A Polynomial-Chaos based Algorithm for Robust optimization in the presence of Bayesian Uncertainty

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Abstract: The paper presents a computationally efficient approach for solving a robust optimization problem in the presence of parametric uncertainties, where the uncertainty description is obtained using the Bayes' Theorem. The approach is based on Polynomial Chaos Expansions (PCE) that are used to propagate the uncertainty into the objective function for each function evaluation, resulting in significant reduction in the computational time when compared to Monte Carlo sampling. A fed-batch process for penicillin production is used as a case study to illustrate the strength of the methodology both in terms of computational efficiency as well as in terms of accuracy when compared to results obtained with more simplistic (e.g. normal) representations of parametric uncertainty.

1. INTRODUCTION

Model-based optimization methodologies rely, primarily, on the accuracy of the model used to predict outputs over the entire space of operating conditions. Uncertainty in the model, if not accounted for, may result in non-optimal operating policies, which may lead to significant loss in the economic objectives, or even result in violations of environmental and safety constraints. However, due to either measurement noise or model structure error, the model parameters are always uncertain. In that case, it becomes very important to quantify the effect of the associated parametric uncertainty on the optimization objectives and if this effect is significant, it is necessary to either reduce the uncertainty in parameters or search for an optimum that is robust to these uncertainties.

The current study is focused on finding an optimal solution that is robust to parametric uncertainties assuming that measurements, beyond a limited set of initially available measurements, are either very difficult to obtain or not available to further reduce the uncertainty. As such, it is expected that the proposed methodology could also be applied, in the future, in other areas of process systems engineering where the effect of uncertainty needs to be considered such as Robust Nonlinear Model Predictive Control.

In contrast to nominal optimization, where the objective function calculated at the nominal values of parameters is minimized, in robust optimization, some statistical metrics of the objective function calculated over the entire parameter space is minimized instead (Beyer et al., 2007; Diwekar et al, 1996; Samsatli et al., 1998; Nagy et al., 2004). A common formulation involves minimization of a weighted sum of both the expected value of the cost and its variance due to

uncertainty, thus providing a trade-off between maximum performance and robustness as follows:

$$\min_{u} J = W_1 * E\big(f(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta})\big) + W_2 * V\big(f(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta})\big)$$

$$s.t. \quad \mathbf{g}(\mathbf{x}, \mathbf{u}, \boldsymbol{\theta}) \leq \mathbf{0} \tag{1}$$

Where, $\boldsymbol{\theta}$ is a vector of uncertain model parameters, $\mathbf{u}$ is a vector of decision variables, $\mathbf{x}$ is a vector of states, f is an objective function, $\mathbf{g}$ is a vector of equalities or inequalities which include the model equations and additional process limits, E is the expected value of the objective function f, V is the variability in the objective function f and W_1 and W_2 are weights that are problem specific.

The calculation of any statistical metrics, to be performed in the robust optimization framework, involves integrals related to the calculation of the functions E and V in equation (1) which generally do not have analytical solutions. The most common approach is to approximate the objective function f in (1) by either a first order or second order Taylor Series Expansion around the nominal parameter values (Darlington et al., 1999; Nagy et al., 2004). Although these approximations work well when the uncertainty in the parameters is not too large and the objective function is nearly linear or quadratic, for most nonlinear processes, these assumptions are not valid. For general nonlinear cases, an alternative is to use a Monte Carlo approach where the parameter values are randomly selected from the joint probability distribution and then the corresponding objective function is calculated (Diwekar et al, 1996; Beyer et al., 2007). However, in this approach, a large number of samples are required for obtaining an accurate estimate of the above integrals. Thus, when using Monte Carlo techniques, the need for extensive sampling combined with the fact that the cost function in (1) has to be computed at each function

evaluation during an iterative search for an optimum, results in a large computational burden. Another major limitation in most of the previous studies is that the parameters are estimated using either least squares or maximum likelihood method and the uncertainty description is obtained by assuming the model output to be linear around the nominal parameter values. However, for nonlinear systems, this assumption is generally inaccurate. Instead, a more accurate description of the uncertainty may be obtained from the Bayes' Theorem which gives a probability distribution instead of a point estimate. In a Bayesian approach, the posterior distribution of the parameters is proportional to a likelihood which is a function of measurements and a prior probability which represents any available information about the parameters before collecting data. If the model is highly nonlinear, the posterior distribution can potentially be of non standard form with no analytical expression. In that case, the propagation of the parametric uncertainty into the optimum is not trivial and it must be obtained, using Monte Carlo sampling methods which are computationally expensive as explained above.

