Computers and Chemical Engineering 000 (2018) 1–10

Contents lists available at ScienceDirect

Computers and Chemical Engineering

journal homepage: www.elsevier.com/locate/compchemeng

An efficient polynomial chaos expansion strategy for active fault identification of chemical processes

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ARTICLE INFO

Article history:
Received 21 January 2018
Revised 1 July 2018
Accepted 14 August 2018
Available online xxx

Keywords:
Active fault detection and isolation
Robust process design
Dynamic optimization
Least angle regression
Polynomial chaos expansion

ABSTRACT

This paper is concerned with a highly efficient active fault detection and isolation (FDI) framework. An auxiliary, fault-revealing input is derived by solving an optimization problem. As we implement a model-based approach, the active FDI framework is robustified against model parameter uncertainties, including parameter correlations which are common for experimentally derived parameters. Moreover, critical safety limits are considered, and an optimal process performance is fulfilled in parallel. In this work, which is an extension to our ESCAPE-2017 contribution, a novel highly effective polynomial chaos expansion (PCE) approach is used to address parameter uncertainties and to include process design parameters directly. To reduce the computational load, we combined the PCE with a least angle regression (LAR) strategy. The overall effectiveness of the novel one-shot sparse polynomial chaos expansion (OS^2-PCE) concept is demonstrated by analyzing a tubular plug flow reactor illustrating the need for uncertainty and parameter correlation analysis in FDI while ensuring an optimal and safe process operation, respectively.

1. Introduction

Chemical processes have to be operated efficiently and monitored reliability to meet the standard of a profitable and growing industry. In the literature mathematical models have been proven beneficial for computer-aided process design, process control, and condition-monitoring (Downs and Vogel, 1993; Kameswaran and Biegler, 2006; Venkatasubramanian et al., 2003). In this work, the focus is on condition monitoring primarily, as well as optimal process performance. For an improved detection and isolation of faults, mathematical models are used to calculate axillary control inputs to stimulate the monitored process deliberately. To provide reliable inferences, mathematical imperfections caused by model simplifications and uncertain model parameters have to be considered (Braatz et al., 1996; Pistikopoulos, 1995; Schenkendorf, 2016). A model imperfection study, in turn, requires advanced methods in uncertainty quantification at manageable computational costs (Telen et al., 2014a). Uncertain model parameters result in model output variations, and thus, model-based inferences can be suboptimal or even misleading (Schuëller and Jensen, 2008) when they are not part of the model-based process design. In addition, parameter correlations are a relevant factor in model output variations (Haaker and Verheijen, 2004) but are frequently ignored in model-based fault identification and process design concepts. For most chemical engineering problems, model parameters cannot be measured directly. Instead, numerical parameter identification routines processing experimental data have to be applied. Parameter identification routines, in turn, may lead to significant parameter correlations of the parameter estimates (Telen et al., 2014b). The state-of-the-art tools for uncertainty propagation, e.g., Monte Carlo simulations or Gaussian quadrature approaches, are prohibitive for complex problems in terms of computational costs (Smith, 2013). On the other side, CPU-friendly implementations based on linearization suffer in terms of precision and credibility, and they typically ignore parameter correlations (Telen et al., 2015). In this context, polynomial chaos expansion (PCE) provides a promising alternative: low computational costs, good approximation results, and a straightforward option to include relevant parameter correlations. The fundamental idea is to replace the original but CPU-intensive model with a PCE surrogate model that – once derived – is light in computational costs (Xiu and Karniadakis, 2002). Please note that different approaches of surrogate modeling (e.g., Kriging and nonlinear regression models) can be applied to lower the computational cost in optimization (Bhosekar and Ierapetritou, 2018). In case of uncertainties, however, PCE models have proven beneficial

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https://doi.org/10.1016/j.compchemeng.2018.08.022
0098-1354/

regarding convergence according to the Cameron-Martin theorem (Cameron and Martin, 1947). To set up a PCE model, several reference simulations of the original model are required to generate a sufficient number of training data sets. Moreover, the process operating conditions are fixed, and the PCE model is valid only under these conditions. When it comes to active fault identification, the operating conditions are changed deliberately to reveal potential faults as quickly as possible (Du et al., 2015). New operating conditions, in turn, imply that for every new scenario the PCE model has to be re-calibrated with costly reference simulations; i.e., new simulated training data sets have to be created. To overcome the need for new reference simulations, it is essential to include the auxiliary control parameters directly in the PCE model. Here, a promising idea is to treat the auxiliary control parameters as uniformly distributed random variables and to integrate auxiliary control parameters in the PCE model (Shen and Braatz, 2016). The so-called one-shot approach, however, is likely to suffer the curse of dimensionality. When model parameters and process design parameters are considered at the same time, the complexity of the PCE model and the number of required reference simulations increase dramatically. The main contribution of this work is to demonstrate how the total number of CPU-intensive reference simulations can be reduced considerably for a highly efficient active FDI implementation. To keep the computational cost tractable, we use the sparsity effect. In detail, we implement the least angle regression (LAR) approach (Blatman and Sudret, 2011) to obtain a workable PCE model, which represents the impact of the model parameters and fault-revealing auxiliary control parameters in equal measure. The scheme of the proposed work flow is illustrated in Fig. 1. Moreover, the flexibility of the proposed concept enables a direct integration of model parameter correlations which are typically ignored by most model-based studies – despite the potential strong effect of the model parameter correlations on simulation results as demonstrated by our case study.

The remainder of the paper is organized as follows. In Section 2, the general concepts of model-based active fault detection and isolation (FDI), the basic idea of PCE, and the principles of the sparsity effect are given. In Section 3, we introduce the case study for active FDI (i.e., analyzing a tubular plug flow reactor), and discuss the derived results. Finally, we provide conclusions in Section 4.

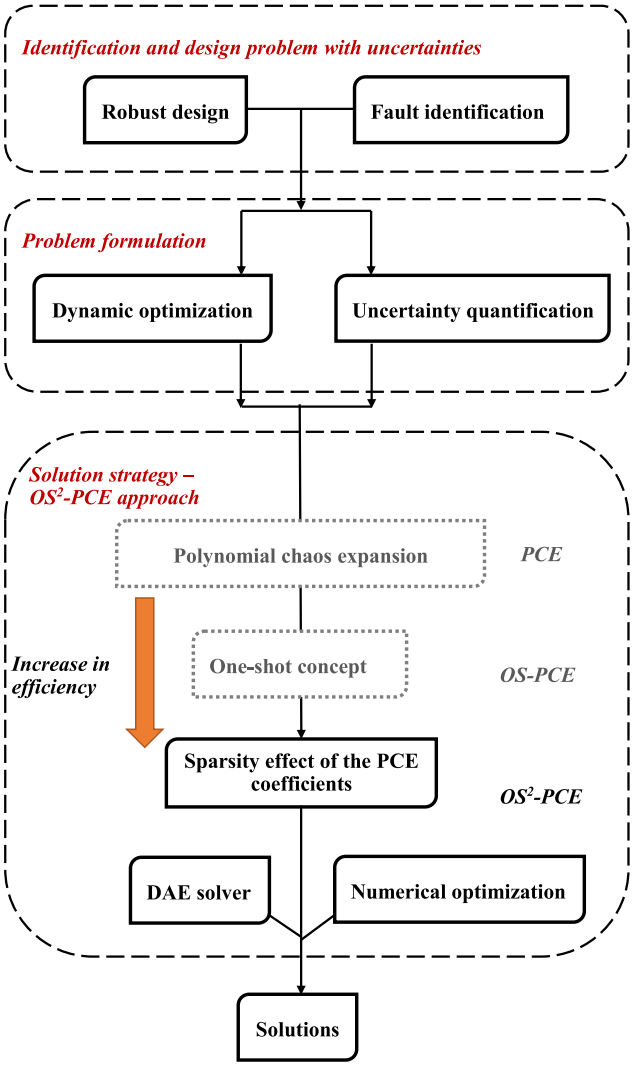


Fig. 1. Scheme of the one-shot PCE-based (OS^2-PCE) implementation for robust process design and active fault identification.

