An Approach to Mechanistic Event Recognition Applied on Monitoring Organic Matter Depletion in SBRs

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A fundamental practice in process engineering is monitoring the state dynamics of a system. Unfortunately, observability of some states is related to high costs, time, and efforts. The mechanistic event recognition (MER) aims to detect an event (defined as a change of the system with specific significance to the operation of the process) that cannot be directly observed but has some predictable effect on the dynamics of the systems. MER attempts to apply fault diagnosis techniques using mechanistic "recognition" models to describe the process. A systematic method for building recognition models using optimal experimental design tools is presented. As proof of concept, the MER approach to detect organic matter depletion in sequencing batch reactors, measuring only ammonia, dissolved oxygen, and nitroxides is applied. The event, that is, consumption of organic matter to a level below 50 gCOD/m^3, was successfully detected even though microbial activity is known to continue after organic matter depletion. © 2014 American Institute of Chemical Engineers *AIChE J*, 60: 3460–3472, 2014
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Introduction

Emerging sensor and computer technology, data management techniques, and a mechanistic understanding of the system are used to create a deeper insight into industrial processes. Nevertheless, monitoring of many processes has been shown to be extremely cost and time demanding, or even not possible. In such cases, the recognition of "faulty" events might still be viable if some symptoms of them can be detected. There is a broad field of research devoted to fault detection, identification, isolation, and diagnosis[1–5] including the use of statistical tools, like principal component analysis[5] or partial least squares,[6] nonlinear models like neural networks[7] and also multivariate statistics.[6] Furthermore, Isermann[8] gives a nice introduction showing the advantages of model-based fault diagnosis (FD) methods like parameter estimation, parity equations, Kalman filters[9] with its variations,[10] and observers.[11,12] Using model-based methods, gives a deeper insight in the process in comparison to limit or trend checking of some measurements and allows not only a fault detection, but also a diagnosis. Within this framework, it is tempting to go one step further and use first principle models in order to apply all the knowledge available for the isolation and diagnosis of the fault. Generally speaking, first principle modeling (white box) is the preferred approach to describe a system when mechanistic understanding (mass balances, thermodynamics, kinetics, etc.) is at hand.[13–16] Scale up, a deeper understanding, and optimizations, are some of many advantages of mechanistic models over black and gray box ones.

Still mechanistic models are rarely used for FD, the main reasons being that white box models are typically very complex, suffer from low tractability, and are very difficult to identify using typical online information.[17] Today, there is neither a systematic approach to take advantage of first principle knowledge for FD nor a methodology to strategically reduce complex mechanistic models for its use together with FD methods.

We propose to use existing methods for optimal experimental design (OED) for nonlinear models[18] in order to build local simplified "recognition" models derived from complex first principle ones to obtain tractable models that can be used for

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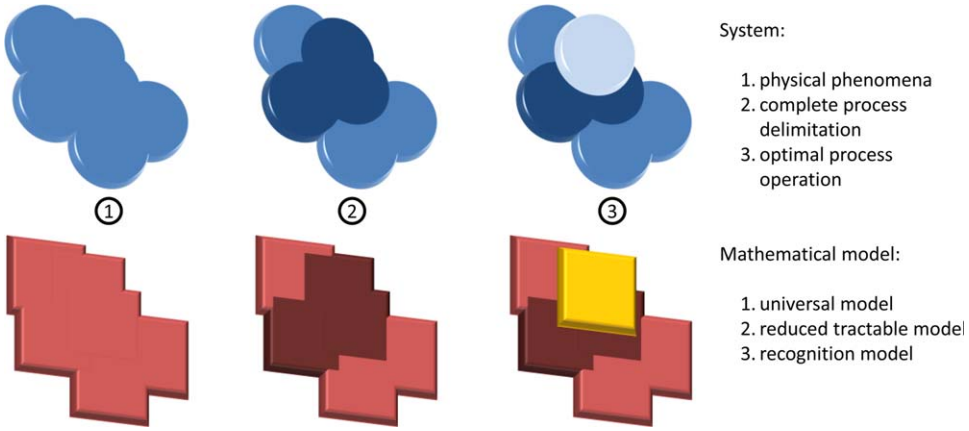

Figure 1. Graphic representation of the model reduction to create the recognition model.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

FD purposes. By these, we can use FD techniques to take advantage of the mechanistic understanding of the system even for cases with insufficient data.[19] Because it is also possible to detect changes in the operation that do not necessarily represent a fault, we use the term event (defined as a change of the system with specific significance to the operation of the process). The mechanistic event recognition (MER) uses the information contained in complex nonidentifiable model structures to create more tractable recognition models that are capable of identifying specific nonobservable events in a dynamic process. These simplified models are easier to identify, allowing for a better parameter and state estimation. In terms of monitoring, proper recognition models allow detection of symptoms comprised by complex and nonlinear feature combinations.

Mechanistic Event Recognition

Mechanistic models, developed through basic research, aim for an exact and extensive description of the system. Conversely, industrial processes can be enclosed in a tight operability regime, and any description of the system beyond this region should be neglected. If we are able to extract only the information that is relevant to the operation of the process, we might be able to obtain a tractable model with all the mechanistic information that is relevant to our system.

Furthermore, if we reduce the model to an extent, where it can only describe the ideal operating conditions, we can detect deviations in our process. In other words, if the process shows a different behavior than the reduced model, we know that the process is deviating from this optimal regime as seen in Figure 1.

Assume the system Φ with dynamics defined in $t \in [t_0, t_{end}]$ where t_0 and t_{end} represent the initial and endpoint, respectively. Consider now that a relevant event is happening at $t=\tau$ which affects the dynamics of Φ but cannot be measured or observed. If that is so, the system Φ can be set as $\Phi=\{\phi_1, \phi_2\}$, where ϕ_1 represents the system at $t \in [t_0, \tau]$ and ϕ_2 represents it at $t \in (\tau, t_{end}]$.

Let Γ be a mechanistic model that properly describes the process Φ (i.e., the residual has mean zero and constant variance for $t \in [t_0, t_{end}]$). Now, let $\gamma_1 \subset \Gamma$ be a reduced version of Γ such that it can mirror the dynamics of ϕ_1 properly but fails to describe ϕ_2.

If this is true, we can use γ_1 as a recognition model together with methods for model-based fault detection to detect the event τ by exploiting the fact that for any $t > \tau$, γ_1 cannot describe the process Φ properly.

One could argue that reducing a complex model requires more effort than creating a tractable model from scratch, and this is indeed the case. Still, using a reduced model offers many advantages over "new" models as are:

- a knowledge supported delimitation of the description capacity of the model
- a transition of the information gained with the model to other systems and models
- scale up
- a mechanistic diagnosis of the cause of the event

These characteristics of reduced models are especially important for MER, as the recognition capacity depends on the proper delimitation of both, the system and the description capability of the recognition model.

Flow Diagram

We present a flow diagram of the methodology of MER in Figure 2. The diagram is divided into three main blocks representing the main steps: (1) building the recognition model, (2) selection of the horizon size, and (3) detection of the event. A short description of each step contained in the blocks of the flow diagram is presented in Building the Recognition Model, Selection of the horizon size, and Detection of the event subchapters, the order is based on the flow diagram.

