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Active Fault Diagnosis for Stochastic Nonlinear Systems: Online Probabilistic Model Discrimination

Marc Martin-Casas * **Ali Mesbah** *

* *Department of Chemical and Biomolecular Engineering, University of California, Berkeley, CA 94720 USA. (mesbah@berkeley.edu)*

Abstract: Reliable and timely diagnosis of system faults under uncertainties is imperative for safe, reliable, and profitable operation of technical systems. This paper presents an input design method for active fault diagnosis for nonlinear systems that are subject to probabilistic model uncertainty and stochastic disturbances, and are under operational constraints. A computationally efficient sample-based method is presented for joint propagation of model uncertainty and stochastic disturbances using non-intrusive generalized polynomial chaos and unscented transformation. A tractable sample-based distance measure, inspired by the k-nearest neighbors algorithm, is used for fault diagnosis, which seeks to discriminate between probabilistic predictions of the model hypotheses for normal and faulty operation. Simulation results on a benchmark bioreactor case study demonstrate the effectiveness of the proposed input design method for reliable fault diagnosis under uncertainty through online model discrimination.

Keywords: Input design, joint propagation of probabilistic model uncertainty and stochastic disturbances, generalized polynomial chaos, unscented transformation.

1. INTRODUCTION

Fault detection and diagnosis is instrumental for reliable and profitable operation of technical systems to prevent safety hazards and economic losses (Nikoukhah, 1998). The majority of reported fault diagnosis methods are *passive*, that is, fault diagnosis is performed by comparing historical data with system measurements under nominal operation (Patton and Chen, 1997; Chiang et al., 2000; Ding, 2008; Campbell and Nikoukhah, 2015). However, system uncertainty due to incomplete knowledge of system dynamics, exogenous disturbances, and measurement noise, as well as the corrective action of feedback controllers, can impede reliable fault diagnosis by masking the effects of faults on system measurements (Blanke et al., 2006). These considerations have motivated the development of *active* fault diagnosis (AFD) methods, which use a set of model hypotheses for normal and faulty operation to design an optimal auxiliary input signal that enhances diagnosability of faults in the presence of system uncertainty (Blanke et al., 2006; Campbell and Nikoukhah, 2015).

Two of the key challenges in AFD for stochastic systems include: (i) efficient propagation of probabilistic uncertainty, particularly in the case of joint model uncertainty and disturbances, and (ii) derivation of tractable AFD criteria for reliable fault diagnosis. For stochastic linear systems, Zhang (1989) introduced a pioneering probabilistic AFD method. Blackmore and Williams (2006) presented a tractable AFD method for handling additive stochastic disturbances by minimizing an upper bound on the probability of model misdiagnosis. Zonotopes are used for guaranteed fault diagnosis for set-based uncertainties (Scott et al., 2016). AFD for nonlinear systems with probabilistic model uncertainty is addressed in (Mesbah et al., 2014), where generalized polynomial chaos (Xiu and Karniadakis, 2002) is used for uncertainty propagation. Paulson et al. (2017) developed an AFD method that minimizes a measure of the Bayes risk of fault misdiagnosis by simultaneously propagating stochastic disturbances and model uncertainty. A review of AFD methods can be found in (Heirung and Mesbah, 2018).

This paper presents a sample-based AFD formulation for nonlinear systems with probabilistic model uncertainty and stochastic disturbances. To this end, non-intrusive generalized polynomial chaos (gPC) is combined with unscented transformation (UT) (Wan and van der Merwe, 2000) using conditional probability rules to jointly propagate both sources of uncertainty. The proposed sample-based uncertainty propagation method, which draws from the benefits of gPC and UT for handling model uncertainty and disturbances, respectively, is particularly suitable for optimization, since it can approximate the statistics of system variables with a fairly small number of samples that are chosen systematically. Inspired by the k-nearest neighbors scheme, classically used for data clustering (Fix and Hodges, 1951; Cover and Hart, 1967), the AFD criterion is defined in terms of a sample-based measure of distance between probabilistic predictions of model hypotheses for the normal and faulty system operation. The AFD criterion does not require the generation of histograms and thus circumvents the need for histogram binning, the accuracy of which is subject to the heuristic choice of bin number. The performance of the proposed AFD method is demonstrated on a continuous bioreactor case study for online diagnosis of multiple operation scenarios.