2. Methods

In what follows, the methods and concepts are introduced separately. The primary focus is on active fault identification and isolation principles. As we combine active FDI with optimal performance measures, the basics of robust process design are summarized, too. In both case, an efficient uncertainty analysis is mandatory. To this end, the general idea of polynomial chaos is introduced, and our novel extension, the one-shot sparse PCE approach, is outlined in more detail.

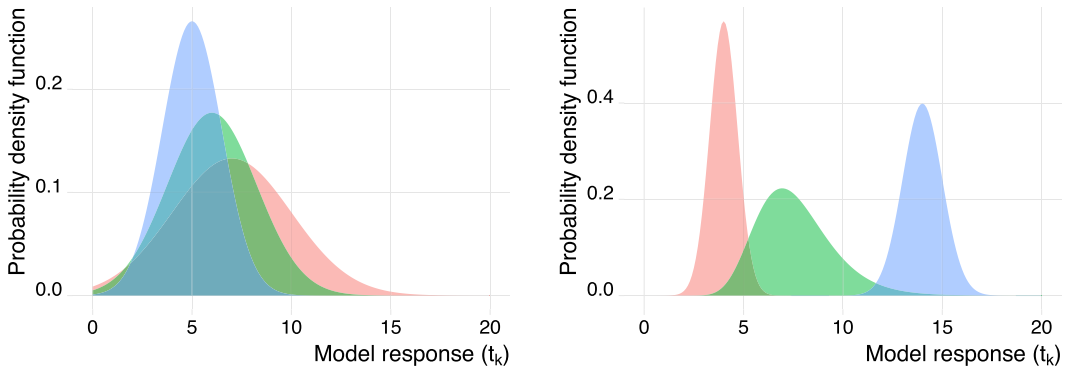
2.1. Active fault detection and isolation

Fault identification concepts are classified as either passive or active. Passive strategies gather and evaluate process data without feedback on the system under study. Active concepts, in turn, aim at applying fault-revealing auxiliary input signals to the analyzed system. An optimal fault-revealing auxiliary input is expected to improve the FDI performance in terms of the fault detection rate and fault isolation. In this work, the focus is on active FDI concepts. To this end, relevant process models, $\mathcal{M}_i,\ i \in \{1,\dots,m\}$, have to be formulated, including the nominal model (i.e., fault-free behavior) and potential error models describing specific fault scenarios. For practical reasons, the fault scenarios are limited to a finite number of the most relevant faults; i.e., $m \ll \infty$. Thus, a failure mode and effect analysis (FMEA) is typically the first step to identify relevant failure modes which are subsequently translated to mathematical models (Kapur and Pecht, 2014; Khan and Abbasi, 1998).

The governing equations of complex technical systems may be given as differential algebraic equations (DAEs) equal to:

$$\mathcal{M}_i \begin{cases} \dot{\mathbf{x}}_\mathbf{d}(t) &= \mathbf{f_i}(\mathbf{x}(t),\mathbf{u}(t),\mathbf{p}), \\ \mathbf{0} &= \mathbf{g_i}(\mathbf{x}(t),\mathbf{u}(t),\mathbf{p}), \end{cases} \quad \mathbf{x_d}(0) = \mathbf{x}_0, \quad \forall i \in \{1,\dots,m\} \tag{1}$$

where $t \in [0,\ t_f]$ is the time, $\mathbf{u} \in \mathbb{R}^{n_u}$ denotes the control input vector, and $\mathbf{p} \in \mathbb{R}^{n_p}$ denotes the time-invariant parameter vector. $\mathbf{x} = [\mathbf{x_d}, \mathbf{x_a}] \in \mathbb{R}^{n_x}$ is the state vector, in which $\mathbf{x}_d \in \mathbb{R}^{n_{x_d}}$ and $\mathbf{x}_a \in \mathbb{R}^{n_{x_a}}$ are the differential and algebraic states, respectively. $\mathbf{x}_0$ is the vector of the initial conditions. $\mathbf{f_i}$ and $\mathbf{g_i}$ denote the differential and algebraic vector fields of the system and define the physical and chemical interactions in accordance with the ith model. In the field of active FDI, these models are an essential part of the algorithmic fault detection and isolation implementation. The quality of the FDI performance depends critically on the reliability of the evaluated model candidates. Thus, uncertainties associated with model parameters $\mathbf{p}$ have to be incorporated in the model-based active FDI concept conscientiously. Uncertainty measures (e.g., probability density functions) are assigned to the pa-



(a) Strong overlap (b) Reduced overlap

Fig. 2. Active FDI principle: overlap of model responses of the nominal model, fault model F_1, and fault model F_2. (a) Strong overlap cause slow FDI rates while a reduced overlap of the model densities (b) guaranties improved FDI rates.

rameters resulting from experimental data imperfections. Technically, we assume parameter uncertainties of finite variance which are described by second-order random variables. The probability space $(\Omega, \mathcal{F}, \mathbf{P})$ is defined by the sample space Ω, the σ-algebra $\mathcal{F}$, and the probability measure $\mathbf{P}$ on Ω. Moreover, we assume that the time-invariant probabilistic uncertainties are functions of random variables $\omega := [\omega_1, ..., \omega_{p_n}]^T$ with known independent probability density functions $\{\mathbf{P}_{\omega_i}\}_{i=0}^{n_p}$ over Ω. Because of the parameter uncertainties, the simulation results can be considered as random vectors according to the Doob–Dynkin lemma (Bobrowski, 2005). For instance, exemplary probability density functions of a nominal model and two fault models at a given time point t_k are illustrated in Fig. 2. The strong overlap of the density functions shown is prohibitive regarding reliable and fast FDI results. The reduced overlap of the corresponding density functions in Fig. 2b, in turn, ensures an improved FDI rate (Schenkendorf, 2016). The objective of active FDI is to identify an auxiliary control input that reduces the overlap of the simulation results and their confidence intervals, i.e., maximizing the differences between the models according to their associated uncertainties. Thus, in the next step, the uncertainties have to be incorporated in calculating the fault-revealing auxiliary inputs numerically. Following a control vector parameterization (Biegler, 2010) strategy, the optimization problem reads as:

$$\mathbf{u}^{FDI} := \arg\max_{\mathbf{u}^{FDI}} \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} D(\mathcal{M}_i(\mathbf{u}^{FDI}, \mathbf{p}), \mathcal{M}_j(\mathbf{u}^{FDI}, \mathbf{p})). \tag{2}$$

In the literature, various distance measures D exist to quantify the difference between two or more model candidates and their density functions (Mesbah et al., 2014). In this work, a distance measure based on the Kullback–Leibler distance is used (Schenkendorf, 2016):

$$D(\mathcal{M}_i(\mathbf{u}, \mathbf{p}), \mathcal{M}_j(\mathbf{u}, \mathbf{p})) = d_{KL}(pdf_i || pdf_j) + d_{KL}(pdf_j || pdf_i), \tag{3}$$

with

$$d_{KL}(pdf_i || pdf_j) = \int_{\Omega} pdf_i(\mathbf{x}) ln \frac{pdf_i(\mathbf{x})}{pdf_j(\mathbf{x})} d\mathbf{x}, \tag{4}$$

where pdf_i and pdf_j are probability density functions corresponding to models $\mathcal{M}_i$ and $\mathcal{M}_j$, respectively.

