k) = 1. \tag{16}$$

The *a priori* model probability $p(M^i|Y_{k-1})$ is known from the last time interval (t_{k-1}, t_k); see Stage 2. The likelihood function $p(y_k|M^i, Y_{k-1})$ can be approximated by a normally distributed function

$$p(y_k|M^i, Y_{k-1}) = \frac{1}{(2\pi)^{m/2} \cdot (\det S_k^i)^{1/2}} \cdot \exp\left(-\frac{1}{2} \cdot (\gamma_k^i)^T \cdot (S_k^i)^{-1} \cdot \gamma_k^i\right) \tag{17}$$

where γ_k^i and S_k^i are the innovation and covariance of the innovation, respectively, which are calculated by a Kalman filter based on model M^i. For nonlinear systems the validity of this approximation must be examined by looking at the overall system performance in simulation studies and experiments.

Stage 2. To improve model discrimination the model probabilities are corrected in the interval between two measurements by including even more *a priori* knowledge in the decision stage. If it is known, for example, that undesired consecutive reactions take place at some higher temperature, a transition from normal operation mode to decomposition mode should be more likely. Mathematical formulation leads to a so-called inhomogeneous Markovian process. In a Markovian process (Bharrucha-Reid, 1960) every operating mode or "class" is associated with a certain probability, p^i. Transition probabilities p_{ij} take into account the possibility of transition from class i to class j, Figure 3.

The model probability p^i of model M^i, $i = 0, 1, \ldots, N$ is calculated with

$$\dot{p}^i(t) = -\left[\sum_{\substack{j=0 \\ j \neq i}}^{N} b_{ij}(t)\right] \cdot p^i(t) + \sum_{\substack{j=0 \\ j \neq i}}^{N} [b_{ji}(t) \cdot p^j(t)] \tag{18}$$

The time dependence of the transition rates or intensities $b_{ij}(t)$ is now replaced by a state dependence

$$b_{ij}(t) = b_{ij}[x(t)] \tag{19}$$

The intensities can be determined by examining binary subsystems. For a binary Markovian process $M^i \leftrightarrow M^j$ the

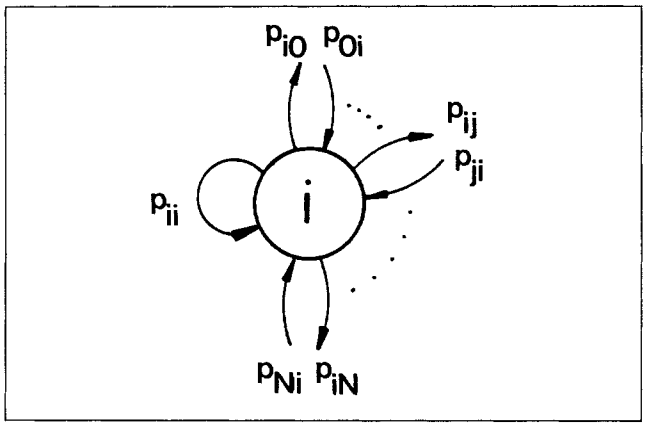

Figure 3. Markovian process.

following relations are valid:

$$\dot{p}^i(t) = -[b_{ij}(x) + b_{ji}(x)] \cdot p^i(t) + b_{ji}(x) \tag{20}$$

with stationary probability p_s^i

$$p_s^i = \frac{b_{ji}(x)}{b_{ij}(x) + b_{ji}(x)} \tag{21}$$

and time constant τ_{ij} of Eq. 20:

$$\tau_{ij} = \frac{1}{b_{ij}(x) + b_{ji}(x)} \tag{22}$$

For simplicity we choose

$$\begin{aligned} b_{ij}(x) &= b_{ij}^* \cdot g_{ij}(x) \\ b_{ji}(x) &= b_{ji}^* \cdot g_{ji}(x) \end{aligned} \tag{23}$$

as a functional dependence of the intensities b_{ij} on the state vector $x(t)$. The functions $g_{ij}(x)$ and $g_{ji}(x)$ are fixed with known parameters. To determine b_{ij}^* and b_{ji}^* the following procedure is proposed.

In a simulation study with model Λ, Eq. 1, a region of state space is determined which is characterized by model M^i but not by model M^j. For typical values of $x(t)$ in that region we demand that the stationary probability p_s^i be very high, that is, $1 - p_s^j$ is very low. The time constant τ_{ij}, which is a measure for the speed of a discrimination, is as well a function of $x(t)$. Hence, with a proper choice of g_{ij} and g_{ji}, parameters b_{ij}^* and b_{ji}^* can be expressed as a function of the maximum value τ_{ijmax}. Especially for some more complex functions $g_{ij}[x(t)]$ and $g_{ji}[x(t)]$ it is impossible to determine a maximum value of τ_{ij}. Now, the time constant might be fixed for an arbitrary value of $x(t)$. However, in both cases simulations should prove the proper working of the model discrimination and the intensities should be corrected where necessary. An example of this procedure is given below.