Building the recognition model

Detailed mechanistic models are typically too complex to be applied in large-scale processes. Instead, a combination of "local" models to describe specific instances of a system has been addressed in various forms. Qualitative process theory,[20,21] interactive multiple model,[3,22] jump Markov linear systems,[23] qualitative algebra and graph theory methods,[24] semiquantative simulation,[25] and variable structure theory[26] are some examples. These methods rely on simple models, striving to fast but short-term predictions. Similarly, efforts to apply models that are limited to defined operation regimes are also popular in process engineering. The idea is to increase model tractability through multiple local simplifications of the global behavior. Adaptive model control,[27,28] operating regime-based modeling,[29] and gain scheduling[30] are the most representative ones. These simplified models are more tractable hence allow a better parameter and state estimation. For monitoring, this means that states which cannot be observed with a global model are observable in defined regimes when a simplified local model is applied.

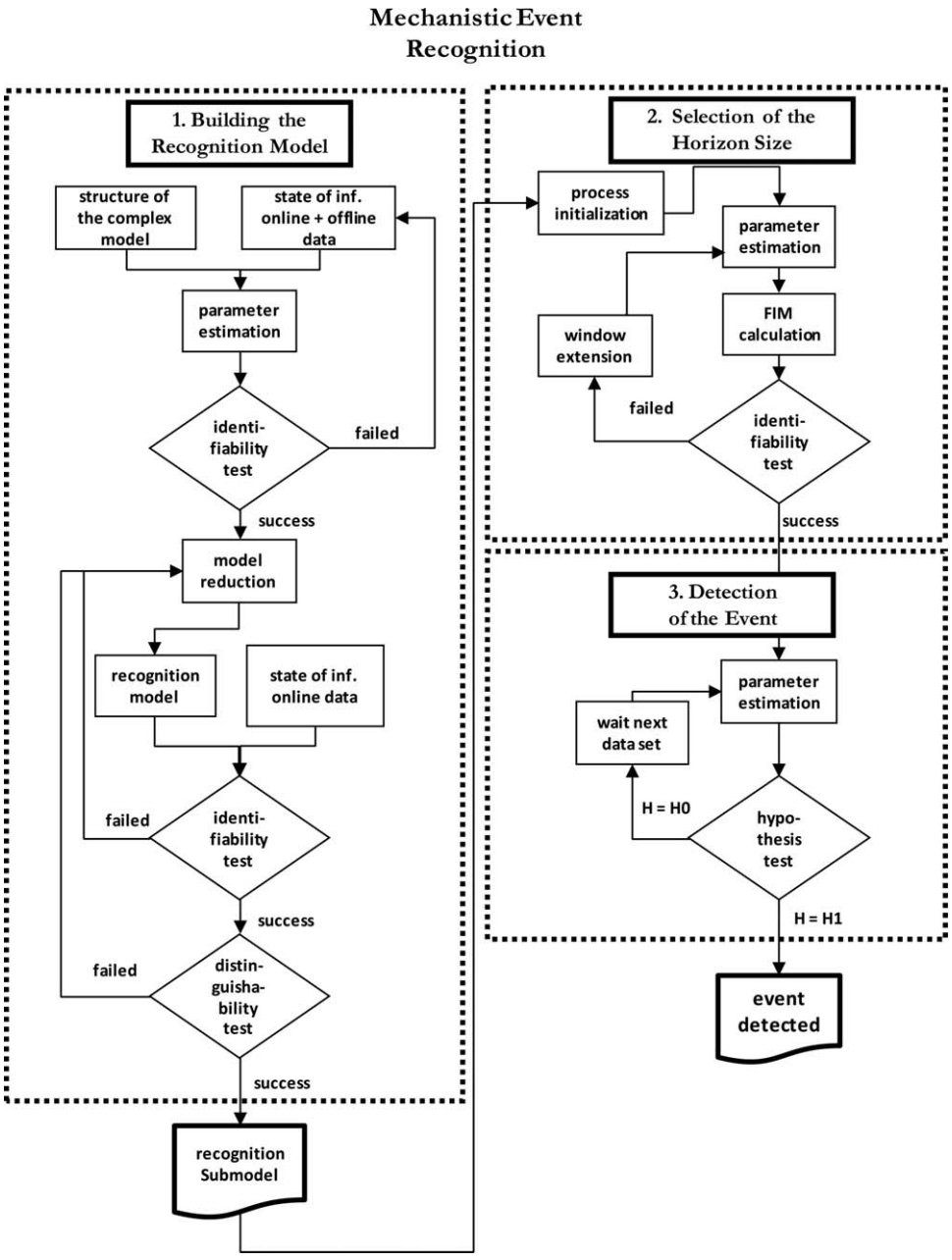

Figure 2. Flow diagram mechanistic event recognition.

Unfortunately, all previous techniques require at least one state to define the operating interval hence cannot deal with systems at low states of information; the most relevant states need to be observed. To overcome this problem, we can use FD methods to detect the instance when the local model ceases to be valid. But, how can we build a mechanistic local model that is identifiable for our system and only describes the desired regime? We can use methods developed for OED in combination with model reduction techniques to find the adequate recognition model for our purposes.

To dictate the level of model complexity that the data are able to support, we first need to determine the quantity and quality of the information that we get from the process. Once we know the state of information of the system,[31] we can define the characteristics of the recognition model. In the following, we give a short introduction to the methods used in OED to determine the information content of a data-set in relation to a structured model.

We consider systems of the form

$$f(\dot{x}(t), x(t), u(t), w, \theta, t) = 0 \tag{1}$$

where $\dot{x}(t)$ is a vector with the derivatives of the state variables, $x(t)$ is a vector with n_s time-dependent variables which define the system, $u(t)$ a vector of n_u time-dependent input variables, w is a vector with n_w constant input variables, θ is a vector with P parameters, and t represents time.

The initial conditions are also to be defined

$$f(\dot{x}(t_0), x(t_0), u(t_0), w, \theta, t_0) = 0 \tag{2}$$

where t_0 is the time at point 0.

To fit a model to data, we require enough information (i.e., sufficient and accurate measurements) to assure a unique solution of the parameter estimation problem. Otherwise, we have an ill-conditioned problem.[32,33] To prevent this, we must study the state of information of our system to ensure a well-conditioned parameter estimation problem.[31,34]

This means we have two important factors to consider, namely the data and the structure of the model.

The steps of the flow diagram are briefly described (see Figure 2, Block 1):

State of Information of the Data. "Measurements are inevitably subject to uncertainties, and for this reason datasets should not be considered observations, but rather a "state of information" acquired from observable variables."[31] The online data obtained from the process might be insufficient to fit the complex mechanistic model. In this case, we need additional information (literature and offline data, experiments, etc.). Nevertheless, we have to keep in mind that for the resulting recognition model, identifiability has to be reached using online information exclusively.

Structure of the Complex Model. The structure of the model defines the interrelations and effects of the parameter values in the output vector. Those outputs which are highly sensitive to changes in the parameters allow for a precise estimation of the "exact" parameter set.[33]

Parameter Estimation. The parameter estimation problem is formulated as follows:

Experiment outputs are represented by the vector $y(t)$

$$y^{\text{mes}}(t)=f\left(y_E^0, u_E(t),\ w_E,\ \eta_s,\ \eta,\ t_E\right) \quad \forall t \in t_{\text{sp}} \tag{3}$$

where the sub index E represents the variables of the experiment and t_{sp} represents the time span of the experiment.