To solve the optimization problem in Eq. (2), at every iteration the corresponding probability density functions have to be quantified for all incorporated model candidates. In parallel, while searching for fault-revealing control actions, the process under study has to meet given design specifications, i.e., ensuring safety margins and high productivity. Thus, the concepts of robust process design need to be considered simultaneously but typically are ignored in the literature of active FDI.

2.2. Robust process design

The uncertainty measures introduced above can be used to formulate robustified process design performance indicators (Telen et al., 2015) as:

$$\min_{\mathbf{u}(t)} \ \mathbf{E}[\mathcal{J}(\mathbf{x}_{t_f})] + \alpha \mathbf{Var}[\mathcal{J}(\mathbf{x}_{t_f})]^{0.5}, \tag{5a}$$

subject to: Eq. (1),

$$\mathbf{Pr}[\mathbf{h_{nq}}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{p}) \geq 0] \leq \varepsilon_{nq}, \tag{5b}$$

$$|\mathbf{E}[\mathbf{h_q}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{p})]| \leq \varepsilon_{q,\mu}, \tag{5c}$$

$$\mathbf{Var}[\mathbf{h_q}(\mathbf{x}(t), \mathbf{u}(t), \mathbf{p})] \leq \varepsilon_{q,\delta}, \tag{5d}$$

$$\mathbf{u}_{min} \leq \mathbf{u} \leq \mathbf{u}_{max}. \tag{5e}$$

Here, $\mathbf{E}[\cdot]$ and $\mathbf{Var}[\cdot]$ denote the mean and variance values of the random variables, $\mathcal{J}$ is the objective function of the states at t_f, α denotes a scalar weight factor, $[\mathbf{u}_{\min}, \mathbf{u}_{\max}]$ are the upper and lower boundaries for the control input vector, $\mathbf{Pr}$ denotes the probability of an event, $\mathbf{h_{nq}}$ and $\mathbf{h_q}$ are the functions for the inequality and equality constraints, respectively and ε_{nq}, $\varepsilon_{q,\mu}$, and $\varepsilon_{q,\delta}$ are tolerance factors (Rangavajhala et al., 2009). The individual chance constraint in (5b) is approximated with the Cantelli-Chebyshev inequality with a scalar weight factor β_c (Telen et al., 2015) as:

$$\mathbf{E}[\mathbf{h_{nq}}] + \beta_c \mathbf{Var}[\mathbf{h_{nq}}]^{0.5} \leq 0. \tag{6}$$

The robust optimization framework can reduce the influence of uncertain model parameters on the optimization outcome. This is because of the following reasons. First, by optimizing the objective function, an averaged measure of the objective function is improved under parameter uncertainties while minimizing the overall variation of the objective function in parallel. Second, by considering the chance constraints in Eq. (6) and the approximated inequality constraints in Eqs. (5c) and (5d), relevant statistics of constraint violations under parameter uncertainties are incorporated into the optimization problem systematically.

The statistical moments required to solve the robust process design problem, i.e., $\mathbf{E}[\cdot]$ and $\mathbf{Var}[\cdot]$ for the state vector $\mathbf{x}$, are defined as:

$$\mathbf{E}[\mathbf{x}] = \int_{\Omega} \mathbf{x} \ pdf(\mathbf{x}) d\mathbf{x}, \tag{7}$$

$$\mathbf{Var}[\mathbf{x}] = \int_{\Omega} (\mathbf{x} - \mathbf{E}[\mathbf{x}])(\mathbf{x} - \mathbf{E}[\mathbf{x}])^T pdf(\mathbf{x}) d\mathbf{x}. \quad (8)$$

The integral terms, however, given in Eqs. (7) and (8) have to be evaluated numerically. This evaluation may render the robust model-based process design approach into an intractable problem, especially when using standard methods of numerical integration, e.g., Monte Carlo simulations or Gaussian quadrature-based concepts. The same holds true for the implementation of active FDI (Eq. (4)) – with or without the consideration of process performance and safety aspects. Alternatively, a novel one-shot sparse PCE (OS^2-PCE) concept is introduced in the following as a highly flexible and efficient algorithmic backbone layer for the robust process design and active FDI or, in particular, a combination thereof.

2.3. One-shot sparse PCE approach (OS^2-PCE)

The non-intrusive concept of PCE has been proven beneficial in uncertainty analysis because of its demonstrated convergence (Cameron and Martin, 1947), i.e., the PCE model can describe any process of finite variance. Due to the Askey scheme (Xiu and Karniadakis, 2002), PCE is applicable to any parameteric probability density function. Empirical distributions can be included using iso-probabilistic transformation techniques (Sudret and Caniou, 2013). The general idea of PCE is to use orthogonal polynomials to approximate the model output. The applied orthogonal polynomials, in turn, depend on the given probability density functions of the parameteric uncertainties while the corresponding polynomial coefficients are estimated to fit a finite set of reference simulations (Xiu and Karniadakis, 2002). The main contribution of this paper is to demonstrate how the number of polynomial terms needed and the total number of CPU-intensive reference simulations can be reduced considerably for a highly efficient active FDI implementation. The proposed OS^2-PCE concept is outlined below starting with the conventional PCE setting. Subsequently, we show how the conventional PCE approach can be reduced to a *one-shot* realization avoiding prohibitive re-parameterizations of the polynomial coefficients when solving the dynamic optimization problem, and second, how PCE benefits from the sparsity effect by applying least angle regression.

2.3.1. Generalized polynomial chaos expansion

The generalized PCE approach (Xiu and Karniadakis, 2002) represents any random variable of finite variance, $Y(\omega) \in \mathcal{L}^2(\Omega, \mathcal{F}, \mathcal{P})$, as an expansion of orthogonal polynomial basis functions:

$$Y(\omega) \approx Y(\omega)^{PCE} = \sum_{k \in \mathcal{A}} \alpha_k \Psi_k(\omega), \quad (9)$$

where ω is a random variable vector, α_k is the polynomial coefficient, $\Psi_k(\omega)$ is the polynomial basis function of degree less than or equal to p. $\mathcal{A}$ represents the set of multiple indices depending on the applied truncation scheme (Blatman and Sudret, 2011). In summary, the number of terms of the truncated series is defined as:

$$\mathrm{card}\,\mathcal{A}_{PCE} = \binom{n_\omega + p}{p} = \frac{(n_\omega + p)!}{n_\omega!\, p!}, \quad (10)$$

where n_ω is the number of uncertain quantities (e.g., model parameters) and may lead to an exponential increase in the computational costs due to the *curse of dimensionality* when it comes to the computation of the unknown polynomial coefficients and providing the reference simulations (Blatman and Sudret, 2011). This is particularly true for the active FDI concept because for any analyzed fault-revealing input configuration the model output results are different compared to the nominal case, i.e., when no auxiliary control input for FDI is applied. Thus, for any new model input-output realization, the polynomial coefficients of the related PCE models have to be recalculated based on a new set of CPU-costly reference simulations. The problem of updating the PCE model within the dynamic optimization loop is illustrated in Fig. (3a). To de-bottleneck the PCE-based active FDI approach, the PCE model has to be derived in a single step first, and the dynamic optimization has to be solely based on the fixed PCE model without the need for cumbersome re-parameterizations; i.e., running a one-shot PCE approach.