Hence, at time t_k an update of the model probability is made using the Bayes rule, Eq. 15, with *a priori* probability

$$p(M^i|Y_{k-1}) = p^i(t_k) \tag{24}$$

After the update, model probabilities are evaluated with Eq. 18, and the initial conditions are

$$p^i(t_k) = p(M^i|Y_k), \quad i = 0, 1, \ldots, N \tag{25}$$

Disjunctive model formulation

When using multiple-filter techniques in a nonfaulty plant we should guarantee that the filters based on fault models do not diverge. Bonivento and Tonielli (1984) proposed a system in which only a nominal model is used as long as its estimates are good according to a hypothesis test. When a fault occurs, a fault model is switched on. Another possibility is the inclusion of the nominal behavior in every fault model by appropriate modeling. As a consequence the models are not disjunctive, as is required for the Bayes rule and Markovian processes. In general, the problem is stated as follows: With given disjunctive models M^i describing either nominal behavior or a fault mode, we search for the likelihood functions

$$p(y_k|M^i, Y_{k-1}), \quad i = 0, 1, \ldots, N \tag{26}$$

used in Eq. 15 when only information

$$p(y_k|\Omega^j, Y_{k-1}), \quad j = 0, 1, \ldots, N \tag{27}$$

of nondisjunctive filter models Ω^j is available. In King (1986) this was done for a specific model configuration with just three models. In the appendix, the solution is shown for the general problem statement with $N + 1$ models. A detailed discussion can be found in King (1989).

Applications

The intention of this work was the application of the proposed detection systems to an industrial plant. The semibatch reactor considered was designed to perform a sulfonation reaction of an aromatic compound. More details are found in King (1989). To demonstrate the working of the detection algorithms, simulation studies and laboratory experiments are considered first. This is necessary because the industrial process cannot be operated in a dangerous region of state variables just to verify the detection system.

Simulation studies

For the simulation, a cooling strategy is considered which does not exhibit oscillatory states. Four reactions are considered in a semibatch reactor:

An aromatic compound, A_1, is sulfonated by sulfur trioxide, A_2, to yield the desired monosulfonic acid, A_3:

$$A_1 + A_2 \xrightarrow{r_1} A_3 + (-\Delta H_R)_1 \tag{28}$$

From numerous heat storage tests, a formal kinetic is found to describe the measured temperature–time readings

$$r_1 = k_{10} \cdot \exp(-E_1/R/T) \cdot c_1^{\alpha} \cdot c_2^{\beta} \tag{29}$$

In a next reaction step the remaining sulfur trioxide, A_2, will form higher sulfonic acids, for example, disulfonic acid

$$A_2 + A_3 \xrightarrow{r_2} A_4 + (-\Delta H_R)_2 \tag{30}$$

In a third reaction two monosulfonic acids will be produced out of one disulfonic acid as long as there is the unsulfonated compound A_1:

$$A_4 + A_1 \xrightarrow{r_3} 2 \cdot A_3 + (-\Delta H_R)_3 \tag{31}$$

Reactions 30 and 31 are approximated by appropriate formal kinetics. In the process industry, the heat of reactions is removed very carefully, for it is known that the sulfonic acids A_3 and A_4 may decompose in an undesired highly exothermic autocatalytical reaction (Grewer, 1975)

$$(A_3, A_4) \xrightarrow{r_4} \text{products} + (-\Delta H_R)_4 \tag{32}$$

To motivate the use of multiple-filter techniques some of the possible operating modes of a semibatch reactor are given in Table 1 together with adequate countermeasures.

Totally different countermeasures must be taken into account when a temperature increase is detected in comparing modes 2 and 3. In mode 3 penetrating cooling water will form, with dissolved SO_3, new H_2SO_4 under almost instantaneous release of heat. Hence, increased cooling would be an absolutely inappropriate response to prevent a major accident. In the most dangerous situation, mode 4, the emergency strategy is changed during operation. Increased cooling, as a result of a detected decomposition reaction, is replaced by a shutdown of the cooling.

This example demonstrates the importance of distinguishing between different faults. A possible warning system is given by the multiple-filter method introduced here. For every mode a special filter is designed. For the following simulations the normalized mathematical models consist of a balance of enthalpy, a number of appropriate material balances, a mass balance, and a proportional controller with a lower bound for the cooling temperature. Three filter models are used.