Model outputs (model predictions) are represented by the vector $y^{\text{calc}}(t)$

$$y^{\text{calc}}(t)= f(\dot{x}(t), x(t), u(t), w, \theta, t) \tag{4}$$

The quantification of the goodness of fit is calculated with the maximum likelihood (MXL)

$$\text{MXL} = \frac{1}{2}\frac{\left(y^{\text{calc}}(t,x)-y^{\text{mes}}(t)\right)^2}{C_y} \tag{5}$$

The variance-covariance matrix C_y serves two purposes. On the one hand, the outputs related to very noisy data have a smaller impact on the criterion. On the other hand, different scales between the outputs are also weighted. The probability density function of the parameter set and its correlation define the confidence region for parameter estimation. The size of the confidence interval is a direct indicator of model identifiability.

Identifiability. Asprey and Macchietto[35] define identifiability as the quality of a model to present a monotonic behavior. For MER, we use the widely used approximation of the variance-covariance matrix, namely the fisher information matrix (FIM)[36]

$$C_\theta \geq \text{FIM}^{-1}(\theta_{\text{es}}) \tag{6}$$

where C_θ and θ_{es} are the variance-covariance matrix of the parameter set and the vector with n_P estimated parameters, respectively. The FIM is computed using the information of the dynamic sensitivities and the variance-covariance matrix of the measurements

$$\text{FIM}(\theta_{\text{es}})=\sum_{k=1}^{N}\left(\left(\frac{dy(x(\theta,t),u(t))}{d\theta}\right)_{\theta_{\text{es}},t_k} C_y^{-1}(t_k)\left(\frac{dy(x(\theta,t),u(t))}{d\theta}\right)^T_{\theta_{\text{es}},t_k}\right) \tag{7}$$

where y is the measurement vector, θ_{es} is the estimated parameter vector, x is the state variables vector, t_k is the time point of the measurement k, u is the control variables, and C_y is the variance-covariance matrix of the measurements. The criterion selected in this work for the quantification of identifiability is the A criterion (A_{crit})[37]

$$A_{\text{crit}} = \text{trace}\left(\text{FIM}^{-1}\right) \tag{8}$$

Model Reduction. Once we are able to quantify the effect of the process information on the accuracy of our estimated parameter set, we need to find methods to systematically change the structure of our models. The reduction of complex models to achieve a higher tractability while maintaining its relevant characteristics has been thoroughly addressed in literature. Representative examples are lumping,[38,39] sensitivity analysis,[40] quasi steady-state assumption,[41] and time-scale analysis.[42–44] The reader is referred to Okino and Mavrovouniotis for an extended review.[45]

Nonetheless, a general method with reasonable computer expenses is still to be developed.[46] Phenomena delimitation and model adaptation for each regime is still a difficult task. When dealing with complex nonlinear systems in a dynamic change, these methods are difficult to apply. In the case of real industrial processes, model reduction is still a heuristic, iterative, and long procedure. Still, the case study presented in this and previous works shows the reduction potential of complex models and its advantages.[47]

Distinguishability. To assure distinguishability, the residual between two different models needs to be larger than the variance of the measurements. Using Eq. 9 it is possible to quantify the measurements required to fulfill a specified threshold for model distinguishability D^B

$$\frac{\sum_{i=1}^{n_y}\left(y_1(x_1(\theta_1,t),u(t))-y_2(x_2(\theta_2,t),u(t))\right)^T\times\left(y_1(x_1(\theta_1,t),u(t))-y_2(x_2(\theta_2,t),u(t))\right)}{n_y}=D^B \geq \sigma_y^2 \tag{9}$$

where y is a vector with n_y outputs of Models 1 and 2 respectively, $u(t)$ a vector of n_{u^u} time-dependent input variables, and θ the parameter set of Models 1 and 2, respectively.

Selection of the horizon size

Once we have built the recognition model, we need to apply method for model-based FD. Methods for model-based residual generation that offer analytical redundancy have been widely discussed in literature.[4,48–51] Typical methods include, state estimation (the parity space approach, observer-based schemes, and fault detection filter approach) and parameter estimation techniques. In our case, the best results were obtained using a moving horizon method[52,53] for the recursive calculation of the MXL estimator. The MXL function is computed every new measurement takes

place, and the recognition program considers a change of regimes if the MXL exceeds a nominal value as in Eq. 15.

Window Extension. The size of the horizon is fitted to assure identifiability. Once the process has been initiated, the recognition model is fitted to the data. Following, the condition number of FIM is calculated to evaluate its nearness to singularity, see Eq. 10. The upper condition bound $k_{\max}$ is set to 1000 according to[54]

$$\frac{\sigma_1(\text{FIM})}{\sigma_m(\text{FIM})} \leq k_{\max} \cong 1000 \tag{10}$$

where σ represent the first and last singular values respectively. Once the state of information is sufficient to assure a well-conditioned problem, the recursive computation of the identifiability criterion is started.

The boundary selected for A_{crit} is based on the distinguishability boundary of the system D^B described in Eq. 9. At the beginning of the estimation, the number of measurements is allowed to grow until the threshold is reached (e.g., the number of measurements is enough to make a distinction between the outputs off different models)

$$A_{\text{crit}} \leq D^B \tag{11}$$

where D^B represents the criterion boundary obtained from the distinguishability test in Eq. 9.

At the next time step, the first measurement is discarded as the current measurement is made available. This procedure is repeated at each time step, and the optimization remains at constant size for all future times.[53]

Detection of the event

In this work, an event is defined as a specific change in the system that is of interest for the operation of the process. The position in time, where the event takes place, is defined as $t=\tau$. MER can be applied to detect events that are not observable but have a known effect on the dynamics of the process (symptoms). Although not necessarily representing a fault in the system from a mathematical and physical point of view, the program is required to detect irregular behavior by the system in comparison to some model predictions. Taking this into account, we can use existing methods for FD with analytical redundancy to maximize the probability of event recognition.

Similar to the condition of detectability,[48] there are four conditions that must be met to allow the detection of the event, and thus need to be considered during the reduction of the detailed model to obtain a recognition model:

1. Knowledge of the normal behavior of the system $\Phi=\{\phi_1, \phi_2\}$, and an adequate representation with a first principle model Γ
2. Mechanistic understanding of the effects of the event on the dynamics of the process and an adequate recognition model γ_1
3. Distinguishability between the models describing the dynamics before and after the event $\phi_1(t)-\phi_2(t)=D^B \geq \sigma_y^2; \forall\ t\ (\tau,\ t_{\text{end}}]$
4. A satisfactory state of information to identify the model applied for the event recognition $A_{\text{crit}} \leq D^B$.

Hypothesis Test. In this work, we focus on the application of parameter identification methods due to the common theoretical background with design of experiments. But, MER is not limited to parameter estimation methods, and the application of faster methods should be tested in the future.

Frank and Ding[49] propose a robust parameter estimation method in order to increase the probability of correct detection of the event. To decide whether the process is running in the present regime or a change is taking place, a residual calculation is carried out to prove one of the following hypotheses

$$\begin{aligned} H_0 &: \theta_{\text{n}} = \theta_{\text{e}} \\ H_1 &: \theta_{\text{n}} \neq \theta_{\text{e}} \end{aligned} \tag{12}$$

where θ_{n} and θ_{e} represent the nominal parameter set and the estimated parameter, respectively, hypothesis zero assumes there is no regime change, whereas hypothesis one assumes the event has been reached.

