Computers and Chemical Engineering 90 (2016) 23–30

Contents lists available at ScienceDirect

Computers and Chemical Engineering

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

Uncertainty quantification and global sensitivity analysis of complex chemical process using a generalized polynomial chaos approach

Pham Luu Trung Duong[a], Wahid Ali[b], Ezra Kwok[c], Moonyong Lee[b,*]

[a] Luxembourg Centre for Systems Biomedicine, Systems Control Group, University of Luxembourg, Luxembourg
[b] School of Chemical Engineering, Yeungnam University, Gyeongsan, Republic of Korea
[c] Chemical & Biological Engineering, University of British Columbia, Vancouver, Canada

ARTICLE INFO

Article history:
Received 6 December 2015
Received in revised form 18 February 2016
Accepted 22 March 2016
Available online 29 March 2016

Keywords:
Generalized polynomial chaos
Uncertainty quantification
Process uncertainty
Sensitivity analysis
Monte-Carlo approach

ABSTRACT

Uncertainties are ubiquitous and unavoidable in process design and modeling. Because they can significantly affect the safety, reliability and economic decisions, it is important to quantify these uncertainties and reflect their propagation effect to process design. This paper proposes the application of generalized polynomial chaos (gPC)-based approach for uncertainty quantification and sensitivity analysis of complex chemical processes. The gPC approach approximates the dependence of a process state or output on the process inputs and parameters through expansion on an orthogonal polynomial basis. All statistical information of the interested quantity (output) can be obtained from the surrogate gPC model. The proposed methodology was compared with the traditional Monte-Carlo and Quasi Monte-Carlo sampling-based approaches to illustrate its advantages in terms of the computational efficiency. The result showed that the gPC method reduces computational effort for uncertainty quantification of complex chemical processes with an acceptable accuracy. Furthermore, Sobol's sensitivity indices to identify influential random inputs can be obtained directly from the surrogated gPC model, which in turn further reduces the required simulations remarkably. The framework developed in this study can be usefully applied to the robust design of complex processes under uncertainties.

1. Introduction

Most rigorous process design problems are carried out under a deterministic setting with fixed specifications. In reality, however, the process inputs and parameters exhibit some randomness as depicted in Fig. 1, which can have a significant effect on the safety, reliability and economic decisions. Therefore, it is important to examine the effects of these uncertainties and analyze the sensitivity of the process model with respect to these uncertainties in the design stage. Monte-Carlo (MC) and Quasi Monte-Carlo (QMC) methods are representative probabilistic approaches for the propagation of uncertainties in the model input to its output (Niederreiter et al., 1996; Liu, 2001; Kroese et al., 2011; Abubakar et al., 2015). The brute-force implementation of these models first involves the generation of an ensemble of random realizations with each parameter drawn randomly from its uncertainty distribution. Deterministic solvers are then applied to each member to obtain an ensemble of results. The ensemble of results is then post-processed to estimate the relevant statistical properties, such as the mean, standard deviation and quantile. Despite this, estimations of the mean converge with the inverse square root of the number of runs, making MC- and QMC-based approaches computationally expensive and even infeasible for complex chemical process problems.

Recently, uncertainty analysis using a generalized polynomial chaos (gPC) expansion was studied in various applications including modeling, control, robust optimal design, and fault detection problems. Nagy and Braatz (2007) considered the gPC approach for uncertainty quantification and robust design of batch crystalized process. In their work, it was shown that the gPC approach to be more computationally efficient than the MC/QMC methods for a system with a moderate number of random inputs. Duong and Lee (2012, 2014) applied the gPC method to the PID controller design for fractional order and integer order systems. Du et al. (2015) considered the fault detection problem by combining maximum likelihood with the gPC framework. The gPC method originated from Wiener chaos (Wiener, 1938). This method is a spectral representation of a random process by the orthonormal polynomials of a random variable. Exponential convergence is expected for the gPC expansion of infinitely smooth functions (i.e., analytic and infinitely differentiable). Ghanem and Spanos (1991) reported that the gPC

* Corresponding author. Fax: +82 53 811 3262.
E-mail address: mynlee@yu.ac.kr (M. Lee).