Model Ω^0. Only desired reaction steps r_1 through r_3 are included in this model. Therefore, this model can only give good estimates of the state variables as long as no decomposition reaction or other fault occurs.

Model Ω^1. It describes nominal behavior, that is, r_1 through r_3, as well as the dynamic behavior caused by reaction r_4.

Table 1. Working Modes of a Sulfonation Process

No.	Mode	Countermeasures
1	Normal operation	None
2	Exothermic decomposition	Increase cooling
3	Penetration of cooling water	Stop cooling, quench reaction
4	Exothermic decomposition and then penetration of cooling water	Increase cooling and then stop cooling

Model Ω^2. The most complex model treats desired and undesired reactions and the possibility of penetration of water. This can be done by estimating the amount of penetrating water, too.

The structure of model Ω^0 differs from model Ω^1 and Ω^2 due to the absence of r_4. Hence, Ω^0 is disjunctive to Ω^1 and Ω^2. In the case of no water penetration, which has a probability greater than zero, models Ω^1 and Ω^2 are the same and therefore not disjunctive, Figure 4a. To apply the Bayes rule and a Markovian process, new disjunctive classes are introduced, Figure 4b:

$M^0 = \Omega^0$ desired reaction steps only
$M^1 = \Omega^1$ class representing simultaneous appearance of desired and undesired reactions
$M^2 = \Omega^2 \cap \neg\, \Omega^1$ class representing simultaneous appearance of desired and undesired reactions with water penetration

To calculate the appropriate likelihood functions, Eq. 26, the formulas in the appendix are used. Three different binary Markovian processes must be considered to determine, for example, the following intensities b_{ij}:

$M^0 \leftrightarrow M^1$. Proportional to the normalized heat release $\bar{q}_4$ due to the undesired reaction step r_4: $\bar{q}_4 = \bar{q}_4[r_4(x)]$

$$b_{01} = b_{01}^* \cdot \bar{q}_4 \tag{33}$$

$$b_{10} = b_{10}^* / \bar{q}_4 \tag{34}$$

$M^0 \leftrightarrow M^2$. Proportional to the normalized amount of penetrating water $\bar{J}^{(CL)}$

$$b_{02} = b_{02}^* \cdot |\bar{J}^{(CL)}| \tag{35}$$

$$b_{20} = b_{20}^* / |\bar{J}^{(CL)}| \tag{36}$$

$M^1 \leftrightarrow M^2$. Proportional to the normalized amount of penetrating water $\bar{J}^{(CL)}$

$$b_{12} = b_{12}^* \cdot |\bar{J}^{(CL)}| \tag{37}$$

$$b_{21} = b_{21}^* / |\bar{J}^{(CL)}| \tag{38}$$

Of course, a different choice of the state dependence of the transition probabilities is possible.

To guarantee positive probabilities and to avoid numeric instabilities, all intensities b_{ij} are bounded to positive values below an upper limit. As an example we consider the binary Markovian process $M^0 \leftrightarrow M^2$. In a simulation it was found that

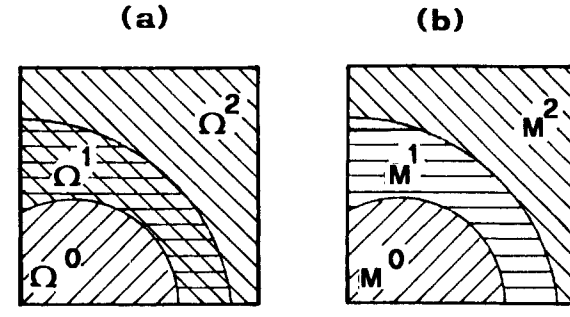

Figure 4. Schematic model space.

for the normalized amount of penetrating water $\bar{J}^{(CL)} = 1$, the system was markedly influenced by this fault. Therefore, we demand a high stationary probability, for example, $p_s^2 = 0.98$ for $\bar{J}^{(CL)} = 1$. Inserting Eqs. 35 and 36 into Eq. 21 yields

$$b_{02}^* = 49 \cdot b_{20}^* \tag{39}$$

From Eqs. 35 and 36 and Eq. 22 a maximum time constant can be evaluated which amounts to

$$\tau_{20\max} = \frac{1}{2 \cdot (b_{02}^* \cdot b_{20}^*)^{0.5}} \tag{40}$$

As a reasonable figure for the maximum time constant a value of 1,000 s can be introduced to calculate the unknown coefficients with Eqs. 39 and 40. Now, for low and high values of $\bar{J}^{(CL)}$ the time constant τ_{20} is very low, that is, a very fast decision is made. For $\bar{J}^{(CL)} = 1/7$ the slowest response ($\tau_{20} = 1{,}000$ s) is observed. As a matter of fact, in this region a discrimination between the two models is difficult. The parameters of all binary Markovian subprocesses are given in Table 2.