To enable the evaluation of the hypothesis taking the uncertainties of the observations into account, a residual between θ_{n} and θ_{e} is calculated weighted by the variance-covariance matrix of the expected parameter set

$$\text{res} = (\theta_{\text{n}}-\theta_{\text{e}})^T C_p^{-1} (\theta_{\text{n}}-\theta_{\text{e}}) \tag{13}$$

where res is the residual, and C_p is the variance-covariance matrix of the parameter set.

We can also take advantage of the previous calculation of FIM in Eq. 7 and substitute C_p by its approximation, resulting in the equation

$$\text{res} = (\theta_{\text{n}}-\theta_{\text{e}})^T \text{FIM}\, (\theta_{\text{n}}-\theta_{\text{e}}) \tag{14}$$

Finally, a fixed threshold D^B is selected based on Eq. 9 to accept or reject hypothesis zero. Although variable threshold approaches have shown to be more efficient,[55] thanks to the implementation of FIM in the equation, the residual also reflect the actual state of information with respect to the parameters.

The method showed a very robust and accurate prediction of the regime change. Nevertheless, the comparison of θ presented a high variation in the optimal threshold when applying it with different effluent qualities, which might have been caused by the extreme complexity of biochemical reactions. Instead, the comparison of the MXL function proved to be more reliable

$$\begin{aligned} H_0 &: \text{MXL}_{\text{n}} \geq \text{MXL}_{\text{e}} \\ H_1 &: \text{MXL}_{\text{n}} < \text{MXL}_{\text{e}} \end{aligned} \tag{15}$$

where MXL_{n} and MXL_{e} represent the nominal and the estimated MXL functions, respectively, hypothesis zero assumes that there is no regime change, whereas hypothesis one assumes that the event has been reached.

Case Study

In wastewater treatment (WWT), running a process beyond fulfillment of effluent restrictions reduces its overall efficiency. This is specially the case for batch and sequencing batch reactor (SBR) systems where cycle length plays an important role in energy consumption and load capacity. A complete cycle of the SBR process consists of five steps; (1) Idle, (2) Fill, (3) React, (4) Settle, and (5) Draw, which are carried out in one or more stirred batch reactors with an aeration system. In an SBR, the retention time, the duration of the aeration and anoxic phases, the settling time, and other conditions can be easily fitted to variations on load quality as well as effluent requirements. When properly designed and operated, SBRs offer important advantages over continuous processes, not only because of its efficiency and economical aspects,[56–58] but also because of its small footprint[59,60] and high flexibility and operation range.[61]

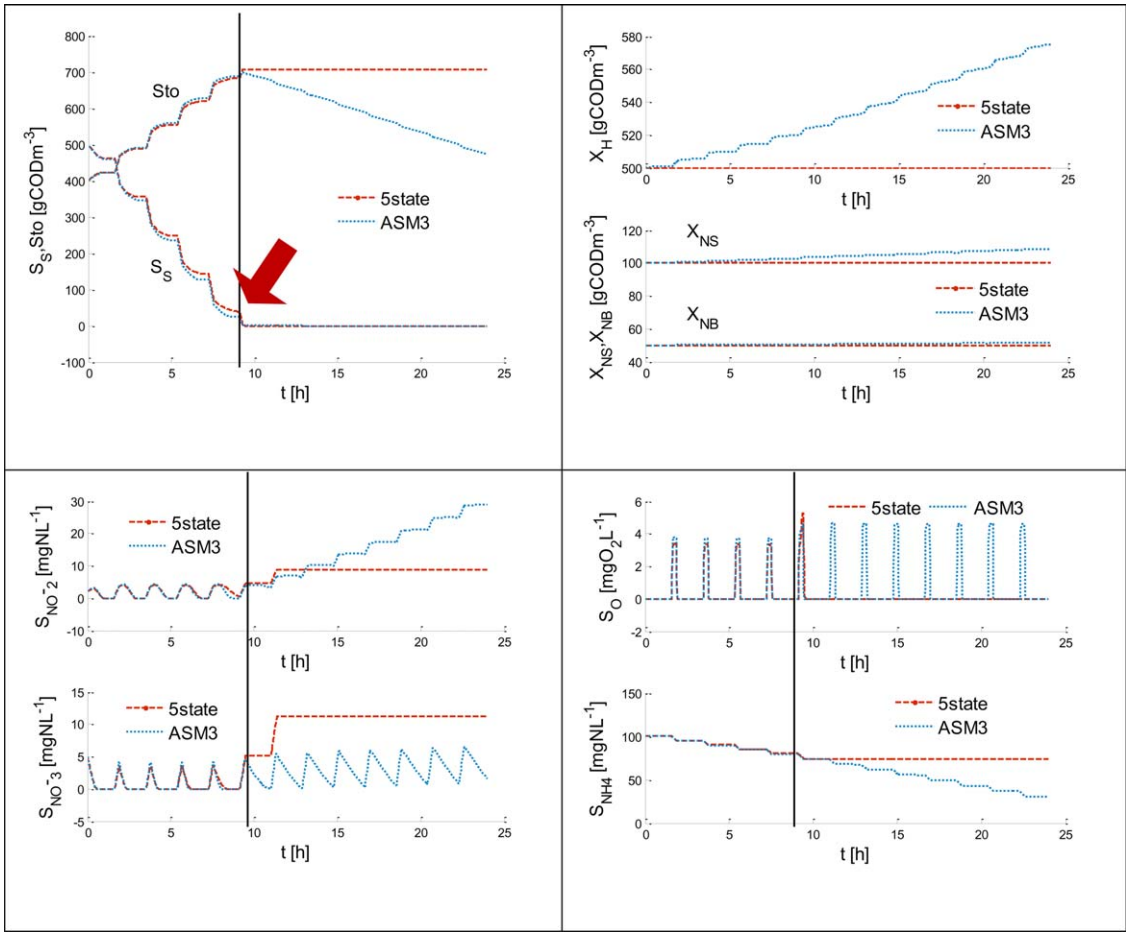

Figure 3. Description of the recognition model in both regimes, with and without substrate.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Today, SBRs are strongly affected by the lack of an efficient method for the detection of depletion of organic matter. Variables measured in standard WWT plants are pH, DO, respirometry, redox capacity, and titrimetry, among others.[62,63] Nevertheless, despite many efforts to monitor nutrient removal,[64–66] online monitoring of chemical oxygen demand (COD), nitrites, nitrates, and ammonia, but especially biological oxygen demand (BOD) is difficult, inaccurate, and costly. A method to distinguish between the dynamics of wastewater degradation using organic matter as an energy source and bacterial activity after its depletion offers important advantages to the process. Within this framework, it is of interest to apply MER to detect the instance when the concentration of ready biodegradable organic matter drops below the level allowed by environmental regulations.