2.3.2. One-shot PCE approach

To avoid the repeated need for polynomial coefficient re-calibrations and consequently, additional costly simulation runs, the PCE model has to be made sensitive to the auxiliary input directly; i.e., the PCE model is also a function of the auxiliary input parameters. The general idea of this implementation is illustrated in Fig. (3b). Here, the PCE model is derived only in the first single step, and the optimization is directly based on the OS-PCE model without the need for additional simulation runs of the original model candidates (Eq. (1)). Practically, the auxiliary input is integrated in the OS-PCE model as a control vector parameter realization. Within the framework of optimal control vector parameterization, inputs are parameterized by piecewise constant functions where the corresponding control parameters might be specified by upper and lower bounds (Biegler, 2010). Because of these upper and lower bounds, the control vector parameters can be considered as uniformly distributed random variables. Uniform random variables, in turn, are an inherent part of generalized PCE (Xiu and Karniadakis, 2002). Thus, the control vector parameters of the fault-revealing auxiliary input can be incorporated in the PCE framework directly (Shen and Braatz, 2016). The extended PCE model reads as:

$$M_{PCE}(\mathbf{p}, \mathbf{u}) = \sum_{\mathcal{A}_u} \sum_{\mathcal{A}_p} \alpha_{kl} \Psi_k^p(\omega) \Psi_l^u(\omega), \quad (11)$$

with specific polynomial basis functions $\Psi_k^p(\omega)$ and $\Psi_l^u(\omega)$ for the uncertain model parameters $\mathbf{p}$ and auxiliary inputs $\mathbf{u}$, respectively. The joint analysis, however, causes an exponential increase in the number of orthogonal polynomial terms. The dimension of the random vector is now the sum of the number of model parameters, $p \in R^{n_p}$, and the number of elements of the discretized control vector, $p_u \in R^{n_{p_u}}$; i.e., the dimension of the random parameter vector reads $\omega \in \mathcal{R}^{n_p + n_{p_u}}$. According to Eq. (10), the computational load to build the extended PCE model (Eq. (11)) increases exponentially with the number of elements of the control vector. This is the main reason why OS-PCE has been applied only for very simple control vector realizations. In Shen and Braatz (2016), a single parameter for the control vector is considered. More flexible and powerful control vector realizations, however, correlate with high computational costs (Paulson and Mesbah, 2018). Because of the increased number of reference simulations needed, OS-PCE may become prohibitive for problems of practical relevance. To avoid this limitation, the so-called *sparsity-of-effects principle* (Blatman and Sudret, 2011) has to be exploited, that is, to include only the most relevant terms of Eq. (11) resulting in a representative but sparse PCE model. An effective algorithm to identify the most relevant polynomial terms is based on least angle regression.

2.3.3. Least angle regression

For a workable PCE implementation, an efficient computation of the polynomial coefficients is mandatory in the field of active FDI. To this end, the LAR concept selects exclusively those polynomial functions $\Psi^{\theta,\, u}(\cdot)$ that have the most impact on the PCE model (Eq. (11)) and its residuals. For many engineering problems, it has been proven that a relatively low number of polynomial

Please cite this article as: R. Schenkendorf et al., An efficient polynomial chaos expansion strategy for active fault identification of chemical processes, Computers and Chemical Engineering (2018), https://doi.org/10.1016/j.compchemeng.2018.08.022

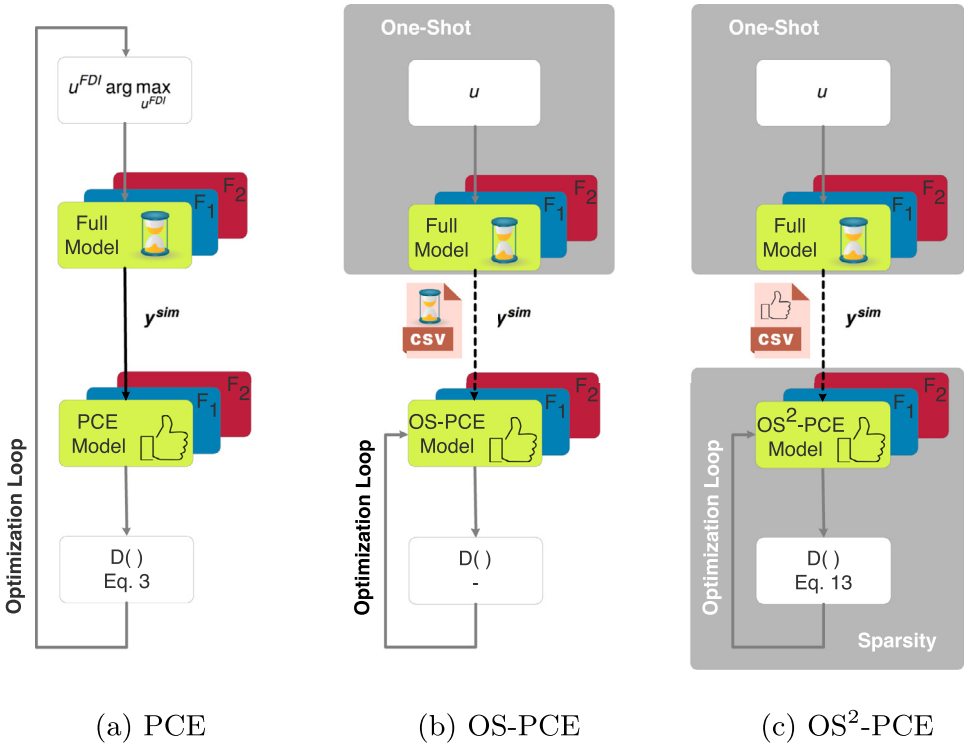


Fig. 3. Non-intrusive PCE-based strategies for active FDI: (a) each PCE model has to be re-parameterized during optimization, (b) direct PCE-based optimization, but the number of reference simulations (e.g., nominal model and fault models F_1 & F_2 stored in a CSV file) are prohibitive, (c) dramatic reduction of needed reference simulations due to the sparsity effect.