Additionally, after each update with the Bayes rule and prediction by the Markovian process, the model probabilities are bounded by a small value from below:

$$p^i > p_{\min}, \quad p_{\min} \ll 1 \tag{41}$$

Figure 5 shows temperature readings of a simulated semibatch reactor. The disturbed reactor and cooling temperatures are the only measurements available for a multiple-filter method. At the beginning the probabilities of all three models amount to 1/3. Almost immediately the multiple-filter method increases the probability for normal operation mode p^0 to a value of 0.96. This is the result of a very small estimated heat release $\hat{\bar{q}}_4$, which together with $\hat{\bar{J}}^{(CL)} = 0$ yields very high intensities b_{20} and b_{10}. After some time the heat release due to the undesired reaction step r_4 is no longer negligible. Therefore, the very simple model M^0 cannot explain the further decrease in cooling temperature. Its probability decreases, whereas probability p^1 of the class representing decomposition mode increases to almost 1. An alarm can be created, for instance, if p^1 is greater than 0.5. However, the simulation was continued applying no countermeasures at all. At $t = 5{,}000$ water penetrates into the reactor. Now, not even model M^1 can explain the further increase in reactor temperature. Hence, probability p^1 is reduced and probability p^2 increases to 0.96. So, for both kinds of hazardous states a meaningful alarm is created.

Introducing different faults, one can show that in every case a correct alarm is created. If a possible fault is not included in a multiple filter for some reason, the Markovian process should be designed in such a way that if it occurs, a safe state of operation will be the result of an applied countermeasure. An unnecessary

Table 2. Parameters of Intensities

Transition $i \leftrightarrow j$	For	p_s^i	max (τ_{ij})	b_{ij}^*	b_{ji}^*
$1 \leftrightarrow 0$	$q_4 = 3 \times 10^{-4}$	0.98	2,000 s	1.1×10^{-8}	5.89
$2 \leftrightarrow 0$	$\bar{J}^{(CL)} = 1.0$	0.98	1,000 s	7.1×10^{-5}	0.0035
$2 \leftrightarrow 0$	$\bar{J}^{(CL)} = 1.0$	0.98	1,000 s	7.1×10^{-5}	0.0035

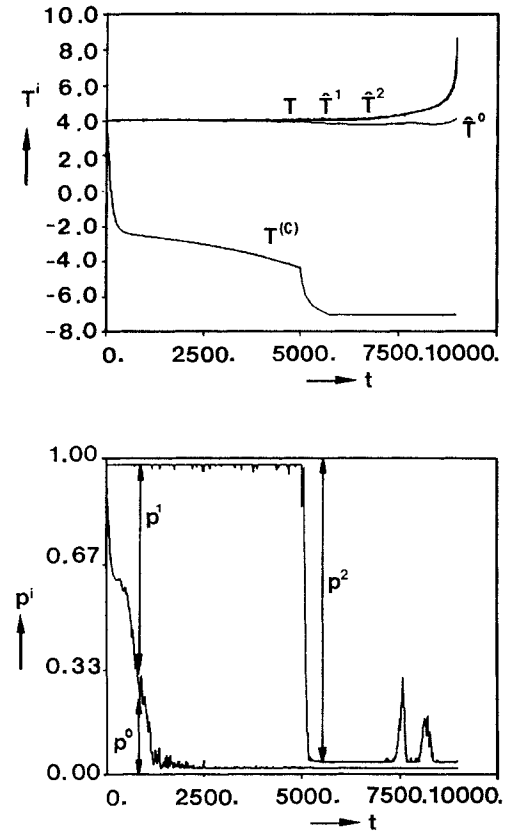

Figure 5. Temperatures and model probabilities of a simulated semibatch reactor.

shutdown of a plant must then be looked at as an "active" error. However, these methods are introduced as a means of early detection of hazardous states, as can be seen in Figure 5. Hence, a multiple-filter method can be used as a supervisory system which must not necessarily apply countermeasures itself. It can inform the operator or, more sophisticated, its information can be used by an appropriate expert system which processes additional fault information.