The complexity of the system is increased when implementing the bypass nitrification (BN) in SBRs as shown in Figure 3. In the active sludge process (ASP), nitrogen is removed from wastewater by the nitrification/denitrification process. In the first stage, *Nitrosomonas* and other ammonia oxidizers convert ammonia and ammonium to nitrite, and in the second stage, *Nitrobacter* and other nitrite oxidizers finish the conversion of nitrite to nitrate. Turk and Mavinic[67] proposed the BN process, which can be achieved by inhibiting the production of nitrate, and suggested various methods for bringing about this effect. BN has been shown to offer a number of advantages over the conventional nitrification-denitrification, such as: 40% reduction of COD demand during denitrification, 63% higher rate of denitrification, 300% lower biomass yield during anaerobic growth, and no apparent nitrite toxicity effects for the microorganisms in the reactor. Katsogiannis et al.[68] showed that a frequent change between aerobic and anoxic conditions, a so called intermittent aeration profile, is the best method to suppress nitrate accumulation. This system poses many challenges for the detection of substrate depletion due to its high nonlinearity combined with the on/off aeration profile.

FD methods have been widely applied in WWT, in continuous[69] and in batch processes.[70] Comparison of historical data,[71,72] and local monitoring methods using multiway principal component analysis[70] are the most representative examples. Still, previous work does not take advantage of the knowledge embedded in first principle models like the extended ASM3 (see section model building). As a result, these methods rely on historical data in order to differentiate normal from abnormal dynamics, which hampers its application in new plants or after important changes in the process. In addition, the results can only be applied to the system under study. A transfer of the results to other processes without a complete recalibration is difficult.[70] Hence, a mechanistic method is of interest.

Now, let us attempt to apply MER in an effort to detect the depletion of organic matter. A detailed flow diagram is shown in Appendix A. First, we need to make sure that the system fulfills all conditions to allow a mechanistic detection of the event. To ensure the recognition of the different regimes during the process, the system is required to fulfill the following conditions in Table 1.

Table 1. Conditions for MER Applicability

Process must have more than one regime	1. Biomass growth based on consumption of organic matter 2. Biomass growth using stored energy.
Detailed model of the general process	The extended ASM3
The initial regime is known including its initial conditions	Biomass growth based on consumption of organic matter
The minimal length of the regime assures model identifiability	Initial concentrations of organic matter must be high enough to assure sufficient data samples before depletion.
Knowledge of the normal behavior of the system	Defined by the extended ASM3
definitiveness of the changing behavior	Demonstrated with the distinguishability tests

The variables that can be measured in the process are presented in Table 2. In real plants, these measurements are available in online information with relatively cheap sensor technology.

Building a recognition model for organic substrate depletion in SBRs

The family of activated sludge models (ASM) represents a state-of-the-art model framework for ASP simulation.[73] ASM1 is the most widely used,[74] ASM2[75] is applied to simulate processes that include biological phosphorus removal,[64] and the latest version, ASM3,[76] includes the quantification of energy storage in order to describe substrate and oxygen uptake with higher accuracy. A newer version of ASM3, referred to in this contribution as extended ASM3, where nitrification and denitrification are considered as two-step processes taking nitrite into account as an intermediate, has been published.[77] This model is composed by a system of 15 differential equations and 20 reaction rates. Even though the size of the extended ASM3 is not particularly large (15 differential equations and 20 reaction rates), it is very stiff and contains a large number of parameters which cannot be estimated due to a lack of sufficient information.

The extended ASM3 is unidentifiable with the state of information that can be obtained from a running SBR and describes many states, which can be neglected for its operation.[78,79] This is a lead that we can reduce the extended ASM3 to a more tractable form and use it as a recognition model to detect deviation from the optimal operation regime.

In SBRs, it is of interest to stop the process once the concentrations in the tank fulfill environmental regulations. An accurate detection of depletion of organic is essential for maximal process efficiency. For this reason, the recognition model is built to describe the process regime under high substrate concentrations aiming at detecting organic matter depletion.

The recognition model should distinguish between two regimes:

1. A regime with readily biodegradable organic matter in the medium
2. A regime where readily biodegradable organic matter has been depleted.

As mentioned before, the biological degradation of organic and inorganic compounds in batch processes is set to different conditions compared to continuous plants. The most relevant assumptions made to create the recognition model are:

a. The concentration of bacteria is constant throughout one cycle

b. Heterotrophic bacteria cannot utilize the energy they store

c. The conversion from slow biodegradable substrate to readily biodegradable is not rate limiting

d. Alkalinity, ammonia, and stored energy do not limit any rate of reaction.

In the resulting recognition model, there are five differential equations which describe the basic variables (concentrations), namely: (1) carbonaceous substrate, (2) dissolved oxygen, (3) ammonia, (4) nitrite, and (5) nitrate. A detailed description of the reduction process from the extended ASM3 to the five-state model is presented in Ref. 47, the system of differential equations is shown in Appendix B.

The identifiability of the model depends not only on the structure but also on the number of parameters that are selected for parameter estimation. Parameters which show a low sensitivity and cannot be estimated with sufficient accuracy should be set to a nominal value (e.g., obtained from literature) and not be included during model fitting. We included all growth rates and yield coefficients in the parameter vector of the optimization program. These parameters were selected based on their high sensitivity and relevance to the description of bacterial biochemical reactions. The parameter vector is presented in Table 3. The reader is referred to Refs. 47 and 77 for further details.

Now that we have obtained an adequate recognition model, we can make use of FD techniques (Figure 1, Blocks 2 and 3) to detect our event, namely the depletion of ready biodegradable organic matter.

Detection of organic matter depletion

The five-state model has proven to be an eligible recognition tool for our purposes; on the one hand, it can mimic the dynamics of the extended ASM3,[80] on the other hand, the five-state model is not capable of describing the behavior of the process after the substrate has been depleted as shown in Figure 3. From this, we conclude that the recognition model can be applied as an indirect method to detect the depletion of organic matter.

MER Initialization. The threshold D^B for A_{crit}, set at 0.2, is reached after 0.22 days (5.28 h) as shown in Figure 4B. From this point on, MER is initiated to detect depletion of organic matter.

Figure 4 depicts the performance of MER, and includes three short aerobic intervals as well as three large anoxic ones. This scenario was selected to test MER in a process with a very low state of information. The anoxic intervals offer measurements with low information content because, (1) the parameters set to estimation have its main effect during the aerobic phase and (2) the concentrations of oxygen

Table 2. Measurements

Variable	Description	Units
SNH_4	Ammonia concentration	$[mgNL^{-1}]$
SO_2	Dissolved oxygen in the medium $[mgO2L^{-1}]$	$[mgO2L^{-1}]$
SNO_X	Concentration of nitroxides ($NO_2 + NO_3$)	$[mgNL^{-1}]$

Table 3. Optimization Parameters, Units are taken from Ref. 77

Parameter	Short Description	Nom. Value	LB	UB
μ_H	Maximal growth of heterotrophous	0.6021	0.4817	0.7225
μ_{A1}	Maximal growth of nitrosomones	0.6552	0.5242	0.7862
μ_{A2}	Maximal growth of nitrobacter	0.3468	0.2774	0.4162
Y_{Haer}	Yield coefficient of S_S to X_H in aerobic conditions	0.1302	0.1042	0.1562
Y_{A1}	Yield coefficient nitrite to Nitrosomonas in aerobic conditions	0.1327	0.1062	0.1592
Y_{A2}	Yield coefficient nitrite to Nitrobacter in aerobic conditions	0.0985	0.0788	0.1182
Y_{A3}	Yield coefficient nitrate to Nitrobacter in aerobic conditions	0.0331	0.0265	0.0397

and nitroxides drop to zero. Still, MER exhibits very good performance in terms of accuracy and robustness.