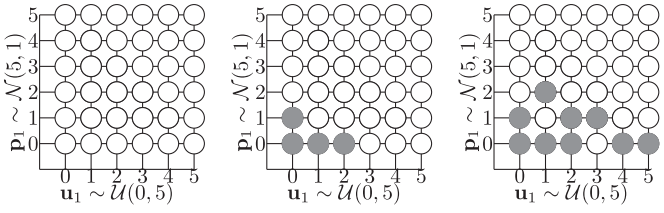


Fig. 4. Exemplary illustration of the least angle regression concept for two random variables. In an iterative process, relevant PCE coefficients α_{kl} are assigned to the active set (●) and have to be identified via reference simulations. The non-active PCE coefficients (○) are set to zero.

terms are required to mimic the approximated system behavior, i.e., $\text{card}(\mathcal{A}^{LAR}) << \text{card}(\mathcal{A})$. Fewer polynomial terms, in turn, mean fewer model evaluations and computational costs. The basic idea of LAR is to start off with an empty polynomial function set and to add those polynomial terms that reduce the difference between the original model (Eq. (1)) and the sparse PCE model the most, i.e., which are highly correlated with the residuals. In parallel, the relevant polynomial coefficients are calculated via linear regression. A selecting criteria, which is based on cross-validation, avoids overfitting and identifies the best sparse PCE model candidate with the lowest estimation error. For the technical details of LAR, please see (Blatman and Sudret, 2011) and references therein. The working principle of LAR is illustrated in Fig. 4 via an academic example. Here, one model parameter is assumed to follow a Gaussian distribution, e.g., $\mathbf{p_1} \sim \mathcal{N}(5,1)$, while one control vector parameter is characterized by a uniform distribution, e.g., $\mathbf{u_1} \sim \mathcal{U}(0,5)$. Assuming a maximum polynomial order of five which is common in many engineering problems (Sudret and Caniou, 2013), 36 polynomial coefficients have to be identified theoretically; see Fig. 4a. LAR identifies polynomial terms that have the highest correlation with the residuals; i.e., the difference between the PCE model and the reference simulation. Only these polynomial coefficients are added to an active set as shown in Fig. 4b. The remaining coefficients are set to zero. The active set of polynomial coefficients is systematically extended to meet given specifications. Typically, 20% to 30% of the polynomial coefficients become part of the active set as illustrated by way of example in Fig. 3c; i.e., a large reduction in computational costs. The resulting OS^2-PCE-based optimization problem reads as:

$$\mathbf{u}^{FDI} := \arg\max_{\mathbf{u}^{FDI}} \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} D\left(M^{LAR}_{PCE,i}\left(\mathbf{u}^{FDI}, \mathbf{p}\right), M^{LAR}_{PCE,j}\left(\mathbf{u}^{FDI}, \mathbf{p}\right)\right), \quad (12)$$

with

$$M^{LAR}_{PCE}(\mathbf{p}, \mathbf{u}) = \sum_{\mathcal{A}^{LAR}_{\mathbf{u}}} \sum_{\mathcal{A}^{LAR}_{\mathbf{p}}} \alpha_{kl} \Psi^{\mathbf{p}}_k(\omega) \Psi^{\mathbf{u}}_l(\omega). \quad (13)$$

In summary, the work flow of the proposed OS^2-PCE framework for active FDI is the following: (1) To build the sparse PCE model which includes uncertain model parameters and control vector parameters of the auxiliary control input alike and (2) to evaluate this sparse PCE model within the optimization routine (Eq. (13)). The original dynamic optimization problem is transferred into a CPU-friendly algebraic optimization problem (see Fig. 3c), i.e., instead of solving ODEs in Eq. (2), the analytical formula in Eq. (13) is evaluated for the auxiliary control input parameters at every iteration. Technically, the PCE-based framework is realized with UQLAB© (Marelli and Sudret, 2014) and *fmincon* in MATLAB® with a multi-start strategy to avoid local optima.

2.4. Parameter correlation

The existence of parameter correlations might increase the difficulty of quantifying the resulting model uncertainties properly

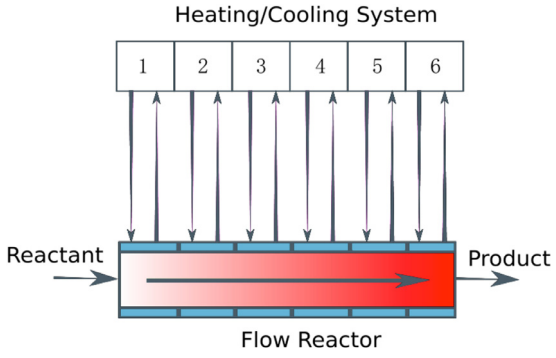


Fig. 5. Scheme of the analyzed jacketed tubular reactor with the heating and cooling system to control the jacket temperature of the six elements individually.

(Xie et al., 2018). Thus, an additional goal of this paper is to demonstrate how parameter correlations can be integrated into the proposed concept of active FDI. Note that parameter correlations are unavoidable when model parameters are identified with experimental data, but despite their considerable impact, parameter correlations are typically ignored in uncertainty analysis and robust model-based design (Li et al., 2010; Valkó et al., 2017; Xu and Gertner, 2008). Here, the framework of PCE allows a straightforward integration of parameter correlations via isoprobabilistic transformations (Lebrun and Dutfoy, 2009; Rosenblatt, 1952; Valkó et al., 2017) or by using copula-based strategies (Nelsen, 2007; Sklar, 1959). In this work, an isoprobabilistic transformation is implemented for simplicity. For more details regarding isoprobabilistic transformation concepts, the interested reader is referred to Xie et al. (2018a) and references therein.

3. Case study

To demonstrate the proposed concept of active FDI, a jacketed tubular reactor under steady-state condition is studied assuming an irreversible first-order reaction; see Fig. 5. Please note that the steady-state assumption is not mandatory but is selected for simplicity. Time-dependent problems can be solved similarly. The governing equations are given in Eqs. (14) and (15) (Telen et al., 2015):

$$\frac{d\mathbf{x}_1}{dz} = \frac{\alpha_{kin}}{v}(1-\mathbf{x}_1)e^{\frac{\gamma \mathbf{x}_2}{1+\mathbf{x}_2}}, \tag{14}$$

$$\frac{d\mathbf{x}_2}{dz} = \frac{\alpha_{kin}\delta}{v}(1-\mathbf{x}_1)e^{\frac{\gamma \mathbf{x}_2}{1+\mathbf{x}_2}} + \frac{\beta(z)}{v}(\mathbf{u}-\mathbf{x}_2). \tag{15}$$

The states $\mathbf{x}_1$ and $\mathbf{x}_2$ are the dimensionless forms of the reactant concentration and the reactor temperature, respectively. The jacket temperature $\mathbf{u}$ is defined as the auxiliary input for active FDI. Following the control vector parameterization strategy, the auxiliary control input is discretized into six equidistant elements (see Fig. 5) constrained by 280K and 400K or in terms of random variables: $u_i \sim \mathcal{U}[280, 400]$, $\forall i = 1, \ldots, 6$. The kinetic coefficient α_{kin} and the heat transfer coefficient β are assumed to follow a Gaussian distribution with a standard deviation of 10% of their nominal values to integrate the model parameter uncertainties. Please note that the proposed OS^2-PCE concept is not limited to Gaussian distributions, i.e., various parameteric and empirical distributions can be included via the Askey scheme (Xiu and Karniadakis, 2002) and iso-probabilistic transformation techniques (Sudret, 2008), respectively. The applied model parameters are summarized in Table 1 and further details of the reactor model can be found in Telen et al. (2015). In what follows, the proposed concept of active FDI is demonstrated, and we show how to add process performance and safety measures to active FDI. To this end,

Table 1
Model parameters and assumed parameter uncertainties.