In recent years, uncertainty propagation using Polynomial Chaos Expansions (PCE) has been studied by several authors from different areas (Najm, 2009; Knio et al., 2006; Nagy et al., 2007; Xiu et al., 2002, 2003; Ghanem et al., 1991) and has been shown to be much efficient and accurate when compared to Monte Carlo sampling approaches. The two major advantages of the PCEs are that they can be used to propagate any complex probability distribution into the desired output and that the mean, variance and any other higher order moments can be calculated analytically. Although few studies have also implemented the PCE in the robust optimization (Molina-Cristobal et al., 2006; Xiong et al., 2011), in all these earlier studies very simplistic descriptions of uncertainty, e.g. normal or exponential distributions, were used.

The current study proposes a systematic methodology to propagate the more accurate representation of the uncertainty in parameters, obtained using a Bayesian approach, into the optimum. The results are compared with those obtained when normal representation of uncertainty is used. Furthermore, the methodology also addresses the presence of correlation in model parameters and its effect on the PCE approximation.

The paper is organized as follows. Section 2 presents the PCE based methodology. Section 3 illustrates the proposed method for a penicillin manufacturing process followed by Section 4 with summary and conclusions.

2. METHODOLOGY

A brief description of PCE, necessary for explaining the proposed method is presented first. If $\{\xi_i(\omega)\}_{i=1}^{\infty}$ is a set of independent random variables with a standard probability density function (e.g. normal or uniform), then the PC representation of any random variable, X, with a finite variance is given as:

$$X(\omega) = a_0\Gamma_o + \sum_{i_1=1}^{\infty} a_{i_1}\Gamma_1(\xi_{i_1}) + \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1} a_{i_1 i_2}\Gamma_2(\xi_{i_1}, \xi_{i_2})$$
$$+ \sum_{i_1=1}^{\infty}\sum_{i_2=1}^{i_1}\sum_{i_3=1}^{i_2} a_{i_1 i_2 i_3}\Gamma_3(\xi_{i_1}, \xi_{i_2}, \xi_{i_3}) + \cdots$$

$$\text{(2)}$$

Where, Γ_p is the PC of order p, ω is the random event and $a_{(.)}$ is the deterministic coefficient. The above expansion can further be rewritten in a simpler form (Ghanem et al., 1991) as:

$$X(\omega) = \sum_{k=0}^{\infty} \hat{a}_k \Psi_k(\xi_1, \xi_2, \xi_3, \dots) \tag{3}$$

Where, there is a one-to-one correspondence between the functions and the coefficients of the two representations shown in (2) and (3). For computation feasibility, the expansion has to be considered in a truncated form. An underlying property of a PC expansion is that all basis functions or polynomials involved in the expansion are orthogonal. Thus the coefficients in the expansion can be calculated by projecting the expansion on a particular basis function and then taking its inner product. The resulting expression for the kth coefficient is given as:

$$\hat{a}_k = \frac{\int X \Psi_k p(\xi) d\xi}{\int \Psi_k^2 p(\xi) d\xi} \tag{4}$$

Where, $\boldsymbol{\xi}$ is the vector of independent random variables. The type of the orthogonal basis functions depends on the type of independent random variables to be used in the expansion, e.g. Hermite polynomials for normal random variables, Langrage polynomials for uniform random variables and so on.