Detection of Events. The detection of the event was achieved by recursive calculation of MXL_e in Eq. 15. The constant threshold was set to a MXL_n value of 7.4. Substrate depletion is accurately detected despite the fact that we cannot measure the concentration of organic matter (online information).

As can be seen in Figure 4, MER detects the event with high precision. Furthermore, the large slope of H at the depletion region assures a robust and accurate detection of the regime change, the initial conditions are depicted in Table 4.

MER performs so well because of one important characteristic of bacterial growth; microorganisms tend to consume as much substrate as possible. Heterotrophic bacteria show similar dynamics in a wide range of organic matter concentration, as can be seen by the substrate limitation constant (k_s=0.1). For this reason, the sensitivity of the MXL function to organic matter concentration is very low at high concentrations. Still, it is of great importance to distinguish the different causes for changes in growth activity. Depletion of organic matter as well as changes in other states have an important effect on the activity of the microbial culture of the sludge. The merit of MER lies in its capability to distinguish between all possible causes for reduction of microbial activity, and to trigger the alarm only when depletion of organic matter is about to happen.

Finally, Figure 5 is presented to prove that MER shows good performance under different conditions. Reducing the initial concentration of organic matter (from 1000 to 500 gCOD/L) poses a difficult challenge to MER. The state of information is smaller in comparison to the first scenario, and the detection has to take place sooner. In the future, a more robust detection method which requires less tuning

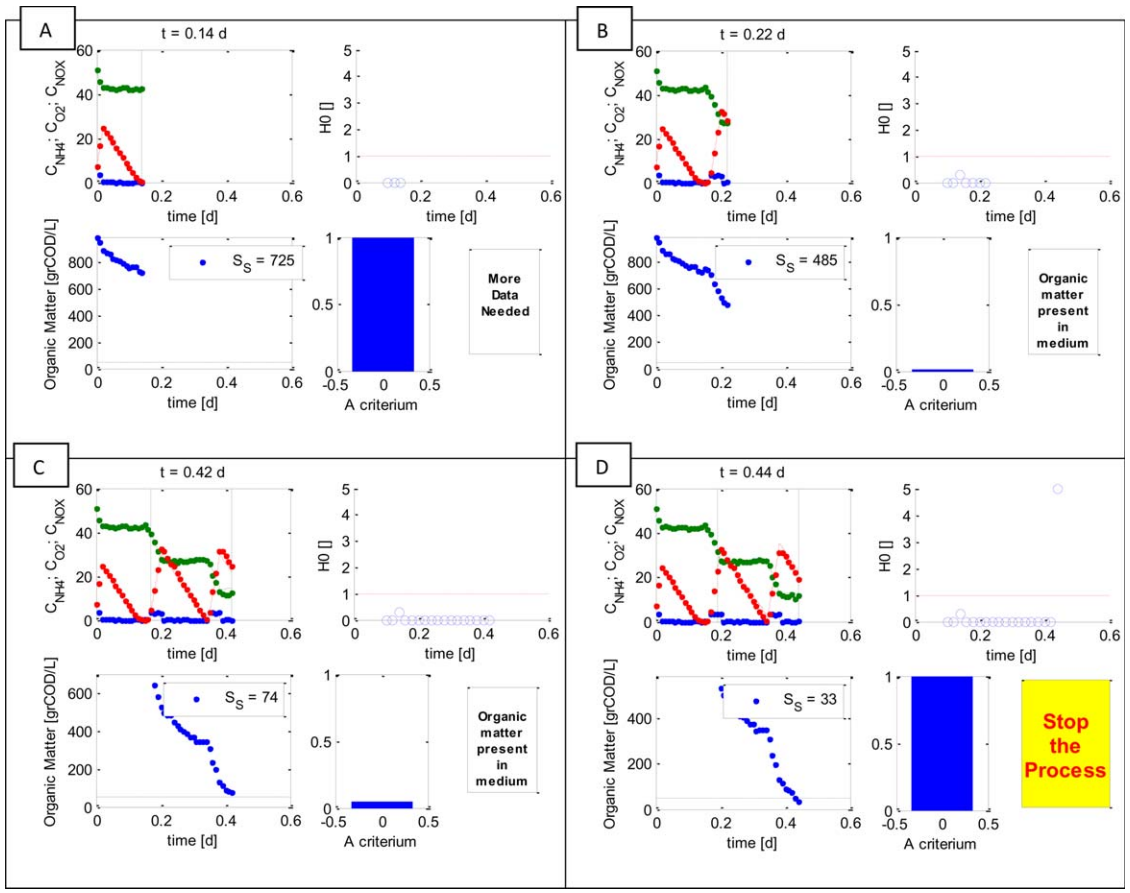

Figure 4. Detection of the organic matter depletion with initial concentration 1000 gCOD/L.

The four figures show the recognition process in one SBR cycle (starting from the top left A and ending in the bottom right figure D). A video of the recognition process is available in the supporting information, *aic14536-sup-0001-suppvideo.avi*.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

Table 4. Initial Conditions $x(t_0)$, Units Are Taken from Ref. 77

Variable	Short Description	Initial Value
S_O	Oxygen	7
S_S	Readily biodegradable substrate	1000
S_{NH}	Ammonium plus ammonia nitrogen	50
S_{NO2}	Nitrite	2
S_{NO3}	Nitrate	50
S_{N2}	Dinitrogen	0
S_{ALK}	Alkalinity	200
S_I	Inert solube organic material	0
X_I	Inert particulate organic material	0
X_H	Heterotrophic organisms	500
X_S	Slowly biodegradable substrates	0
X_{STO}	Cell internal storage product of heterotrophic organisms	400
X_{AOB}	Ammonium Oxidizing Bacteria	100
X_{NOB}	Nitrite Oxidizing Bacteria	100
X_{TSS}	Total suspended solids	0

should increase the reliability of the method. However, the program manages to detect depletion despite these complications. Using MER, it is possible to detect the appropriate point in time to either initiate COD feed or, in the case that all other restriction are fulfilled, stop the process.

Conclusions and Outlook

We have shown that MER is able to detect the depletion of organic matter in SBR systems. To obtain a proper recognition model, we reduced the extended ASM3 creating a more tractable model that is identifiable with common large-scale sensor technology (ammonia, dissolved oxygen, and nitroxides). By this, it is possible to distinguish two different dynamics: (1) heterotrophic bacteria using organic matter as main energy source and (2) heterotrophic bacteria consuming stored energy. This distinction allows a detection of the depletion of readily biodegradable organic matter by combining the recognition model with methods for analytical redundancy. The key element of MER is using the information that complex mechanistic models comprise to create reduced models specifically tailored to the recognition process. These recognition models should be tractable, even with low quality measurements and help us recognize particular changes in the dynamics of a system. As a result, we obtain a tool for event detection, based on mechanistic models that can be scaled up and transferred to similar processes. In other words, we obtain a FD method with first principle information embedded in it.

Further work is required to develop a general framework for building of recognition models. Still, with novel techniques for model reduction and data analysis methods, it should become possible to develop a more general approach in the near future.