2. PROBLEM STATEMENT

Consider a continuous-time, nonlinear system described by

$$M : \begin{cases} \dot{\boldsymbol{x}}(t) = \mathbf{f}(\boldsymbol{x}(t), \boldsymbol{\theta}, \boldsymbol{u}(t), \boldsymbol{w}(t)), \\ \boldsymbol{y}(t) = \mathbf{h}(\boldsymbol{x}(t), \boldsymbol{\theta}, \boldsymbol{v}(t)), \end{cases} \quad (1)$$

where t is time; $\boldsymbol{x} \in \mathbb{R}^{n_x}$ is the states with initial conditions $\boldsymbol{x_o}$; $\boldsymbol{u} \in \mathbb{R}^{n_u}$ is the inputs; $\boldsymbol{y} \in \mathbb{R}^{n_y}$ is the measurable outputs; $\boldsymbol{w} \in \mathbb{R}^{n_w}$ is the time-varying system disturbances; $\boldsymbol{\theta} \in \mathbb{R}^{n_\theta}$ is the time-invariant model parameters; and the nonlinear functions $\mathbf{f}$ and $\mathbf{h}$ describe the system dynamics. The system model (1) is uncertain due to inadequate knowledge of parameters θ and initial conditions x_0, described by the distributions $P(\theta)$ and $P(x_0)$, respectively. The probabilistic model uncertainty is denoted by $\boldsymbol{\Theta} = [\boldsymbol{\theta}^\top \boldsymbol{x_o}^\top]^\top$, which can be expressed in terms of standard random variables $\xi \in \mathbb{R}^{n_\xi}$, with $n_\xi \leq n_\theta + n_x$ (i.e., $\boldsymbol{\Theta}(\xi)$).

The system is subject to input constraints $\boldsymbol{u}(t) \in \mathcal{U} \subseteq \mathbb{R}^n_u$, as well as state constraints $\boldsymbol{x}(t) \in \mathcal{X} \subseteq \mathbb{R}^n_x$ that are enforced as the chance constraint

$$\mathbb{P}(\boldsymbol{x}(t) \leq \mathcal{X}) \geq \alpha \quad (2)$$

due to the probabilistic evolution of states. In (2), α is the permitted probability of state constraint violation. When all uncertainties in (1) are bounded and α is set to 1, the state constraints can be enforced as hard constraints for all uncertainty realizations.

Let there be a given number of model hypotheses of form (1) to describe the system dynamics under nominal and faulty operation, i.e., $\mathcal{M} = \{M_0, M_1, \ldots, M_{n_m}\}$, where the subscripts indicate the model number. The nominal system operation is denoted by model M_0, while the faulty scenarios are denoted by $\{M_i\}_{i=1}^{n_m}$. All models $M_i \in \mathcal{M}$ are assumed to have the same inputs $\boldsymbol{u}$ and outputs $\boldsymbol{y}$. This paper presents a method for active fault diagnosis of the stochastic nonlinear system (1) through designing the input $\boldsymbol{u}$. The AFD problem is stated as follows.

Problem 1 (Active fault diagnosis). For the fault diagnosis horizon $t \in [0, T]$, design an input profile $\boldsymbol{u}(t)$ such that the predicted distributions of the model outputs are separated at least at one measurement time instant while the input constraints $\boldsymbol{u}(t) \in \mathcal{U}$ and state chance constraints (2) are satisfied over the diagnosis horizon $[0, T]$ for all $M_i \in \mathcal{M}$.

The designed input profile is applied to the system to compare the system measurements with the predictions of the competing models (i.e., nominal and faulty). This enables invalidating the model hypotheses that cannot describe the system behavior adequately. Note that AFD is commonly performed in an *open-loop* setting, where the input profile is designed offline and then applied to the system. Alternatively, the input profile can be designed *online* through recursive solution of the AFD problem in a receding-horizon manner. This allows for (partly) counteracting the effects of unmodeled system uncertainties and disturbances (Paulson et al., 2017).