In the current study, the idea is to use the PCE to propagate uncertainty in the model parameters $\boldsymbol{\theta}$, obtained using a Bayesian approach, into the objective function *f*. According to the Bayes' Theorem, the posterior probability of the parameters based on an initially available set of measurements is given by:

$$p(\boldsymbol{\theta}|D) = \frac{L(\boldsymbol{\theta}|D) p(\boldsymbol{\theta})}{\int L(\boldsymbol{\theta}|D) p(\boldsymbol{\theta})d\boldsymbol{\theta}} \tag{5}$$

where, $L(.)$ is the likelihood of the parameters given the measurements, $p(\boldsymbol{\theta})$ is the prior probability of the parameters and D represents the desired output based on the given measurements. Assuming the errors between predictions and measurement are independent and normally distributed, the likelihood function is equal to the product of the normal distributions of these errors.

Since the posterior distribution of the model parameters $\boldsymbol{\theta}$ may be very different from a standard distribution (e.g. normal) as required for the input random variables $\boldsymbol{\xi}$ in PCE's, $\boldsymbol{\xi}$ cannot be replaced with $\boldsymbol{\theta}$ directly in equation (3). Instead, the first step is to transform the model parameters $\boldsymbol{\theta}$

into a set of independent random variables ξ. For the one parameter case, the transformation can be obtained by:

$$\xi = F^{-1}\left(\int_0^\theta p(\theta)d\theta\right) \tag{6}$$

where, F^{-1} is the inverse of the cumulative density function for the independent random variable ξ and $p(\theta)$ is the probability of the model parameter θ.

For more than one parameter, if the parameters are uncorrelated, the transformations will be straightforward where each model parameter can be transformed into a separate independent variable according to equation (6). However, for the case of correlated parameters, the transformation is obtained using the concepts of marginal and conditional probabilities. For example, for two correlated parameters, the transformations will be as follows:

$$\xi_1 = F^{-1}\left(\int_0^{\theta_1} p(\theta_1)d\theta_1\right) \tag{7}$$

$$\xi_2 = F^{-1}\left(\int_0^{\theta_2} p(\theta_2|\theta_1)\,d\theta_2\right) \tag{8}$$

where, $p(\theta_1)$ is the marginal probability of parameter θ_1 and $p(\theta_2|\theta_1)$ is the probability of parameter θ_2 conditional on parameter θ_1

After a mapping is obtained between the parameters θ and the independent random variables ξ using (6-8), the next step is to develop a mapping between the objective function f in problem (1) and the set of independent random variables ξ. One option could be to select random values for parameters θ and then calculate for them, the corresponding objective function f by solving the model equations and the values for the set of independent random variables ξ using the transformations (6-8). However, for solving the integrals in (4) using quadrature rules, the values of the objective function f should be available at specific values of ξ, also known as collocation points and the above method may result in the values of ξ that are not the required ones. An alternate approach is to first formulate a PCE of the parameters θ as a function of the variables ξ using transformations (6-8); then, select values of independent random variables ξ at the required collocation points, calculate the corresponding values of model parameters θ from the formulated PCE's and finally calculate the objective function f by solving the model equations for each combination of model parameters.

For the one parameter case, after a mapping between model parameter θ and independent random variable ξ is obtained from equation (6), the generated pairs of corresponding θ and ξ are used to formulate the following PCE,

$$\theta = \sum_i^O \theta_i \Psi_i(\xi) \tag{9}$$

For the case of two parameters, first the mapping between model parameter θ_1 and the corresponding independent random variable ξ_1, given by equation (7) is used to

formulate the PCE for θ_1 based on its marginal probability as follows:

$$\theta_1 = \sum_i^O \theta_{1_i} \Psi_i(\xi_1) \tag{10}$$

Similarly, the mapping given by equation (8) is used to formulate the PCE for θ_2 as follows:

$$\theta_2|\theta_1 = \sum_i^O \theta_{2_i} \Psi_i(\xi_2) \tag{11}$$

Here, it should be noted that the PCE for θ_2 in (11) is conditional on a particular value of θ_1 and in the general case of correlated parameters, different values for coefficients θ_{2_i} corresponding to different values of θ_1 have to be obtained resulting in different PCEs. In order to explicitly incorporate the effect of θ_1 in the PCE in (11), the coefficients θ_{2_i} are further expanded in terms of the independent random variable ξ_1 as follows:

$$\theta_{2_i} = \sum_k^P \theta_{2_{ik}} \Psi_k(\xi_1) \tag{12}$$

Substitution of (12) into (11) results in one PCE for θ_2 which depends on both random variables ξ_1 and ξ_2 as follows:

$$\theta_2 = \sum_i^O \left(\sum_k^P \theta_{2_{ik}} \Psi_k(\xi_1)\right) \Psi_i(\xi_2) \tag{13}$$