A very important test for model-based technique is its response in the presence of modeling errors. In the models of the example mentioned above all parameters, with the exception of the activation energies, are multiplied by a random figure, with a mean of 1 and a standard deviation of 0.05. The greatest parameter error amounts to 9%. Figure 6 shows the development of the model probabilities for the same case as in Figure 5, that is, a high reactor temperature leads to a nonnegligable decomposition reaction and water penetrates at $t = 5{,}000$. Again, both faults are detected, although the signals are no longer smooth.

Experimental results

To apply all detection methods on-line, experiments in adiabatic storage containers are performed. All experiments are run until decomposition appears. For the chosen initial conditions decomposition occurs between 30 and 1,900 min.

Criteria

An example of different temperature readings is shown in Figure 7. In this figure the arrows marked (a) indicate the time when a criterion, Eq. 5, detects an accelerated release of heat

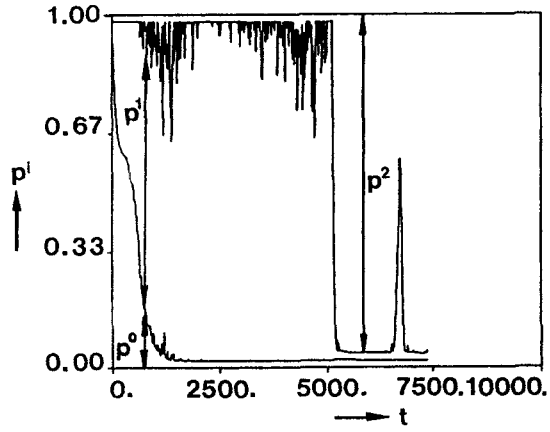

Figure 6. Model probabilities with modeling errors; same faults as in Figure 5.

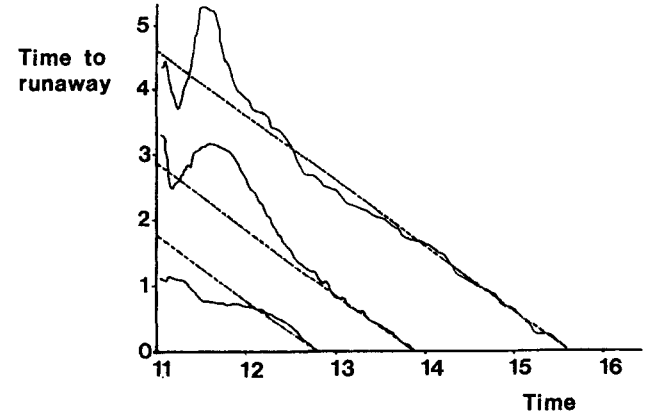

Figure 8. On-line prediction of time to runaway for three different experiments.
---, Theoretical solution

due to the undesired reaction step. The hazardous state is detected at a very early stage.

Prediction

If an alarm is created by using a criterion or a multiple filter, it might be of interest to know how the reaction will go on. This can be done with the actual state estimate $\hat{x}(t)$ and the mathematical model of the process by means of a fast simulation. Here, the time of runaway is of particular interest. Such a prediction is of course based on the assumption that no disturbances will occur in the near future and that the assumed mathematical model is correct. Therefore, a prediction gives only a rough estimate, that is, only the order of magnitude of the time to runaway. Figure 8 shows on-line predictions for three experiments with the sulfonation reaction performed in an adiabatic vessel. All experiments are started at 11.00 h. The predictions of the time to runaway are inaccurate at the beginning due to a high sensitivity in this example. After some time the predictions are quite stable and give satisfying results.

Multiple-Filter Methods

A multiple-filter method was used for the experiments, too. Three different models for normal operation, decomposition, and water penetration mode are implemented. In Figure 7 probability p^0 for the normal operation mode is the largest until the time denoted by the arrows marked (*b*). After that, probability p^1 for decomposition mode is greater than p^0 and p^2.

Two other examples are shown in Figure 9. In case *a*, a small amount of water was injected into the reaction mixture. Here, the normal operation mode was replaced by the water penetration mode. In case *b*, the reaction mixture included a catalytical substance. The usually observed pattern of the temperature reading disappeared completely. Instead after 1 h the mixture decomposed in 6 min. The possibility of the presence of a catalytical substance was not included in any model. Hence, an alarm was created indicating water penetration. Although this is a false alarm, an applied emergency precipitation would be an appropriate countermeasure.