Parameters	Unit	Nominal value	Uncertainty
$x_1(0)$	–	0	–
$x_2(0)$	–	0	–
α_{kin}	s^-1	0.058	$\mathcal{N}$(0.058,0.0058)
β (nominal)	s^-1	0.2	$\mathcal{N}$(0.2,0.02)
β (fault)	s^-1	0.05	$\mathcal{N}$(0.05,0.01)
v	s^-1	0.1	–
γ	–	16.66	–
δ	–	0.25	–

we define the conversion of the reactor as the process output used for process monitoring and process design:

$$C_f = x_1(z=1), \tag{16}$$

where z is the relative reactor position, $0 \leq z \leq 1$. As all proposed strategies are based on a very efficient PCE implementation, we compare the PCE outcome with the original model first. In Fig. 6, the resulting probability density functions for the reactor temperature at different locations are illustrated. Please note that these uncertainties of the reactor temperature are a result of the model parameter uncertainties. When we compare the Monte Carlo simulation result (5,000 simulations) of the original nominal model and the corresponding OS^2-PCE model, we see a good match and low approximation errors. Similar results can be derived for the reactant profiles and the two models of fouling layers, but the results are not shown here due to space limitations. As the PCE models represent the original model candidates sufficiently well, they are good candidates for solving the optimization problems for active FDI efficiently. In addition to a reduced overlap of the model results and an improved FDI rate, the reactor has to ensure high productivity and safety operation, i.e., high conversion and temperature values below 400K. Please note that the entire OS^2-PCE framework requires only 2000 model evaluations computed once in parallel, while the conventional PCE-based design framework without using the sparsity effect and the normal robust design approach need around 10,000 and at least 20,000 evaluations (depending on the optimization condition), respectively.

3.1. Active fault detection and isolation

In the first step, two different fault scenarios are defined: (1) a fouling layer in the front section of the reactor and (2) a fouling layer in the end section of the reactor. Fouling is a relevant failure mode in chemical engineering. Typically, process design and operating strategies are applied to reduce the formation of critical fouling layers (Föste et al., 2013; Ishiyama et al., 2014; Mirzaei et al., 2017), but the fouling process cannot be avoided completely. Thus, identifying the fouling formation progress is essential for scheduling intervention and cleaning actions in time (Diaz-Bejarano et al., 2015; Markowski et al., 2013; Qureshi and Zubair, 2016). Algorithmically, the fouling effect is realized by changing the heat transfer coefficient locally (see Table 1) to mimic the lower thermal conductivity caused by the fouling layer; i.e., for Fault 1 ($0 \leq z \leq 0.5$) and Fault 2 ($0.5 \leq z \leq 1$) $\beta(z) = 0.05$ is used instead of $\beta(z) = 0.2$ as for the nominal case. The OS^2-PCE framework includes eight input random variables, i.e., six control elements and the two uncertain model parameters, which result in 2000 model evaluations for each model candidate to derive the corresponding OS^2-PCE model. The applied OS^2-PCE models (Eq. (13)) benefit considerably from the sparsity effect; i.e., the number of required terms was reduced by a factor of $\text{card}(\mathcal{A}^{LAR})/\text{card}(\mathcal{A}) = 0.2$, on average. After the single *one-shot* PCE model building step, the optimal fault-revealing temperature input profile is derived in the presence of model parameter uncertainties. That is, in the course of optimization no ad-

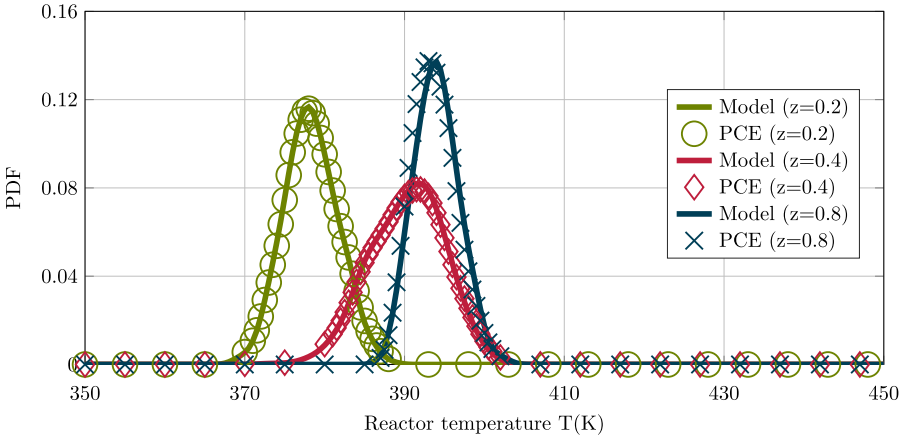


Fig. 6. Probability density functions of the reactor temperature at different relative reactor positions, z $\in$ {0.2, 0.4, 0.8}. 5000 Monte Carlo simulations are used to compare the nominal process model with the derived OS^2-PCE model.

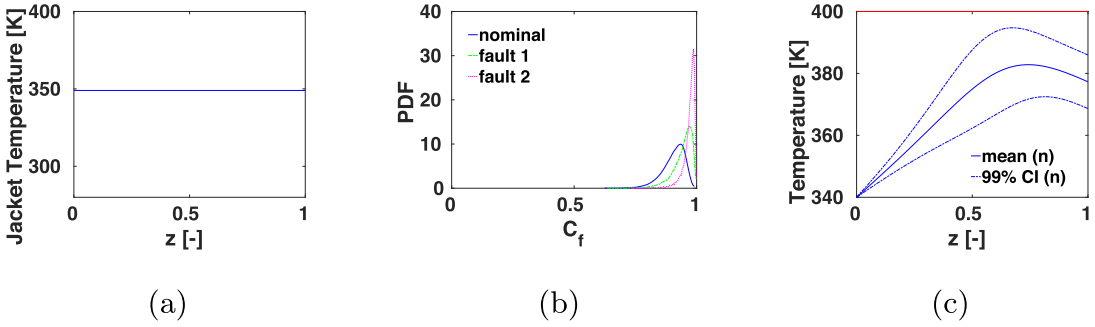


Fig. 7. Results for the default scenario: (a) assuming a constant jacket temperature profile, (b) the probability density functions of the nominal and fault cases, and (c) the reactor temperature profile (nominal model) and its 99% confidence interval.

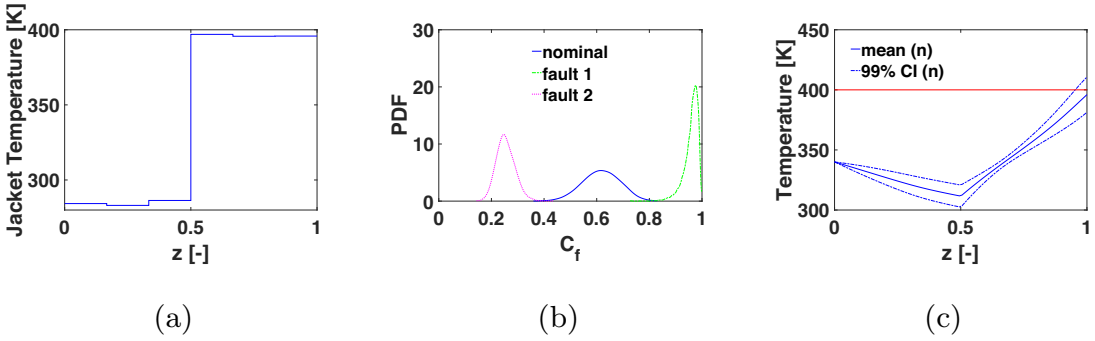


Fig. 8. Results for active FDI: (a) optimized jacket temperature profile, (b) the probability density functions of the nominal and fault cases, and (c) the reactor temperature profile (nominal model) and its 99% confidence interval.