Using the map between f and ξ, the coefficients for the PCE of objective function f are calculated using equation 4 and finally the expected value and the variance are calculated using standard PCE formulae:

$$E(f) = \hat{a}_0 \tag{14}$$

$$V(f) = \sum_{k=1}^P \hat{a}_k^2 < \Psi_k^2 > \tag{15}$$

where, $< \cdot >$ represents the inner product. The calculated expected value and variance of the objective function f are then substituted in the cost function of the problem (1) and the search for the optimum is performed using the *fmincon* function in the MATLAB Optimization toolbox. The overall methodology, to be executed at each function evaluation in the search for the optimum in problem (1), has been summarized for clarity in a stepwise procedure as follows:

1. Calculate the posterior distribution of the model parameters θ from the given data using Bayesian Inference

2. Transform the model parameters θ into a set of independent random variables ξ using (6-8) and formulate their PCEs, as given by (9-13)

3. Select values of independent random variables ξ at collocation points of the orthogonal polynomials

4. Calculate for these $\boldsymbol{\xi}$, the corresponding values of parameters $\boldsymbol{\theta}$ using PCE's 9-13

5. Calculate the values of objective function f for the $\boldsymbol{\theta}$ obtained in the previous step using model equations

6. Formulate a PCE for the objective function f and calculate the expected value and the variance using (14-15)

3. CASE STUDY: PENICILLIN PRODUCTION PROCESS

The proposed methodology is applied to a penicillin production process. The simulated data for identifying the parameters and the parametric uncertainty are obtained using the model based on the process simulator, proposed by Birol et al. (2002). For simplicity, it is assumed that there are no changes in pH and temperature and that oxygen is available in excess. Therefore, the effect of these three variables is removed from the governing equations and only a reduced set of equations, as given by equations 16-19, is used as follows:

$$\frac{dX}{dt} = \left(\frac{\mu_X * S * X}{K_X * X + S}\right) - \frac{X}{V} * \frac{dV}{dt} \quad (16)$$

$$\frac{dP}{dt} = \left(\frac{\mu_P * S * X}{K_P + S + \frac{S^2}{K_I}}\right) - K_H * P - \frac{P}{V} * \frac{dV}{dt} \quad (17)$$

$$\frac{dS}{dt} = -\left(\frac{1}{Y_{X/S}} * \frac{\mu_X * S * X}{K_X * X + S}\right)$$
$$- \left(\frac{1}{Y_{P/S}} * \frac{\mu_P * S * X}{K_P + S + \frac{S^2}{K_I}}\right) \quad (18)$$
$$- m_X * X + \frac{F * s_f}{V} - \frac{S}{V} * \frac{dV}{dt}$$

$$\frac{dV}{dt} = F - V * 6.226 * 10^{-4} \quad (19)$$

where, X is the concentration of biomass, μ_X is the specific growth rate, K_X and K_P are saturation constants, S is the concentration of substrate, V is the volume of the culture medium, P is the concentration of penicillin, μ_P is the specific rate of penicillin production, K_I is an inhibition constant, $Y_{X/S}$ is the yield of biomass per unit mass of substrate, $Y_{P/S}$ is the yield of penicillin per unit mass of substrate, m_X is the maintenance constant, F is the amount of feed and s_f is the concentration of substrate in the feed.

The initial concentrations and the inlet feed profile used to obtain the simulated is given in Table 1.