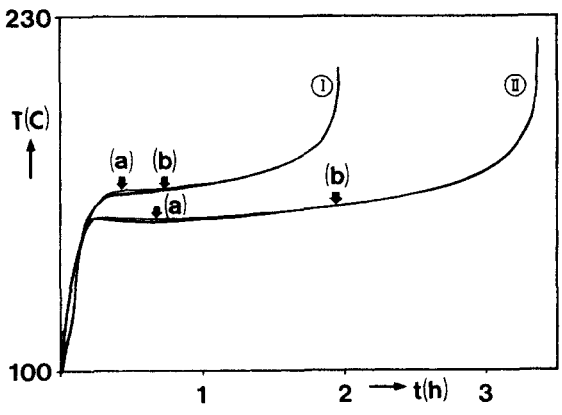

Figure 7. Temperature readings of adiabatic heat storage tests.
(*a*) Alarm with criterion of Eq. 5
(*b*) Alarm with a multiple filter

Industrial reactor

The application of a model-based detection system for an industrial plant differs significantly from a simulation study. In

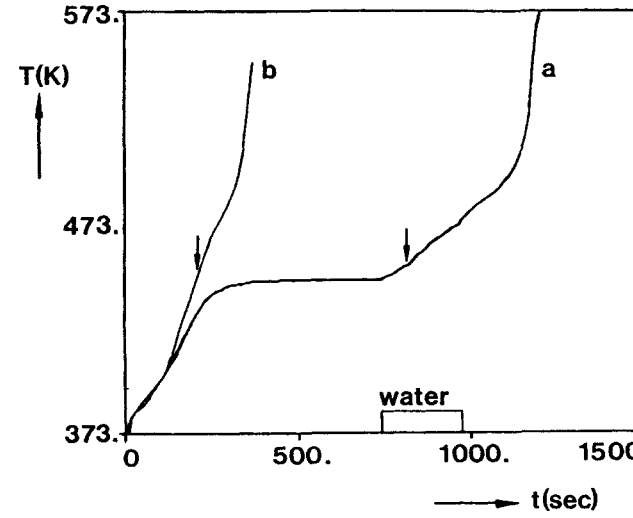

Figure 9. Alarm creation (arrows) with water penetration, *a*, and presence of catalytical substance, *b*.

industry a reactor is not embedded in a well-defined environment. A mathematical model cannot describe all dynamic effects observed in a plant in full detail. Moreover, the initial and boundary conditions are time dependent and very often not exactly measurable. Hence, the design of a model-based detection system has to be done very carefully to avoid false alarms or unnecessary corrections of state estimates that are due to model uncertainties. On the other hand, these uncertainties demand a model-based system to describe the parameter-sensitive behavior of a plant at least approximately.

For the problem considered, the kinetics were determined beforehand in laboratory experiments by evaluating temperature readings of adiabatic heat storage tests. Concentration measurements in isothermal experiments could not be performed (King, 1989). Therefore, as a first step, the kinetics based on temperature readings of adiabatic batch experiments had to be verified in the large-scale reactor, which was operated in an almost isothermal semibatch mode. For one run we could analyze the concentrations inside the industrial reactor. Figure 10 shows the comparison between measured and simulated developments of sulfur trioxide, the aromate, and the desired sulfonic acid. The amounts of all other substances are of minor magnitude in this region of operation. As a very important result, this comparison shows that kinetics found in laboratory experiments, if they are done very carefully, can be used in a large-scale reactor. Moreover, this holds true even if experiments are carried out in an adiabatic batch vessel and the large-scale reactor is operated in an isothermal semibatch mode.

The remaining unknown parameters in the model of the large-scale reactor were some heat transfer coefficients. They were identified by fitting simulated temperature readings to measured ones, Figure 11.

To account for the uncertainties in the industrial plant and for unmeasurable boundary conditions in the building the detection system has been redesigned. This was done by explicitly consid-

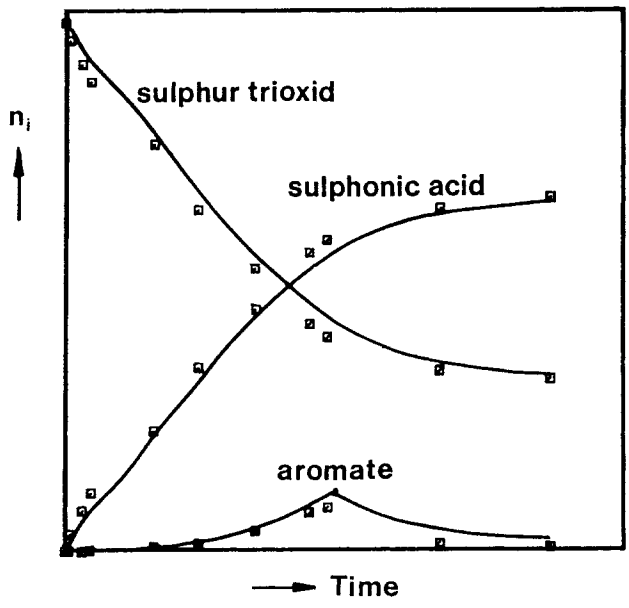

Figure 10. Measured and simulated concentration readings of an industrial process.