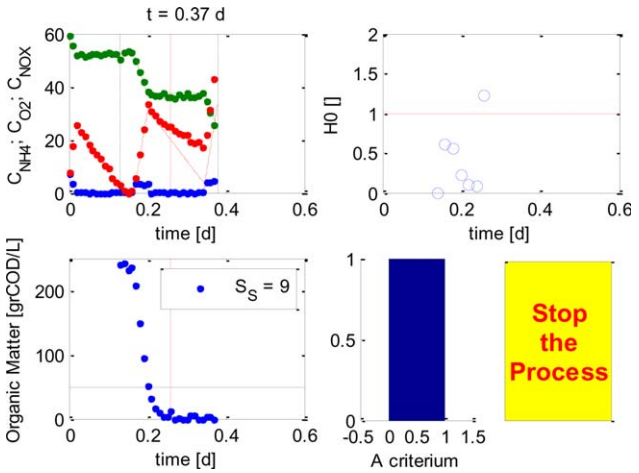

Figure 5. Detection of the organic matter depletion with initial concentration 500 gCOD/L.

[Color figure can be viewed in the online issue, which is available at wileyonlinelibrary.com.]

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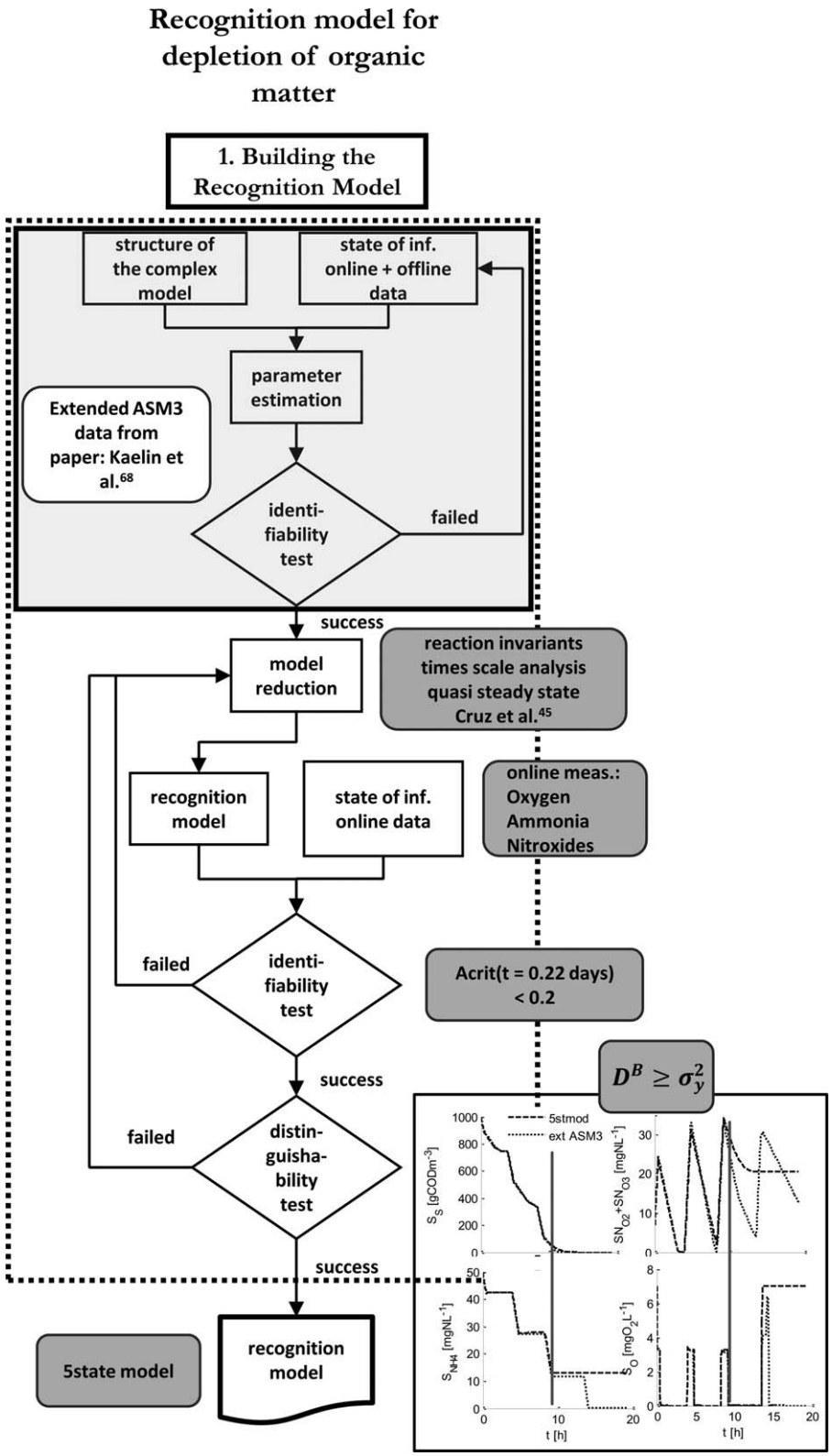
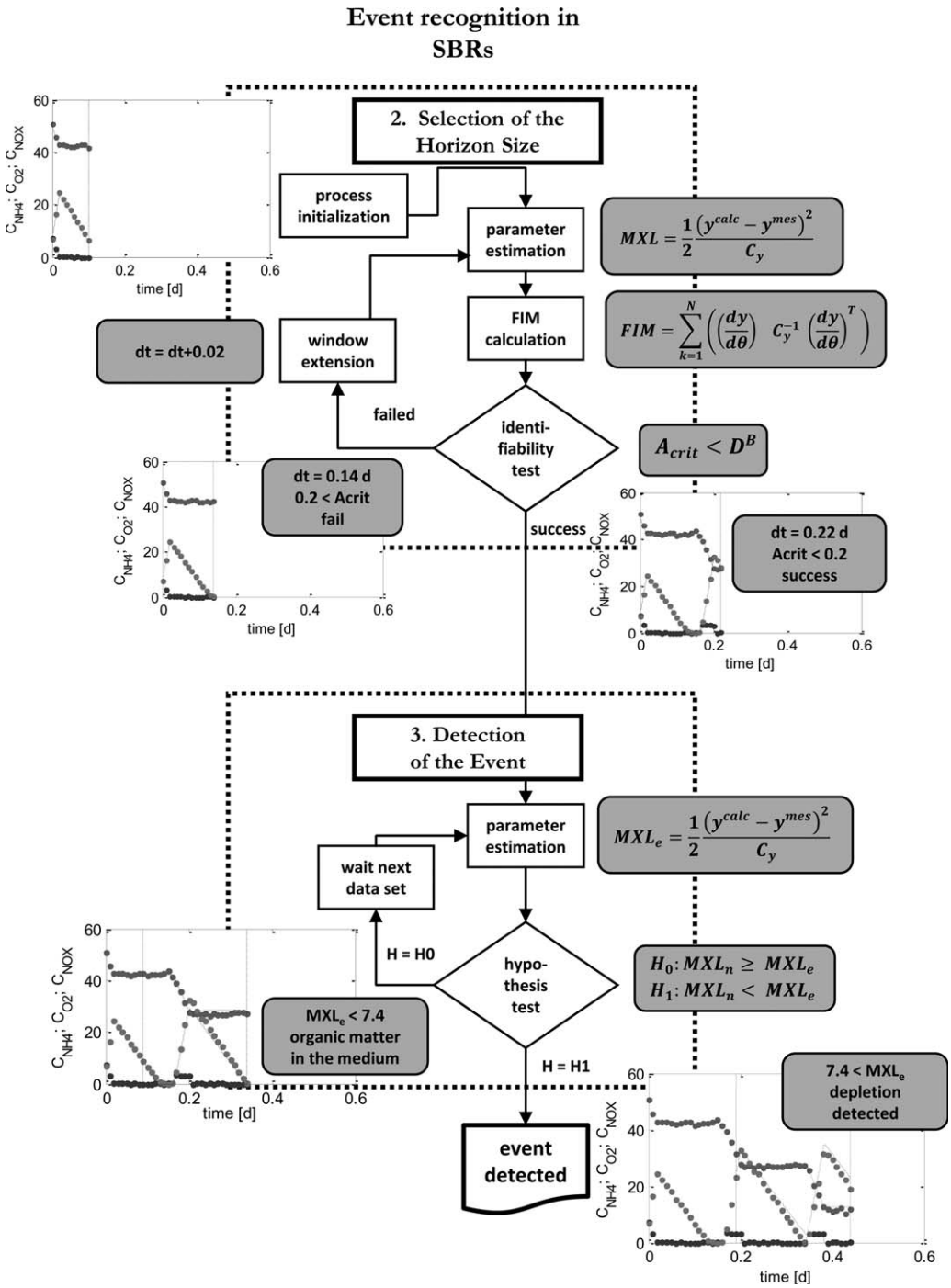
Appendix A