The challenges of solving Problem 1 in light of the probabilistic model uncertainty and stochastic disturbances are two-fold. The first challenge stems from *joint* propagation of model uncertainty $\boldsymbol{\Theta}$ and stochastic disturbances $\boldsymbol{w}(t)$ through the nonlinear system models. The second challenge arises from deriving a tractable measure that quantifies dissimilarity between the probabilistic model predictions.[1] In this work, the first challenge is addressed by proposing a sample-based propagation method based on non-intrusive gPC and UT, which are respectively suitable for the propagation of time-invariant uncertainties and time-varying stochasticity in (1) (Section 3). To alleviate the need to approximate the full distribution of model outputs (Martin-Casas and Mesbah, 2016), or evaluate their statistical moments (Paulson et al., 2017), the model discrimination criterion in the AFD problem is defined in terms of the distance between the k closest samples of the outputs predicted by the different model hypotheses. This choice of the model discrimination criterion significantly simplifies the formulation of the input design problem. The proposed uncertainty propagation method and model discrimination criterion are used to derive a computationally tractable surrogate for Problem 1, which is amenable to online solution (Section 4).

3. PROPAGATION OF MODEL UNCERTAINTY AND STOCHASTIC DISTURBANCES

The most widely-used uncertainty propagation methods typically consider one source of uncertainty: either the time-invariant uncertainty in $\boldsymbol{\Theta}$ (Nagy and Braatz, 2007), or time-varying stochastic disturbances $\boldsymbol{w}(t)$ (Darlington et al., 2000; Wan and van der Merwe, 2000; Caflisch, 1998). We present an efficient uncertainty propagation method that considers both sources of uncertainty in (1). The key notion of the proposed method is to decouple the propagation of probabilistic uncertainty in the model parameters and initial conditions from the propagation of stochastic disturbances using conditional probability rules, so that different methods that are best-suited for handling each uncertainty source can be adopted. To this end, UT (Wan and van der Merwe, 2000) is used for propagation of stochastic disturbances conditioned on a realization of model uncertainty $\boldsymbol{\Theta}$, which is then integrated over different realizations of model uncertainty using non-intrusive gPC (Xiu and Karniadakis, 2002). This results in a sample-based method for joint propagation of stochastic disturbances and model uncertainty, as described below.

3.1 Unscented transformation for propagation of stochastic disturbances conditioned on model uncertainty

Unscented transformation, originally developed for nonlinear state estimation, is a heuristic-based method for propagation of samples of time-varying stochastic uncertainty through nonlinear dynamics (Wan and van der Merwe, 2000). The UT method can effectively deal with nonlinearities, as it does not require linearization of the nonlinear system equations and thus computation of Jacobian. The UT method consists in the propagation of a relatively small number of deterministically-chosen samples (known as *sigma points*), centered around the mean of states, through the system dynamics. In this work,

[1] Another computational challenge in solving Problem 1 arises from the state chance constraint (2), which is computationally intractable in general (Calafiore and El Ghaoui, 2006; Nemirovski and Shapiro, 2006). Chance constraint approximation is not addressed here.

the UT method is used for the propagation of stochastic disturbances $w(t)$ in (1) given a realization of the model uncertainty $\boldsymbol{\Theta}(\xi)$.

Denote the sigma points conditioned on a given realization of model uncertainty by $\mathcal{S}(t;\xi)$. Let $m(t;\xi)$ and $V(t;\xi)$ be the mean and covariance of the states conditioned on a realization of the standard random variables ξ. A set of $2n+1$ sigma points $\{\mathcal{S}_i(t;\xi)\}_{i=0}^{2n}$ is defined as

$$\mathcal{S}_0(t;\xi) = m(t;\xi),$$
$$\mathcal{S}_i(t;\xi) = m(t;\xi) + \big(\sqrt{(n+\lambda)V(t;\xi)}\big)_i, \quad i = 1,\dots,n,$$
$$\mathcal{S}_i(t;\xi) = m(t;\xi) - \big(\sqrt{(n+\lambda)V(t;\xi)}\big)_i, \quad i = n+1,\dots,2n,$$

where $n = n_x + n_w$; $(A)_i$ is the ith column of matrix A; and λ is a scaling parameter. The sigma points $\{\mathcal{S}_i(t;\xi)\}_{i=0}^{2n}$ are propagated through the nonlinear system dynamics (1) to obtain the propagated points $\{\mathcal{P}_i(t;\xi)\}_{i=0}^{2n}$ that characterize the distribution of the states, conditioned on ξ, in terms of the mean and covariance

$$m_{\mathcal{P}}(t;\xi) \approx \sum_{i=0}^{2n} W_i^m \mathcal{P}_i(t;\xi),$$
$$V_{\mathcal{P}}(t;\xi) \approx \sum_{i=0}^{2n} W_i^c \big(\mathcal{P}_i(t;\xi) - m_{\mathcal{P}}(t;\xi)\big)\big(\mathcal{P}_i(t;\xi) - m_{\mathcal{P}}(t;\xi)\big).$$

