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Uncertainty quantification and global sensitivity analysis of complex chemical processes with a large number of input parameters using compressive polynomial chaos

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ABSTRACT

Uncertainties are ubiquitous and unavoidable in process design and modeling while they can significantly affect safety, reliability, and economic decisions. The large number of uncertainties in complex chemical processes make the well-known Monte-Carlo and polynomial chaos approaches for uncertainty quantification computationally expensive and even infeasible. This study focused on the uncertainty quantification and sensitivity analysis of complex chemical processes with a large number of uncertainties. An efficient method was proposed using a compressed sensing technique to overcome the computational limitations for complex and large scale systems. In the proposed method, compressive sparse polynomial chaos surrogates were constructed and applied to quantify the uncertainties and reflect their propagation effect on process design. Rigorous case studies were provided by the interface between MATLAB™ and Aspen HYSYS™ for a propylene glycol production process and lean dry gas processing plant. The proposed methodology was compared with traditional Monte-Carlo/Quasi Monte-Carlo sampling-based and standard polynomial chaos approaches to highlight its advantages in terms of computational efficiency. The proposed approach could mitigate the simulation costs significantly using an accurate, efficient-to-evaluate polynomial chaos that can be used in place of expensive simulations. In addition, the global sensitivity indices, which show the relative importance of uncertain inputs on the process output, could be derived analytically from the obtained polynomial chaos surrogate model.

1. Introduction

The presence of uncertainty is inevitable in the real-world implementation of engineering systems. The problems of process design under uncertainties have attracted considerable attention, especially regarding safety, reliability, and economic decisions (Abubakar et al., 2015). On the other hand, the design level needs to consider the uncertainty in process inputs, such as pressure, temperature, feed flow, pH, density, concentration, etc. (Arellano-Garcia and Wozny, 2009; Ostrovsky et al., 2012; Sun and Lou, 2008; Vasquez and Whiting, 2004). These uncertainties often have negative influences on the design accuracy. Hence, they need to be accounted for when constructing process models (Beck,

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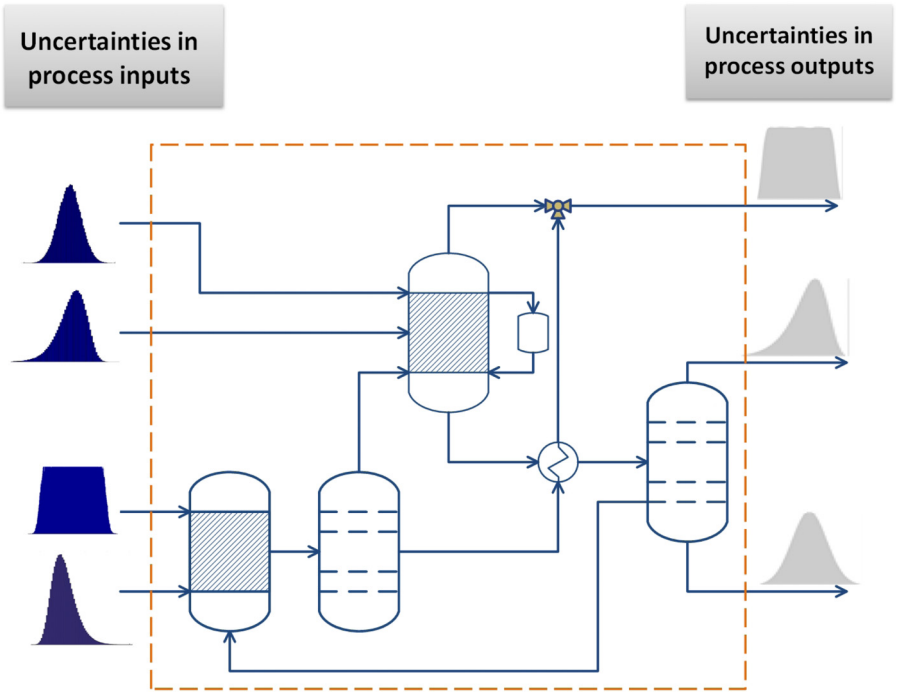

Fig. 1 – Uncertainty propagation and quantification in chemical processes.