Recognition model for depletion of organic matter is given below.



Event recognition in SBRs is given below.



Appendix B : Five-State Model

Ordinary Differential Equations

$$\frac{dS_S}{dt} = \left(-\frac{1}{Y_{Haer}} \times r_{aae} - \frac{1}{Y_{Hanox}} \times (r_{aNO3} + r_{aNO2})\right) \times (1 + St_S) \quad \text{(B1)}$$

$$\frac{dS_O}{dt} = K_{La}(S_O^* - S_O) - \frac{1 - Y_{Haer}}{Y_{Haer}} r_{aae} - \left(\frac{3.43}{Y_{A1}} - 1\right) r_{aaNs} - \left(\frac{1.14}{Y_{A2}} - 1\right) r_{aaNb} \quad \text{(B2)}$$

$$\frac{dS_{NH4}}{dt} = -\left(-\frac{i_{NSS}}{Y_{Haer}} + i_{NB}\right) r_{aae} - \left(\frac{1}{Y_{A1}} + i_{NB}\right) r_{aaNs} - i_{NB}\, r_{aaNb} - \left(-\frac{i_{NSS}}{Y_{Hanox}} + i_{NB}\right) r_{aNO3} - \left(-\frac{i_{NSS}}{Y_{Hanox}} + i_{NB}\right) r_{aNO2} \quad \text{(B3)}$$

$$\frac{dS_{NO2}}{dt} = \frac{1}{Y_{A1}} r_{aaNs} - \frac{1}{Y_{A2}} r_{aaNb} + \frac{1 - Y_{Hanox}}{1.14 Y_{Hanox}} (r_{aNO3} - r_{aNO2}) \quad \text{(B4)}$$

$$\frac{dS_{NO3}}{dt} = \frac{1}{Y_{A3}} r_{aaNb} - \frac{1 - Y_{Hanox}}{1.14 Y_{Hanox}} r_{aNO3} \quad \text{(B5)}$$

Constant State Variables

$$\frac{dX_H}{dt} = 0 \quad \text{(B6)}$$

$$\frac{dX_{Ns}}{dt} = 0. \quad \text{(B7)}$$

$$\frac{dX_{Nb}}{dt} = 0 \quad \text{(B8)}$$

Algebraic Relation

$$0 = \left(C_{Sto} - \frac{S_S}{1 + St_S} \right) \times St_S - Sto \quad \text{(B9)}$$

Reaction Rates

$$r_{aae} = \mu_H \times \frac{S_S}{S_S + K_S} \times \frac{S_O}{S_O + K_{O1}} \times \frac{S_{NH4}}{S_{NH4} + K_{NH}} \times X_H \quad \text{(B10)}$$

$$r_{aaNs} = \mu_{A1} \times \frac{S_O}{S_O + K_O} \times \frac{S_{NH4}}{S_{NH4} + K_{NH}} \times X_{Ns} \quad \text{(B11)}$$

$$r_{aaNb} = \mu_{A2} \times \frac{S_{NO2}}{S_{NO2} + K_{NO21}} \times \frac{S_O}{S_O + K_O} \times \frac{S_{NH4}}{S_{NH4} + K_{NH}} \times X_{Nb} \quad \text{(B12)}$$

$$r_{aNO3} = \mu_{H1} \times \frac{S_S}{S_S + K_S} \times \frac{S_{NO3}}{S_{NO3} + K_{NO3}} \times \frac{K_{O21}}{K_{O21} + S_O} \times \frac{S_{NH4}}{S_{NH4} + K_{NH}} \times X_H \quad \text{(B13)}$$

$$r_{aNO2} = \mu_{H2} \times \frac{S_S}{S_S + K_S} \times \frac{S_{NO2}}{S_{NO2} + K_{NO2}} \times \frac{K_{O22}}{K_{O22} + S_O} \times \frac{S_{NH4}}{S_{NH4} + K_{NH}} \times X_H \quad \text{(B14)}$$

Parameter Values

SOStar	7	[mgO2/L]	Process
K_{La}	1000	[d-1]	Process
i_{NB}	0.086	[gN/gCOD]	Fitted
mou_H	0.6021	[d-1]	Fitted
mou_{A1}	0.6552	[d-1]	Fitted
mou_{A2}	0.3468	[d-1]	Fitted
Y_{Haer}	0.1302	[gCOD/gCOD]	Fitted
Y_{A1}	0.1327	[gCOD/gN]	Fitted
Y_{A2}	0.0985	[gCOD/gN]	Fitted
Y_{A3}	0.0331	[gCOD/gN]	Fitted
i_{NSS}	0.01	[gN/gCOD]	ASM3[81]
Y_{Hanox}	0.0632	[gCOD/gCOD]	Fitted
mou_{H1}	0.0511	[d-1]	Fitted
mou_{H2}	0.0362	[d-1]	Fitted
K_{NH1}	0.01	[mgCOD/L]	ASM3[81]
K_{NH2}	0.1	[mgCOD/L]	ASM3[81]
K_S	10	[mgCOD/L]	ASM3[81]
K_{S1}	0.1	[mgCOD/L]	ASM3[81]
K_{S2}	0.1	[mgCOD/L]	ASM3[81]
K_{NHH}	0.05	[mgN/L]	ASM3[81]
K_{O1}	0.2	[mgO2/L]	ASM3[81]
K_{NH}	0.1	[mgN/L]	ASM3[81]
K_O	0.8	[mgO2/L]	ASM3[81]
K_{NO21}	0.5	[mgO2/L]	ASM3[81]
K_{NO3}	0.5	[mgN/L]	ASM3[81]
K_{O21}	0.2	[mgO2/L]	ASM3[81]
K_{NO2}	0.25	[mgN/L]	ASM3[81]
K_{O22}	0.2	[mgO2/L]	ASM3[81]
st_S	1.7	[ ]	Fitted
st_O	0.08	[ ]	Fitted

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