The mean weights $\{W_i^m\}_{i=0}^{2n}$ and covariance weights $\{W_i^c\}_{i=0}^{2n}$ are defined as

$$W_0^m = \frac{\lambda}{n+\lambda},$$
$$W_0^c = \frac{\lambda}{n+\lambda} + (1-\alpha^2+\beta),$$
$$W_i^m = W_i^c = \frac{1}{2(n+\lambda)}, \quad i = 1,\dots,2n,$$

where α determines the spread of sigma points around the mean and β accounts for prior knowledge of the state distribution (Wan and van der Merwe, 2000).

The computational complexity of the UT method scales linearly with the dimension of the stochastic disturbances n_w, as UT relies on $2n+1$ function evaluations; that is, one function evaluation per sigma point. This can result in considerable computational speed-up in comparison with Monte Carlo-based sampling methods (Caflisch, 1998).

3.2 Non-intrusive polynomial chaos for propagation of model uncertainty of sigma points

Disturbance propagation based on UT yields the (propagated) sigma points $\{\mathcal{P}_i(t;\xi)\}_{i=0}^{2n}$ that are conditioned on model uncertainty. We now employ gPC to integrate the sigma points over the probabilistic model uncertainty $\boldsymbol{\Theta}(\xi)$. gPC consists in approximating a stochastic variable, the sigma points $\mathcal{P}_i$, with the truncated expansion

$$\mathcal{P}_i(t;\xi) \approx \sum_{k=0}^{L} \tilde{\mathcal{P}}_{i,k}(t)\Phi_k(\xi), \tag{3}$$

where $\tilde{\mathcal{P}}_{i,k}$ denotes the expansion coefficients of sigma point $\mathcal{P}_i$, which evolve as a function of system dynamics; and Φ_k denotes multivariate polynomial basis functions constructed from the univariate polynomial basis functions of the individual random variables ξ_j

$$\Phi_k(\xi) = \prod_{j=1}^{m} \phi^{(j)}_{\alpha_j^{(i)}}(\xi_j), \quad \alpha_j^{(i)} \in \{0,1,\dots\}, \ \forall j = \{1,\dots,m\},$$

with $\alpha_j^{(i)}$ being the jth element of a multi-index whose value corresponds to the order of the basis of the jth random variable in the ith multivariate polynomial basis. The univariate polynomials ϕ belong to the Askey-Wiener scheme of polynomials, so that each univariate polynomial has an optimal convergence rate with respect to ξ_j (Xiu and Karniadakis, 2002). The truncation order in the gPC expansion (3) is defined by $L+1 = \frac{(n_\xi+m)}{m!n_\xi!}$, where m denotes the prespecified degree of the multivariate polynomial basis and n_ξ denotes the dimension of $\boldsymbol{\Theta}(\xi)$. An important property of the polynomial basis functions in the Askey-Wiener scheme, key to the computational efficiency of gPC, is their orthogonality with respect to the multivariate distribution of ξ. Note that the polynomials $\Phi_k(\xi)$ are constructed only once, merely based on the known distribution of $\boldsymbol{\Theta}(\xi)$.

Evaluation of the gPC expansions for each of the $2n+1$ sigma points requires computation of the coefficients $\tilde{\mathcal{P}}_{i,k}$ in (3), which can be done using intrusive or non-intrusive methods (Kim et al., 2013). In this work, we adopt the non-intrusive method, which hinges on evaluating the system model at given samples of model uncertainty $\{\boldsymbol{\Theta}(\xi^{(i)})\}_{j=1}^{n_s}$. This enables estimating the gPC coefficients as a weighted sum of the samples $\{\mathcal{P}_i^{(j)}(t,\xi^{(j)})\}_{j=1}^{n_s}$