1987). Sensitivity analysis can then be used to identify key parameters that drive the uncertainty of process output predictions qualitatively or quantitatively (Saltelli et al., 2004a).

Most tools available for rigorous process design predict the performance without considering the uncertainties. Hence, it is essential to develop efficient tools for sensitivity analysis (SA) and uncertainty quantification (UQ). The probabilistic approach is a common framework for tracing the effects of uncertainty on the model output. 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 (Abubakar et al., 2015; Binder, 1998; Caflisch, 1998; Coulibaly and Lécot, 1998; Kroese et al., 2011; Liu, 2008). The principle of MC/QMC methods is to generate an ensemble of random realizations from its uncertainty distribution, to evaluate the model for each element of a sample set, and estimate the relevant statistical properties, such as the mean, standard deviation, and quantile of the output. Despite the simplicity in their implementation, estimations of the mean converge with the inverse square root of the number of runs, making the MC—based approach computationally expensive and even infeasible for most complex chemical process problems. One approach to mitigating the combined simulation cost is to construct an accurate and efficient-to-evaluate surrogate model that can be used in place of expensive simulations (Celse et al., 2015).

Recently, uncertainty analysis using a surrogate model, such as generalized polynomial chaos (gPC) expansion was examined for a range of applications, including modeling, control, robust optimal design, and fault detection problems. The gPC method, which was first proposed by Wiener (1938), is a spectral representation of a random process by the orthonormal polynomials of random variables. Nagy and Braatz (2007) considered the gPC approach for uncertainty quantification and the robust design for a batch crystallization process. They reported that the gPC approach is more computationally efficient for a system with a moderate number of random inputs than MC/QMC methods. Duong and Lee (2012, 2014) considered the PID controller design for fractional order and integer order systems using the gPC method. Du et al. (2015) examined the fault detection problem by combining the maximum likelihood with the gPC framework. Duong et al. (2016) analyzed the problem of uncertainty quantification/sensitivity analysis of rigorous processes with a small number of random inputs using the standard polynomial chaos (PC) method. Xiu and Karniadakis (2002) further generalized the gPC for non-standard distributions through the Askey scheme.

When adequate smoothness conditions were provided, the gPC expansion for engineering purposes with a uniform and Gaussian distribution showed rapid convergence; in some cases, even exponential convergence was obtained (Ghanem and Spanos, 2003). In theory, there are two main computational schemes for building up a PC model: intrusive and non-intrusive. In the intrusive schemes, the gPC coefficients are obtained by a Galerkin scheme that leads to a system of coupled deterministic equations. Alternatively, a non-intrusive scheme allows the computation of a stochastic model using a set of (decoupled) calls to the existing deterministic model. A current limitation of the standard full non-intrusive gPC approach, where the coefficients are estimated using the tensor cubature, is that the number of model evaluations grows exponentially and may not applicable to systems with a large number of uncertainties. To address this problem, this paper describes a non-intrusive method that builds a sparse gPC expansion using the compressed sensing technique. Under the assumption that the model output prediction produces a sparse representation, the compressed sensing technique can reduce the computational cost compared to the classical full gPC (Blatman and Sudret, 2011). In addition, the limitation of classical full gPC to a system with a large number of uncertainties can be overcome effectively using the compressed sensing method. Moreover, the Sobol′ sensitivity indices (Sobol′, 2001) can also be obtained directly from the gPC surrogate analytical model (Crestaux et al., 2009; Haro Sandoval et al., 2012), which can in turn be used to detect the influential inputs in the propagation of process uncertainty.

In this paper, the convergence of an algorithm for UQ and SA is first reported on an analytical function: the Ishigami function. The method is then illustrated using case studies of complex chemical processes, such as a propylene glycol production process and a lean dry gas processing plant. HYSYS™ was used for a rigorous process simulation. The results showed that the proposed compressive gPC-based method could reduce significantly the computational cost (simulation time) for UQ over traditional approaches, such as MC/QMC/gPC methods.

2. Uncertainty quantification using compressive polynomial chaos

Consider a steady-state process described by the following set of nonlinear equations:

$$y = \mathbb{M}(\xi) \tag{1}$$