ditional simulation runs of Eqs. ((14)–(15)) are needed to solve the optimization problem (Eq. (12)). As a reference scenario, we define the temperature profile of a constant jacket temperature of 350K in the entire reactor; see Fig. 7a. In Fig. 7b, we show the resulting probability density functions of the reactor conversion (Eq. (16)). The averaged conversion determined by the nominal model is 0.91, but the strong overlap of the density functions is prohibitive for FDI. The reactor temperature, in turn, is below the critical temperature limit of 400K for the nominal model as illustrated in Fig. 7c. In case of an optimal fault-revealing jacket temperature profile (see Fig. 8a) the difference in the reactor conversion could be increased considerably as illustrated in Fig. 8b. When combined with Bayesian reasoning, the condition of the reactor might be quantified in a subsequent step (Schenkendorf, 2016). The improved FDI outcome, however, goes along with a decreased process performance regarding the conversion of the nominal model, $c_f = 0.62$. Moreover, the reactor exceeds the temperature limit of 400K at the outlet; see Fig. 8c. In active FDI, robust process design principles have to be considered in parallel to avoid such a dramatic loss in the process performance and critical temperature values, respectively.

3.2. Robust process design

Before we combine robust process design principles with active FDI, we introduce the results of a direct robust process design strategy first and use them as additional references. Here, the OS^2-PCE concept is implemented to solve the robust process design problem efficiently. In this case, the optimized jacket temperature profile aims at maximizing the conversion of the reaction while simultaneously satisfying the temperature constraints in the presence of model parameter uncertainties. The weight factor, α, of the

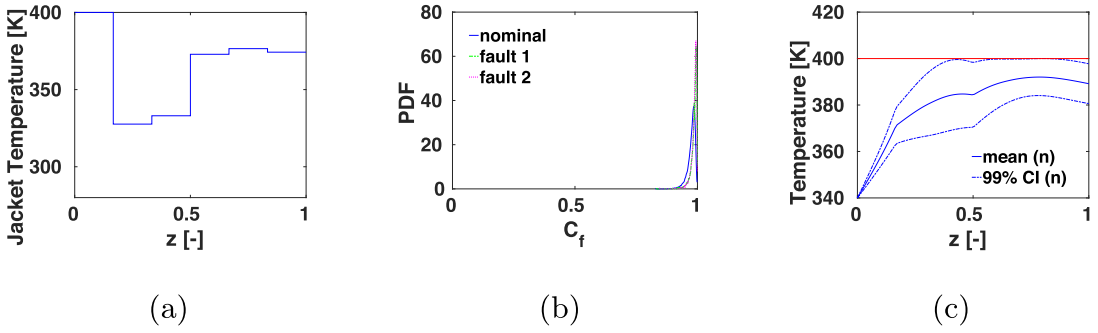


Fig. 9. Results for robust process design: (a) optimized jacket temperature profile, (b) the probability density functions of the nominal and fault cases, and (c) the reactor temperature profile (nominal model) and its 99% confidence interval.

objective function for the robust process design (Eq. (5)) is set to four and thus, a low variation of the conversation C_f (Eq. (16)) is advantageous. Please note that a weight factor of zero results in an exclusive optimization of the averaged conversation value but ignores the associated uncertainty totally. In general, to find an optimal weight factor α, a multi-objective design strategy could be implemented which is out of the scope of this study. Moreover, the backoff value, β_c, of the chance constraint (Eq. (6)) is set to three, i.e., a strong focus on robustness but less on high conversion. Please note that assuming a Gaussian distribution, a backoff value of three results in 99% confidence intervals, i.e., 99 out of 100 realizations fulfill the given constraints under model parameter uncertainties. The resulting optimal jacket temperature profile is illustrated in Fig. 9a. Obviously, a high jacket temperature at the beginning and the end of the reactor seems beneficial for an increased conversion as illustrated in Fig. 9b. The averaged conversion of the reactant is 0.98. The drop of the jacket temperature in the middle of the reactor, in turn, keeps the reactor temperature below the limit of 400K; see Fig. 9c. The robust process design comes at the price of a lower FDI rate, i.e., a large overlap in the density functions as shown in Fig. 9b. To find a jacket temperature profile that ensures an improved process performance and an acceptable FDI rate, both objectives are combined in the next step.

3.3. Combining active FDI with a robust process design

For improved FDI rates and high process performance, we have to combine active FDI and robust process design principles. The joint analysis uses the same OS^2-PCE concept but with a modified cost function. Technically, we incorporate the process performance measures (Eq. (5)) as additional constraints to the introduced active FDI optimization problem (Eq. (3)) in the following way:

$$\max_{\mathbf{u(t)}} \sum_{i=1}^{m-1} \sum_{j=i+1}^{m} D\left(M^{LAR}_{PCE,i}, M^{LAR}_{PCE,j}\right), \tag{17a}$$

$$\mathbf{E}[\mathcal{J}(M^{LAR}_{PCE,n})] + \alpha \mathbf{Var}[\mathcal{J}(M^{LAR}_{PCE,n})]^{0.5} \leq \delta_{pf} \tag{17b}$$

$$\mathbf{E}[\mathbf{h_{nq}}(M^{LAR}_{PCE,n})] + \beta_c \mathbf{Var}[\mathbf{h_{nq}}(M^{LAR}_{PCE,n})]^{0.5} \leq 0 \tag{17c}$$

$$M^{LAR}_{PCE,i}(\mathbf{p},\mathbf{u}) = \sum_{\mathcal{A}^{LAR}_{\mathbf{u}}} \sum_{\mathcal{A}^{LAR}_{\mathbf{p}}} \alpha_{kl,i} \Psi^{\mathbf{p}}_k(\omega) \Psi^{\mathbf{u}}_l(\omega) \tag{17d}$$

$$\mathbf{u}_{min} \leq \mathbf{u(t)} \leq \mathbf{u}_{max}. \tag{17e}$$

Here, δ_{pf} controls the impact of the robust process design on active FDI. Assuming $\delta_{pf} = -0.65$, we derived a new optimized jacket temperature profile; see Fig. 10a. Similar to the robust process design scenario (Fig. 9a), the jacket temperature is high in the beginning and end sections of the reactor but low in the middle section. The essential difference is that the jacket temperature profile operates on its maximum and minimum limits. As shown in Fig. 10b, the overlap of the density functions can be reduced while the conversion for the nominal case can be increased ($c_f = 0.85$) compared to the unconstrained active FDI design (Fig. 8b). Here, too, the jacket temperature drop in the middle of the reactor keeps the reactor temperature below the limit of 400K; see Fig. 10c. By adapting the scaling parameter δ_{pf} a better trade-off between FDI rate and process performance might be derived. Meaningful results, however, can only be calculated when considering the full uncertainty information about the model parameters as demonstrated in the next section.