$$\begin{bmatrix} \tilde{\mathcal{P}}_{i,0}(t) \\ \vdots \\ \tilde{\mathcal{P}}_{i,L}(t) \end{bmatrix} = \begin{bmatrix} \Pi_{0,1},\dots,\Pi_{0,n_s} \\ \vdots \quad \ddots \quad \vdots \\ \Pi_{L,1},\dots,\Pi_{L,n_s} \end{bmatrix} \begin{bmatrix} \mathcal{P}_i^{(1)}(t;\xi^{(1)}) \\ \vdots \\ \mathcal{P}_i^{(n_s)}(t;\xi^{(n_s)}) \end{bmatrix}, \tag{4}$$

where the weights $\Pi_{k,j}$ describe the effect of the sigma point samples $\{\mathcal{P}_i^{(j)}\}_{j=1}^{n_s}$ on the expansion coefficients $\tilde{\mathcal{P}}_{i,k}$ for $k = 0,...,L$. Note that the sigma point samples are simply determined by evaluating the sigma points $\{\mathcal{P}_i(t;\xi)\}_{i=0}^{2n}$ for the uncertainty realizations $\{\xi^{(j)}\}_{j=1}^{n_s}$. The non-intrusive method can be used irrespective of the form and complexity of the nonlinear model equations.

In this work, the weight matrix in (4) is defined in terms of least-squares estimation of the expansion coefficients

$$\boldsymbol{\Pi} = (\Lambda^\top\Lambda)^{-1}\Lambda^\top,$$

with Λ given by (see Paulson and Mesbah (2017))

$$\Lambda = \begin{bmatrix} \Phi_0(\xi^{(1)}) & \Phi_1(\xi^{(1)}) & \cdots & \Phi_L(\xi^{(1)}) \\ \Phi_0(\xi^{(2)}) & \Phi_1(\xi^{(2)}) & \cdots & \Phi_L(\xi^{(2)}) \\ \vdots & \vdots & \cdots & \vdots \\ \Phi_0(\xi^{(n_s)}) & \Phi_1(\xi^{(n_s)}) & \cdots & \Phi_L(\xi^{(n_s)}) \end{bmatrix}.$$

The model uncertainty sample set $\{\xi^{(j)}\}_{j=1}^{n_s}$ can be selected as the roots of the polynomial basis of one degree higher $(m+1)$, so that the number of uncertainty samples is $n_s = \frac{(n_\xi+m+1)!}{n_\xi!(m+1)!}$. Due to the optimal choice of the polynomials in (3) with respect to the multivariate distribution of ξ, non-intrusive gPC requires a relatively small number of samples to propagate the model uncertainty $\boldsymbol{\Theta}$.

3.3 Joint propagation of model uncertainty and disturbances

Joint propagation of the probabilistic model uncertainty and stochastic disturbances entails expressing each one of the $2n+1$ sigma points $\{\mathcal{P}_i(t;\xi)\}_{i=0}^{2n}$ as the gPC expansion (3). Evaluating the coefficients $\widetilde{\mathcal{P}}_{i,k}(t)$ using the non-intrusive method in (4) requires computing the conditional sigma points $\{\mathcal{P}_i(t;\xi)\}_{i=0}^{2n}$ at n_s samples of the model uncertainty, i.e., $\{\xi^{(j)}\}_{j=1}^{n_s}$. Thus, the proposed sample-based uncertainty propagation method uses a total of $n_{\text{tot}} = (2n+1)\times n_s$ samples for the joint propagation of probabilistic model uncertainty and stochastic disturbances, yielding the *total sigma points* $\{\mathsf{P}_s(t)\}_{s=1}^{n_{\text{tot}}} = \{\mathcal{P}_i(t;\{\xi^{(j)}\}_{j=1}^{n_s})\}_{i=0}^{2n}$.

4. TRACTABLE FORMULATION FOR ACTIVE FAULT DIAGNOSIS

We now present a tractable criterion for AFD that readily uses the total sigma points $\{\mathsf{P}_s(t)\}_{s=1}^{n_{\text{tot}}}$, alleviating the need to either construct the distribution of the model outputs, or evaluate their statistical moments. To enable probabilistic model discrimination, the AFD criterion is defined as a measure of the distance between the sigma points belonging to the competing model hypotheses in the model set $\mathcal{M}$. The distance measure used here is inspired by the k-nearest neighbors (KNN) algorithm (Cover and Hart, 1967), which computes the distance between the sigma points of a model M_i to the k closest sigma points of other models in $\mathcal{M}$. Maximization of the kNN distance between the sigma points of the model hypotheses in $\mathcal{M}$ will lead to separation of the output distributions, thus enhancing fault diagnosability.