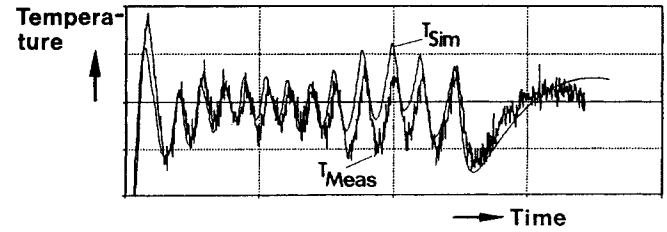

Figure 11. Measured and simulated temperature readings of an industrial process.

ering errors in important parameters of the model. In simulation studies the parameters of the Kalman filters and the Markov process were chosen in a way that a robust state estimation and a reasonable detection were achieved.

Two different methods for detection of hazardous states are implemented in the large-scale reactor:

1. A multiple-filter method with models

Model Ω^0. Only desired reaction steps r_1 through r_3 are included in this model

Model Ω^1. This model describes nominal behavior, that is, r_1 through r_3, as well as the dynamic behavior caused by reaction r_4

Model Ω^2. The most complex model covers desired and undesired reaction and an unknown additional heat source in the balance of enthalpy

2. A statistical mean test based on model Ω^2 to cover other faults.

Up to now the detection system was implemented for only a short period of time in which no faults occurred. However, after a modification of the cooling system, which resulted in an unexpected reduction of cooling capacity, the detection system gave an alarm almost immediately after the process had been started. No other alarms were created in the runs considered.

Besides the proposed benefits of such a detection system, the rather complicated computer program developed in the university should fulfill additional demands. The program has to be maintainable and expansible by the industrial users for a long period of time. Moreover, the program has to fit into company-specific software packages. This could be done only by replacing larger parts of the program by company-specific routines.

Conclusions

Model-based systems provide a very powerful tool to detect hazardous states in a chemical plant at a very early stage. They help to distinguish between different faults. Today, all methods are available and the design is not difficult for an experienced engineer. However, model-based detection is only possible because a great deal of *a priori* information about a process is put together in a mathematical model. This is the most time-consuming step in the application of the methods proposed. Therefore, future work should concentrate on tools to simplify model building.

Acknowledgment

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Notation

D = coefficient matrix of elementary events
$\overline{D}$ = complement to D
$G(\ldots)$ = disturbance matrix
$H_k(\ldots)$ = Jacobian of measurement vector
$\bar{J}^{(CL)}$ = normalized amount of penetrating water
L_Ω = matrix of likelihood functions with nondisjunctive models Ω^j
L_M = vector with likelihood functions with disjunctive models M^i
M^i = disjunctive models or classes
NN = denominator of Bayes formula
P_k = covariance of estimation error
p_M = vector of *a priori* model probabilities
P_M = diagonal matrix of *a priori* model probabilities
R_k = covariance of measurements
S_k, S_k^i = covariance of innovation
$T^{(*)}$ = temperature of liquid (L) or cooling (C)
U_k = sequence of control inputs
Y_k = sequence of measurements

$b_{ij}(t),\ b_{ij}[x(t)]$ = intensities
d_{ij} = logical variable
$g_{ij}[x(t)]$ = state-dependent term of an intensity
k = index of time
$n^{(i)}$ = amount of substance i
p, p^i = probability
$p(M^i|Y_k, U_k)$ = conditional probability of model M^i given
$p_{ij}(t)$ = transition probability
$u(t), u_k$ = control inputs
$v(t), v_k, w(t)$ = stochastic processes
$x(t), x^i(t)$ = state vector
$y(t), y^i(t)$ = measurement vector

Greek letters

$\gamma(t), \gamma_k$ = innovation
Θ = vector of unknown parameters
Λ = original system
τ_{ij} = time constant
Ω^j = nondisjunctive model representation

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Appendix

To calculate the conditional probabilities, Eq. 26, given Eq. 27, we introduce some notation from Boolean algebra: "·" and "+" denote a logical "and" and "or", respectively. "1" is a true event, "0" is a false event. Therefore, nondisjunctive events Ω^j can be expressed using disjunctive elementary events M^i in the following way:

$$\Omega^j = d_{0j} \cdot M^0 + d_{1j} \cdot M^1 \ldots + d_{Nj} \cdot M^N, \quad d_{ij} \in \{0,1\} \tag{A1}$$

or

$$\Omega = D \cdot M$$

with

$$\Omega = (\Omega^0\, \Omega^1 \ldots \Omega^N)^T, \quad D = [d_{ij}], \quad M = (M^0\, M^1 \ldots M^N)^T$$