3.4. Parameter correlation

Finally, we illustrate the impact of parameter correlations on the active FDI outcome. Most often, the model parameters cannot be measured directly and are identified by optimization procedures (e.g., least square methods and maximum likelihood estimations) evaluating given experimental data. The identified model parameters providing the best model fit are typically correlated; i.e., the uncertainties of the model parameters are characterized by the parameter (co)variance matrix. In the previous studies, we only considered the uncertainties of individual model parameters, i.e., ignoring parameter correlations totally. Thus, the available uncertainty information about the model parameters is not considered properly and might result into too conservative or misleading model-based optimizations results. In the following, we additionally assume a parameter correlation of $\rho = 0.8$ while using the same parameter standard deviations of 10% of their nominal values. Please note that the parameter correlation has been defined manually and is not based on experimental data. Different values of the parameter correlation might be of interest when analyzing experimental data (Xie et al., 2018b). However, to demonstrate the relevance of parameter correlations, the focus is solely on the fictitious but representative parameter correlation value given above. In principle, the parameter correlation affects all considered optimizations scenarios. For the sake of space, we mainly discuss the impact of the parameter correlation on the joint optimizations problem, i.e., active FDI with robust process design. In Fig. 11a, we illustrate the resulting jacket temperature profile. The optimized profile follows a similar trajectory but with lower temperature values at the reactor entrance compared to the non-correlation study (Fig. 10a). As highlighted in Fig. 11b, the resulting densities of the conversion of the nominal and the two fault models are well separated, i.e., high FDI-rate and credible fault classification. The conversion, in turn, is slightly decreased, $c_f = 0.80$. The confidence intervals of the reactor temperature (see Fig. 11c) are significantly reduced in comparison to Fig. 10c which allows more flexible and less conservative optimal results. Thus, the conversion might be improved by different scaling parameters δ_{pf} addition-

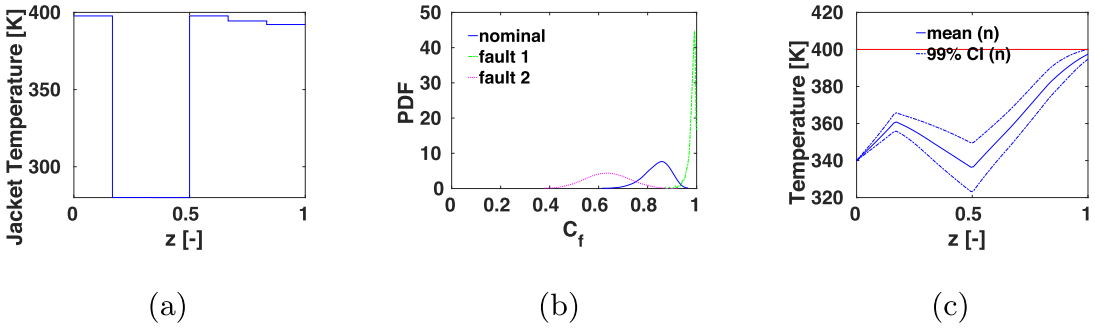


Fig. 10. Results for active FDI with additional constraints and performance functions: (a) optimized jacket temperature profile, (b) the probability density functions of the nominal and fault cases, and (c) the reactor temperature profile (nominal model) and its 99% confidence interval.

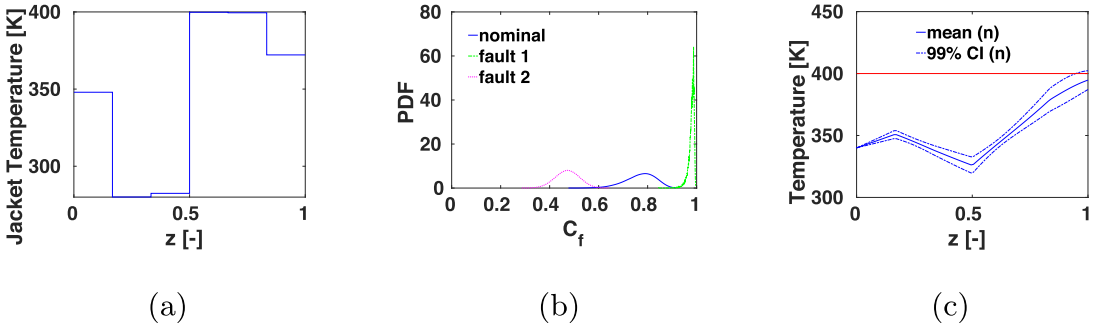


Fig. 11. Results for active FDI with additional constraints and performance functions considering the parameter correlation: (a) optimized jacket temperature profile, (b) the probability density functions of the nominal and fault cases, and (c) the reactor temperature profile (nominal model) and its 99% confidence interval.

Table 2
Active FDI results ignoring parameter correlation: (1) direct active FDI, (2) direct robust process design, and (3) joint design. Active FDI results including parameter correlation: (4) joint design but focus on high FDI rate, (5) balanced joint design, and (6) direct robust process design. Note that the Kullback-Leibler distance is based on Eq. (12).

Parameters	Independent				Correlated		
Scenarios	Base line	(1)	(2)	(3)	(4)	(5)	(6)
Conversion c_f	0.91	0.62	0.98	0.84	0.80	0.90	0.97
KL-Distance	7.28	74.73	2.30	52.35	68.39	29.43	6.30
δ_{pf}	–	–	–	−0.65	−0.65	−0.75	–

ally. Two additional configurations are analyzed: (1) less focus on high FDI rate, and (2) a direct optimal process design (Eq. (5)). The results are summarized in Table 2 and compared with all previous implemented and discussed scenarios. The derived conversion values and the distance measures vary strongly. Thus, depending on the system under study and given specifications, a proper balance between condition monitoring and process performance has to be found. In general, however, parameter correlations should be included in the model-based design framework. Please note, within the proposed concept of OS^2-PCE there is no need for additional reference simulations when considering parameter correlations. Using the full information of the model parameter uncertainties to improve the active FDI results comes with no additional computational costs.

4. Conclusions

A new approach based on the one-short sparse polynomial chaos expansion (OS^2-PCE) concept was proposed to quantify the effect of parameter uncertainties for active FDI efficiently. Moreover, robust process design principle was successfully combined with the active FDI framework. First results regarding the effectiveness and the performance of the proposed concept were demonstrated on an industrial relevant problem, i.e., forming of fouling layers in a jacket tubular reactor. In this study, the uncertainty of kinetic parameter and heat transfer coefficient are taken into account. This work contributes to the literature in three ways. (1) A distinct separation of each fault scenario was achieved by the proposed active FDI framework including model parameter uncertainties. Process performance requirements were added, and critical operation constraints were satisfied simultaneously. (2) A dramatic reduction in the computational cost was achieved by incorporating the design parameters into PCE and utilizing the sparsity of the polynomial coefficients. (3) The impact of the parameter correlation on the model-based design for active FDI and the variation of the process states was described and analyzed. In this work, a fixed ratio of active FDI and process performance was used. Therefore, further work will explore the optimal trade-off between the identification of fault scenarios and to improve the process performance by using multi–objective optimization strategies in the field of pharmaceutical manufacturing processes.

Acknowledgments

X. Xie gratefully acknowledges the financial support from the “Promotionsprogramm μ-Props” by MWK Niedersachsen.

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Please cite this article as: R. Schenkendorf et al., An efficient polynomial chaos expansion strategy for active fault identification of chemical processes, Computers and Chemical Engineering (2018), https://doi.org/10.1016/j.compchemeng.2018.08.022