Let $\{\mathsf{P}_i^{(l)}(t)\}_{i=1}^{n_{\text{tot}}}$ and $\{\mathsf{P}_j^{(o)}(t)\}_{j=1}^{n_{\text{tot}}}$ denote the total sigma points corresponding to the model hypotheses M_l and M_o, respectively. The L_2 distance between each sigma point of M_l to every sigma point of M_o is computed, and the indices of the k closest sigma points of M_o to each sigma point of model M_l are stored. After iterating over all points of model M_l, a total of $t_s = kn_{\text{tot}}$ pairs of sigma points are obtained. Let $\{(p_1,q_1),...,(p_{t_s},q_{t_s})\}$ denote the stacked indices of the k closest sigma points of model M_o to each sigma point of model M_l. The kNN measure of probabilistic discrimination between the two models is defined as

$$d^{(l,o)}(t) = \sum_{(p=p_1,q=q_1)}^{(p_{t_s},q_{t_s})} \left(\|\mathsf{P}_p^{(l)}(t) - \mathsf{P}_q^{(o)}(t)\|_2 \right),$$

which quantifies the distance between t_s pairs of sigma points predicted by models M_l and M_o. For the multiple model hypotheses in the model set $\mathcal{M}$, the AFD criterion can now be defined as

$$J = \sum_{l=0}^{n_m} \sum_{o=0,l\neq o}^{n_m} w_{l,o} d^{(l,o)}(t), \tag{5}$$

where the weights $w_{l,o}$ are user-specified. For example, $w_{m,n} = (\frac{1}{n_m})$ when uniform weights are used for discrimination between all models. The AFD criterion (5) allows for handling multiple model hypotheses and tuning the importance of probabilistic discrimination between different model-hypothesis pairs. The tractable surrogate problem for the AFD Problem 1 can now be formulated as follows.

Problem 2 (Tractable AFD). For the fault diagnosis horizon $t \in [0,T]$ and the (possibly uncertain) initial states $\boldsymbol{x_o}$, the active fault diagnosis for the stochastic nonlinear system described by (1) with model hypotheses $\mathcal{M}$ involves solving the nonlinear optimization problem

$$\max_{u(t)} \; J$$

subject to the propagation of the total sigma points $\{\mathsf{P}_i^{(l)}(t)\}_{i=1}^{n_{\text{tot}}}$ for all model hypotheses $l = 0,1,\ldots,n_m$ in $\mathcal{M}$, the input constraints $u(t) \in \mathcal{U}$, and an approximation of the chance constraint $\mathbb{P}(\boldsymbol{x}(t) \leq \mathcal{X}) \geq \alpha$.

Remark 1. The tractable AFD Problem 2 can be solved online using system measurements obtained at every sampling point to account for the effects of unmodeled system uncertainties. This requires recursive estimation of the initial states as well as the model probabilities for all model hypotheses in $\mathcal{M}$ at every sampling point via Bayesian estimation (Paulson et al., 2017).

5. CASE STUDY

The proposed AFD method is demonstrated on a bioreactor (Henson and Seborg, 1992). Assuming constant reaction volume, the system dynamics are described by

$$dX = (-DX + \mu X)\,dt + \sigma_X dw_X(t), \tag{6a}$$

$$dS = \left(D(S_f - S) - \frac{1}{Y_{X/S}}\mu X \right) dt + \sigma_S dw_S(t), \tag{6b}$$

$$dP = (-DP + (\alpha\mu + \beta)X)\,dt + \sigma_P dw_P(t), \tag{6c}$$

where X, S, and P are the concentration of biomass, substrate, and product, respectively; D is the dilution rate, which is the only process input; S_f is the substrate concentration in the inlet feed; $\frac{1}{Y_{X/S}}$ is the yield of biomass per unit substrate consumed; α and β are yield parameters; and w_X, w_S, and w_P are independent, zero-mean Wiener processes scaled by standard deviations σ_X, σ_S, and σ_P, respectively. μ is the rate of biomass growth as a function of the substrate concentration

$$\mu = \frac{\mu_{\max} S}{K_M + S}, \tag{7}$$

where $\mu_{\max}$ is the maximum growth rate and K_M is an affinity constant. The initial conditions of (6) and the model parameters are taken from Henson and Seborg (1992). $\mu_{\max}$ is the only uncertain model parameter, which is described by a Gaussian distribution with mean 0.6 h^{-1} and variance 0.05.