Table 1: Initial concentrations and input feed profile for the simulated data

Biomass Conc. (X_0)	0.1 (g/l)
Substrate Conc. (S_0)	1 (g/l)
Product Conc. (P_0)	0 (g/l)
Initial Culture Volume (V_0)	100 (L)
Input Feed (F)	0.04 (L/hr)

To introduce the effect of model structure error, the term representing the consumption of penicillin by hydrolysis in (17) is neglected and as a result, the rate of change of penicillin is now given by:

$$\frac{dP}{dt} = \left(\frac{\mu_P * S * X}{K_P + S + \frac{S^2}{K_I}}\right) - \frac{P}{V} * \frac{dV}{dt} \quad (20)$$

In addition, uncertainty in the data is introduced by assuming that the culture volume cannot be measured and that the measurements of the remaining three states are corrupted with Gaussian noise.

In a preliminary study, nominal values for all the parameters in the uncertain model (equations 16,18, 19 and 20) were estimated using a standard least squares' method and their variance-covariance matrix was obtained assuming the model outputs are linear around these estimates (Bard, 1974). To illustrate the methodology, the examples in this study consider only a subset of these parameters to be uncertain. The three parameters with the largest associated uncertainty, as found in the preliminary study mentioned above are K_X, K_I and K_P. The effect of uncertainty in these parameters was studied individually in three examples and the combined effect of uncertainty in K_X and K_I was studied in a fourth example. A key point of the current work was to compare the effect of the actual uncertainty description with the one obtained using standard linear approximation, on the robust optimization problem given in (1). With that goal, in all the examples, the uncertainty description for the respective parameters was obtained using both the Bayesian approach, resulting in an accurate and realistic description, and the linearization approach which for the normally distributed errors, results in the normal description of the parametric uncertainty.

Although the Bayesian based distributions are different than their normal counterparts in each example, as can be seen from their means and variances listed in Table 2, the differences are most significant for parameter K_I and the joint distribution of K_X and K_I.

Table 2: List of means and variances, comparing Bayesian and Normal distributions for each example

$\boldsymbol{\theta}$	K_X		K_P		K_I		K_X & K_I	
	Normal	Bayesian	Normal	Bayesian	Normal	Bayesian	Normal	Bayesian
E($\boldsymbol{\theta}$)	0.2892	0.3253	0.9986	1.2076	0.036	0.0589	[0.2892 0.036]	[0.2498 0.0955]
V($\boldsymbol{\theta}$)	0.0107	0.0098	0.0807	0.1605	0.000263	0.0012	[0.0122 0.0003]	[0.0089 0.004]
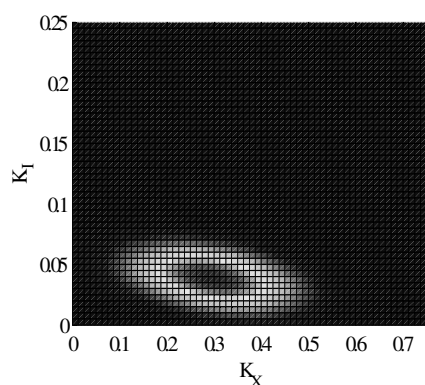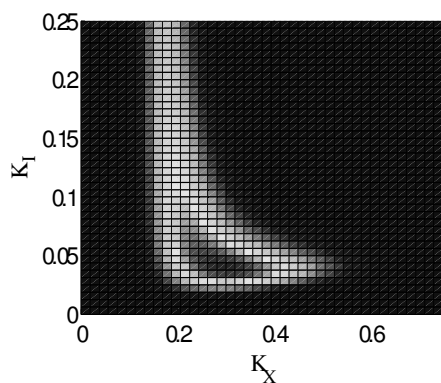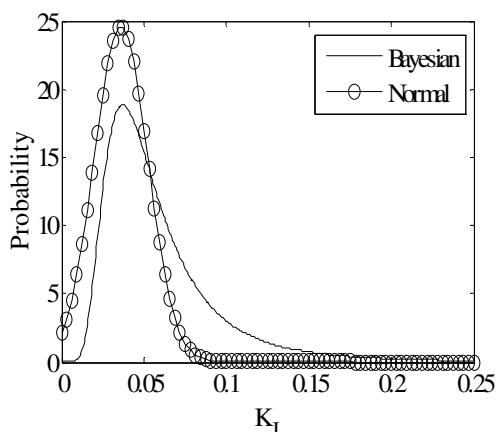
(c)