http://dx.doi.org/10.1016/j.compchemeng.2016.03.020
0098-1354/

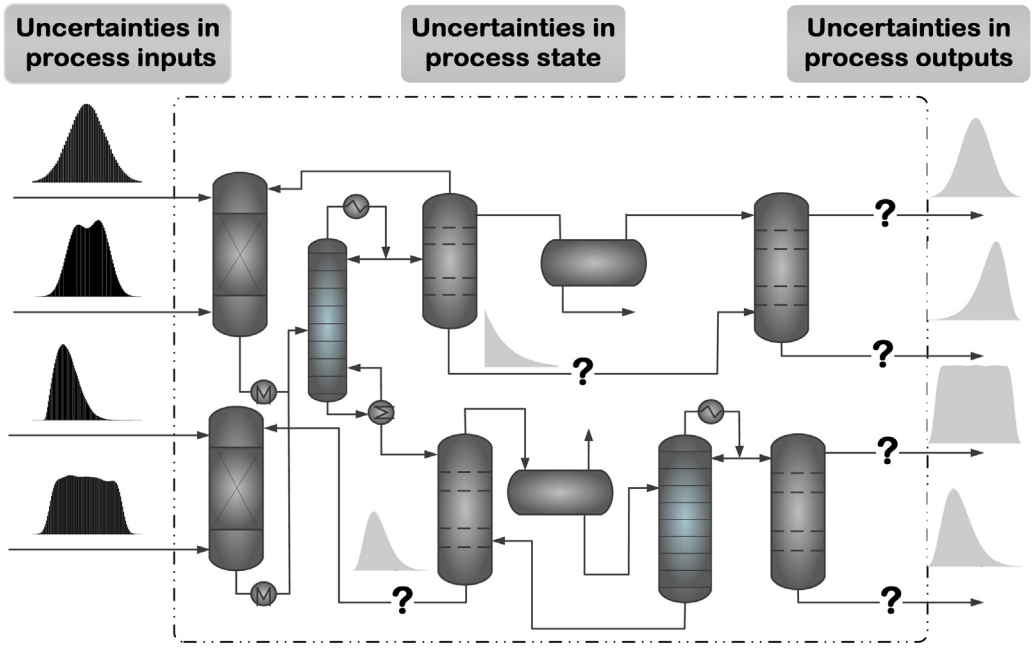

Fig 1. Uncertainty propagation and quantification in chemical processes.

is an effective computational tool for engineering purposes. Xiu and Karniadakis (2002) further generalized PC for use with non-standard distributions.

This work demonstrates and validates the applicability of polynomial chaos theory for uncertainty quantification and sensitivity analysis for complex chemical processes such as natural gas and syngas production. The proposed gPC based method can reduce significantly the computational cost (simulation time) for uncertainty quantification over traditional approaches, such as the MC/QMC methods. Moreover, Sobol's sensitivity indices (Sobol, 2001) can also be directly obtained from the gPC surrogate analytical model (Crestaux et al., 2009; Sandoval et al., 2012), which can in turn be used to detect the influential inputs in the propagation of process uncertainty.

2. Uncertainty quantification using polynomial chaos theory

Consider a steady-state process that is described with a set of following nonlinear equations:

$$\mathbf{F}(\mathbf{y},\xi) = \mathbf{0} \tag{1}$$

where $\boldsymbol{\xi} = (\xi_1, \xi_2, \ldots \xi_N)$ is a process input variable vector expressed by a random vector of mutually independent random components with probability density functions of $\rho_i(\xi_i): \Gamma_i \rightarrow R^+$; and $\boldsymbol{y}$ denotes a process state and output variable vector.

The joint probability density of the random vector, $\boldsymbol{\xi}$, is $\boldsymbol{\rho} = \prod_{i=1}^{N} \rho_i$, and the support of $\boldsymbol{\xi}$ is $\boldsymbol{\Gamma} \equiv \prod_{i=1}^{N} \Gamma_i \in R^N$. The uncertainties in the process inputs $\boldsymbol{\xi}$ are then propagated through the entire process, as shown in Fig. 1. The set of one-dimensional orthonormal polynomials, $\{\phi_i(\xi_i)_{m=0}^{d_i}\}$, can be defined in finite dimension space, Γ_i, with respect to the weight, $\rho_i(\xi_i)$. Based on a one-dimensional set of polynomials, an N-variate orthonormal set can be constructed with P total degrees in space, $\boldsymbol{\Gamma}$, using the tensor product of the one-dimensional polynomials, the basis function of which satisfies the following:

$$\int_{\boldsymbol{\Gamma}} \Phi_m(\boldsymbol{\xi})\Phi_n(\boldsymbol{\xi})\boldsymbol{\rho}(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} = \begin{cases} 1\ , & m = n \\ 0\ , & m \neq n \end{cases} \tag{2}$$

Consider a response function $f(y(\xi))$ for a process state variable, y, with the statistics (e.g., mean, variance) of interest, the N-variate P^{th} order approximation of the response function can be constructed as follows:

$$\begin{aligned} {f_N}^P(y(\boldsymbol{\xi})) &= \sum_{i=1}^{M} \hat{f}_i \Phi_i(\boldsymbol{\xi})\,; \\ M + 1 &= \binom{N+P}{N} = \frac{(N+P)!}{N!P!} \end{aligned} \tag{3}$$

where P is the order of polynomial chaos, and $\hat{f}_m$ is the coefficient of gPC expansion that satisfies Eq. (2) as follows:

$$\hat{f}_i = \boldsymbol{E}[\Phi_i f(y)] = \int_{\Gamma} f(y)\Phi_i(\boldsymbol{\xi})\rho(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \tag{4}$$

where $\boldsymbol{E}[\cdot]$ denotes the expectation operator.

The coefficients of the gPC expansion from Eq. (4) are normally obtained numerically using the following procedure (Xiu, 2010):

- Choose a N-dimensional integration rule (cubature nodes and weights)

$$\ell^{Q}[g] = ({Q_{q_1}}^{(1)} \otimes \ldots \otimes {Q_{q_N}}^{(N)})[g] = \sum_{j_1=1}^{q_1} \cdots \sum_{j_N=1}^{q_N} g(\xi_j^{(j_1)}, \ldots, \xi_j^{(j_N)})$$

$$({w_1}^{(j_1)} \ldots {w_1}^{(j_N)}) \cong \int_{\Gamma} g(\boldsymbol{\xi})\rho(\boldsymbol{\xi})\mathrm{d}\boldsymbol{\xi} \tag{5}$$

where $\otimes$ denotes the tensor product, and $\ell^{Q}[\cdot]$ denotes the multivariate cubature approximation.

- Approximate the gPC coefficients in Eq. (4) using the numerical integration rule in Eq. (5).