Three scenarios for process operation are considered. The nominal process operation is described by (6). The two process fault scenarios include: (i) substrate inhibition in which the biomass growth and hence product yield are hampered by excess concentrations of substrate, and (ii) a decrease in 20% in the substrate in the inlet feed ($S_f = 0.8S_f$). In the substrate inhibition case, the biomass growth rate μ takes the form

$$\mu = \frac{\mu_{\max} S}{K_M + S\left(1 + \frac{S}{K_I}\right)}, \tag{8}$$

where K_I is the affinity constant specifying the extent of growth inhibition; set to 1 g/L here.

The performance of the AFD method is benchmarked against a deterministic AFD method that merely mini-

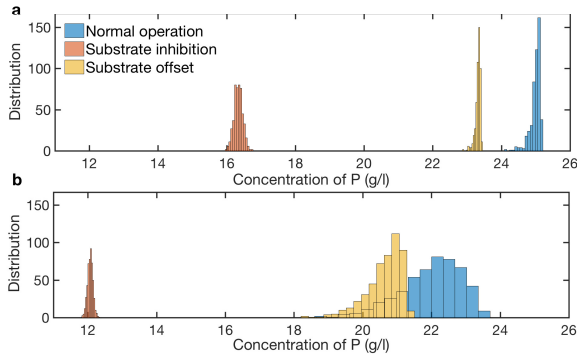

Fig. 1. Predicted distributions of product concentration at time 2 h obtained using the input designed by (a) the proposed AFD method and (b) the deterministic AFD method (based on 500 Monte Carlo runs).

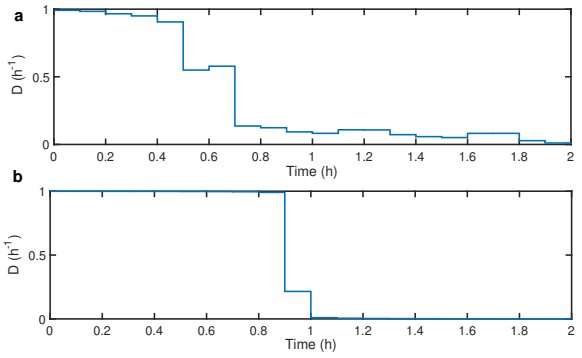

Fig. 2. Input profiles designed by (a) the proposed AFD method and (b) the deterministic AFD method.

mizes the L_2-norm between the mean of the model outputs. Fig. 1 shows the distributions of the product concentration at time 2 h predicted by the three process models under the input profiles designed by the proposed AFD and the deterministic AFD methods. The distributions are constructed based on 500 Monte Carlo runs using the designed input profiles. As can be seen, the proposed AFD method enables discriminating between the three model hypotheses more effectively. This is because the AFD method can reduce the variance of the outputs, which can in turn reduce the overlap between the outputs of the competing models in the presence of process uncertainties. On the other hand, even though deterministic AFD can increase the absolute distance between the means of the output distributions, it cannot effectively reduce the overlap between the distributions to enhance fault diagnosability. The optimal input profiles designed by both AFD methods are shown in Fig. 2. The input designed by the proposed method maintains near maximal dilution rate until approximately 0.5 h, after which it gradually decreases until reaching zero dilution rate at the end of the diagnosis horizon. The input designed via deterministic AFD, on the other hand, maintains maximum dilution rate until it is abruptly decreased to near zero values at around time 1 h. Fig. 2 suggests that deterministic AFD results in more process stimulation, while the fault diagnosis is less effective due to the overlap of the output distributions.

Inspired by industrial practice, the proposed AFD method is implemented in an online setting in which the AFD Problem 2 is solved repeatedly every 6 min when the product concentration is measured (see Paulson et al. (2017) for the online AFD algorithm). The results of online AFD are shown in Fig. 3. The process is initially at steady state. At time 2 h, a fault in the concentration of substrate in the inlet feed becomes active. The fault results in deviation of the product concentration from its desired setpoint ($P = 27$ g/l). At time 4 h, online AFD is initiated for a period of approximately 2 h. As can be seen, the probability of detecting the *active* model increases dramatically during this period until reaching a probability of approximately 1. When the correct scenario of process operation is diagnosed at time 6 h, the process input is adjusted based on the diagnosed operational scenario, which is different from the nominal process input (Fig. 3d). The adjusted process input enables recovering the product concentration to its desired setpoint (Fig. 3a). If the fault remained undiagnosed and the nominal process input continued to be applied, the concentration of product (dashed line in Fig. 3a) would continue to deviate from the desired setpoint. The results of this case study clearly demonstrate the significance of online AFD for effective process operation in the event of faults.