Figure 1: (a) Comparison of Bayesian and Normal uncertainty for K_I; (b) 2-D representation of joint Bayesian uncertainty for K_X and K_I (c) 2-D representation of joint normal uncertainty for K_X and K_I

For K_I, as can be seen in Figure 1a, the Bayesian uncertainty results in lower probability for values ranging between 0 to 0.01, whereas values higher than ~0.075 are more probable when compared to the normal distribution. For the joint distribution of K_X and K_I, the Bayesian uncertainty (Figure 1b) shows very strong correlation between the two parameters, with the region of K_I ranging from 0.075-0.25 and K_X ranging from 0.15-0.25 having higher probability when compared to the normal distribution (Figure 1c) for which this region has very low probability.

In the next step, it is investigated how the differences in the uncertainty descriptions in each example, i.e. Bayesian based versus Normal, affect the corresponding optimal solution. The objective of the optimization problem, in this study, was to maximize the amount of penicillin produced at a preselected final batch time with minimum variability and the volume of culture medium not exceeding 120 L. The initial substrate concentration (X_0) and the inlet feed rate (F) were selected as decision variables and a worst case scenario was considered by setting the cost function in (1) to be equal to the expectation of f minus its variance. Accordingly, the weights for the robust optimization problem posed in (1) were selected to be: $W_1 = -1$ and $W_2 = 1$. To ensure the global optimality of solution, the search was conducted using multiple initial guesses for the decision variables. The mean and variance information of the optimum objective function f is summarized in Table 3. Examination of these results clearly shows that the robust optimal solution obtained using the Bayesian representation of the parametric uncertainty differs significantly from the one corresponds to the normal representation, especially for the two parameters' case where the Bayesian description of uncertainty differs significantly from the normal, as shown in Figure 1b and 1c. The distribution of f at the optimum based on joint uncertainty in K_X sand K_I is shown in Figure 2a and 2b.

Table 3: List of means and variances of the objective function f at the optimum, based on Bayesian and Normal description of uncertainty

θ	$p(\theta)$	X_0	F	E(f)	V(f)
K_X	Normal	12.54	0.078	53.011	28.834
	Bayesian	38.04	0.150	75.953	13.756
K_P	Normal	31.74	0.277	86.58	11.801
	Bayesian	29.38	0.277	80.589	12.118
K_I	Normal	26.35	0.0797	30.546	14.087
	Bayesian	22.91	0.0799	46.933	22.135
K_X & K_I	Normal	26.87	0.0734	17.654	12.58
	Bayesian	29.16	0.1009	52.749	32.726

Since the intention is, in the future, to extend the proposed methodology to on-line schemes, it is important to assess its computational efficiency. The simulation time to propagate the Bayesian uncertainty using PCE was compared to the widely used Monte Carlo method.
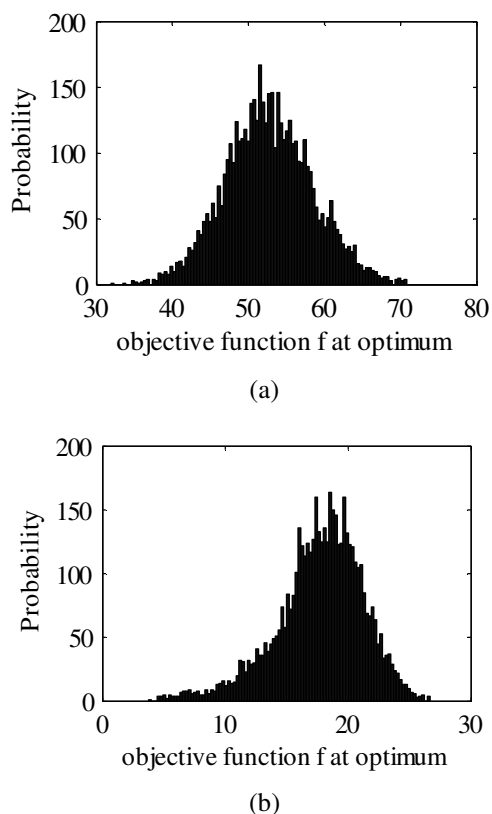
(a)