The denominator of Eq. 15

$$NN = \sum_{i=0}^{N} p(y_k|M^i, Y_{k-1}) \cdot p(M^i|Y_{k-1}) \tag{A2}$$

is now transformed successively. One or more elementary events, for example, M^{i_0} and M^{i_1}, are replaced by the corresponding event Ω^j for $j = 0, 1, \ldots, N$, Figure 12. Now, instead of Eq. A2 we have a sum formed by

$$p(y_k|\Omega^j, y_{k-1}) \cdot p(\Omega^j|Y_{k-1}) \tag{A3}$$

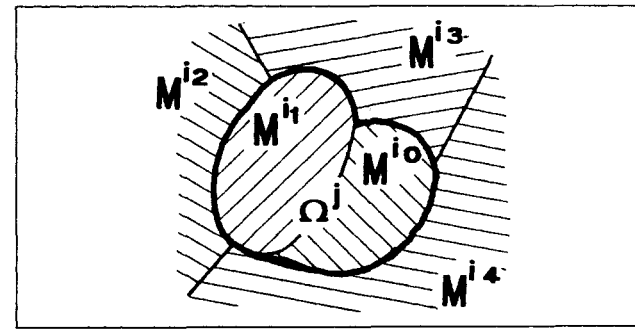

Figure 12. Schematic model space.

and the sum of the "missing" elementary events M^i

$$\sum_{\substack{i=0 \\ M^i \notin \Omega^j}}^{N} p(y_k|M^i, Y_{k-1}) \cdot p(M^i|Y_{k-1}) \tag{A4}$$

Since the sum of all model probabilities equals 1,

$$p(\Omega^j|Y_{k-1}) + \sum_{\substack{i=0 \\ M^i \notin \Omega^j}}^{N} p(M^i|Y_{k-1}) = 1 \tag{A5}$$

it follows for all $j, j = 0, 1, \ldots, N$

$$NN = p(y_k|\Omega^j, Y_{k-1}) \cdot \left(1 - \sum_{\substack{i=0 \\ M^i \notin \Omega^j}}^{N} p(M^i|Y_{k-1})\right) + \sum_{\substack{i=0 \\ M^i \notin \Omega^j}}^{N} p(y_k|M^i, Y_{k-1}) \cdot p(M^i|Y_{k-1}) \tag{A6}$$

If $\overline{D}$ is the logical complement to D and if the logical elements "0" and "1" in $\overline{D}$ and D are replaced by the numerical values 0 and 1, Eqs. A6 and A2 give

$$\mathbf{D} \cdot \begin{pmatrix} p(M^0|Y_{k-1}) & & & 0 \\ & p(M^1|Y_{k-1}) & & \\ & & \ddots & \\ 0 & & & p(M^N|Y_{k-1}) \end{pmatrix} \cdot \begin{pmatrix} p(y_k|M^0, Y_{k-1}) \\ p(y_k|M^1, Y_{k-1}) \\ \vdots \\ p(y_k|M^N, Y_{k-1}) \end{pmatrix}$$

$$= \begin{pmatrix} p(Y_k|\Omega^0, Y_{k-1}) & & & 0 \\ & p(y_k|\Omega^1, Y_{k-1}) & & \\ & & \ddots & \\ 0 & & & p(y_k|\Omega^N, Y_{k-1}) \end{pmatrix} \cdot \left[\begin{pmatrix} 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix} - \overline{D} \cdot \begin{pmatrix} p(M^0|Y_{k-1}) \\ p(M^1|Y_{k-1}) \\ \vdots \\ p(M^N|Y_{k-1}) \end{pmatrix} \right]$$

or, in a shorter notation

$$D \cdot P_M \cdot L_M = L_\Omega \cdot (1 - \overline{D} \cdot p_M) \tag{A7}$$

Because Eq. 41 holds true, an inverse of P_M exists. Hence, if D is of rank $N + 1$, Eq. A7 can be solved to calculate the unknown likelihood functions, Eq. 26, which are put together in vector L_M

$$L_M = \mathbf{P}_M^{-1} \cdot D^{-1} \cdot \mathbf{L}_\Omega \cdot (\mathbf{1} - \overline{D} \cdot p_M) \tag{A8}$$

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