6. CONCLUSIONS

A tractable formulation for active fault diagnosis that can handle probabilistic model uncertainty and stochastic disturbances is presented. A sample-based uncertainty propagation method is proposed for joint propagation of time-invariant model uncertainty and time-varying disturbances using non-intrusive generalized polynomial chaos and unscented transformation. For probabilistic discrimination between multiple model hypotheses, the fault diagnosis criterion is defined in terms of the samples of the model outputs, preventing the need to build output distributions, or compute their statistical moments. The computational efficiency of the proposed active fault diagnosis method enables its online implementation to mitigate the effects of unmodeled system uncertainties on reliable fault diagnosis.

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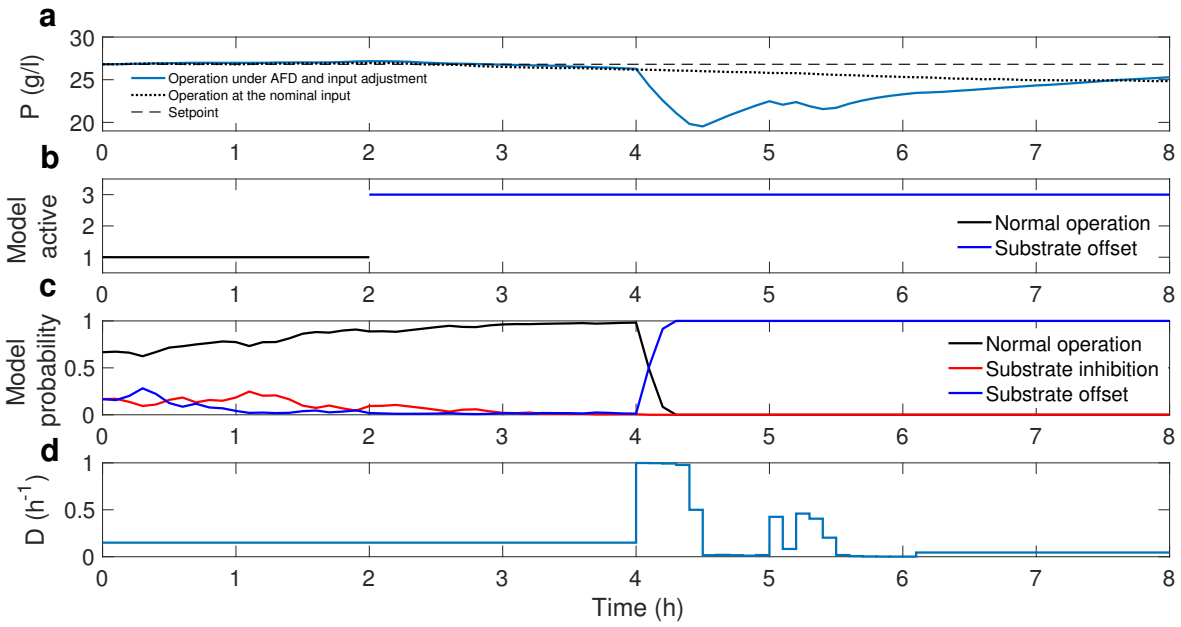

Fig. 3. Online active fault diagnosis. Different segments of time correspond to different operation stages: 0 to 2 h is normal operation, 2 to 4 h is the fault detection period during which the product concentration starts to deviate from its setpoint; 4 to 6 h is the period during which online AFD is performed, and 6 to 8 h is the process recovery stage to return to the desired steady-state operation. The plots show (a) the product concentration in the AFD run with subsequent adjustment of the dilution rate (solid line) and the product concentration under the nominal dilution rate (dashed line), (b) the active process model over time, (c) the probabilities of each model estimated via Bayesian recursion (see Paulson et al. (2017)), and (d) the dilution rate.

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