(b)

Figure 2: Probability distribution of objective function *f* at the optimum, based on the (a) Bayesian uncertainty and (b) Normal uncertainty

Using PCE, the calculation of the objective function posed in (1) for one function evaluation was completed in 2-3 seconds on average on quad-core 3 GHz Core-i7 workstation and the search for the optimum was completed after approximately 50-60 function evaluations which results in an overall simulation time of 3-4 min. On the other hand, using Monte Carlo methods, 1 hr of computation time was needed to calculate the objective function in (1). Thus 50-60 function evaluations, needed for finding the optimum would take 50-60 hours, significantly higher as compared to the proposed PCE based method

6. CONCLUSIONS

A PCE-based methodology is used to propagate uncertainty in model parameters into the objective function of a robust optimization problem. Significant differences in the optimum are obtained when realistic descriptions of parametric uncertainty are used instead of simplistic ones. The proposed methodology proved to be significantly more efficient than Monte Carlo based method thus making it attractive for future application in on-line problems. The proposed methodology, as such, can be applied for more complex cases where more than two or even all parameters are uncertain and will be studied in future work.

REFERENCES

Bard, Y. (1974). *Nonlinear Parameter Estimation*, Academic Press, New York

Beyer, H. and B. Sendhoff (2007). Robust optimization - A comprehensive survey. *Computer Methods in Applied Mechanics and Engineering*, **196(33-34)**, 3190-3218

Birol, G., C. Undey and A. Cinar (2002). A modular simulation package for fed-batch fermentation: penicillin production. *Computers and Chemical Engineering*, **26(11)**, 1553-1565.

Darlington, J., C. C. Pantelides, B. Rustem and B. A. Tanyi (1999). An algorithm for constrained nonlinear optimization under uncertainty. *Automatica*, **35(2)**, 217-228.

Diwekar, U. M. and J. R. Kalagnanam (1996). Robust Design using an Efficient Sampling Technique. *Computers and Chemical Engineering*, **20**, S389-S394.

Ghanem, R. G. and P. Spanos (1991). *Stochastic Finite Elements: A Spectral Approach*, Springer, Berlin

Knio, O. M. and O. P. Le Maître (2006). Uncertainty propagation in CFD using polynomial chaos decomposition. *Fluid Dynamics Research*, **38(9)**, 616-640.

Molina-Cristobal, A., G. T. Parks and P. J. Clarkson (2006). Finding Robust Solutions to Multi-Objective Optimization Problems using Polynomial Chaos. *Proceedings of the 6th ASMO UK/ISSMO Conference on Engineering Design Optimization*, CD-ROM. Oxford

Nagy, Z. K. and R. D. Braatz (2007). Distributional uncertainty analysis using power series and polynomial chaos expansions. *Journal of Process Control*, **17(3)**, 229-240.

Nagy, Z. K. and R. D. Braatz (2004). Open-loop and closed-loop robust optimal control of batch processes using distributional and worst-case analysis. *Journal of Process Control*, **14(4)**, 411-422.

Najm, H. N. (2009). Uncertainty Quantification and Polynomial Chaos Techniques in Computational Fluid Dynamics. *Annual Review of Fluid Mechanics*, **41**, 35-52.

Samsatli, N. J., L. G. Papageorgiou and N. Shah (1998). Robustness metrics for dynamic optimization models under parameter uncertainty. *American Institute of Chemical Engineering Journal*, **44(9)**, 1993-2006.

Xiong, F., B. Xue, Z. Yan and S. Yang (2011). Polynomial Chaos Expansion Based Robust Design Optimization. *International conference on Quality, Reliability, Risk, Maintenance and Safety Engineering*, 868-873. China

Xiu, D. and G. E. Karniadakis (2002). Modeling uncertainty in steady state diffusion problems via generalized polynomial chaos. *Computer Methods in Applied Mechanics and Engineering*, **191(43)**, 4927-4948.

Xiu, D. and G. E. Karniadakis (2003). Modeling uncertainty in flow simulations via generalized polynomial chaos. *Journal of Computational Physics*, **187(1)**, 137-167.