

Non-Intrusive Polynomial Chaos for a Realistic Estimation of Accident Frequency

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Abstract

The pivotal role of frequency analysis in quantitative risk assessments necessitates realistic and efficient prediction of their metrics. Uncertainty analysis, which aims to determine the effects of the involved input uncertainties on the output of interest form a strong basis for all the decisions to be taken based on the results of such assessments. The main purpose of this paper is to employ a non-intrusive polynomial chaos approach to simplify the model relating to the estimation of the frequency of major accidents. Such application facilitates the propagation of the associated parametric uncertainties and makes the whole process less expensive while assuring the desired accuracy when compared with the classical application of the Monte Carlo simulation.

Keywords: industrial safety; frequency of major accidents; uncertainty propagation; polynomial chaos expansion; Monte Carlo simulation

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1. Introduction

Notations:

α	Deterministic coefficient
β	Beta factor model's coefficient
λ	Failure rate
π	Probability density function
Ψ	Multivariate polynomial basis
ψ	Univariate polynomial basis
E	Number of events in one sequence
$f(X)$	Original model
$f_M(X)$	Truncated model
$f(x^{(i)})$	i^{th} evaluation of $f(X)$
$E(\cdot)$	Expected value
M	Truncation order
N	Dimension of X
n	Sample size
p	Highest polynomial order
S	Number of sequences with undesired consequences
T	Time interval
$V(\cdot)$	Variance
V_e	Probability of occurrence or non-occurrence of e
$w(\cdot)$	weighting function
w	Frequency
X	Input random vector
$x^{(i)}$	i^{th} realization of X

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<i>Y</i>	Output
Nomenclature:	
<i>avg</i>	Average
CCF	Common cause failures
<i>e</i>	Generic event in event tree analysis
<i>IE</i>	Initiating event
LE	Level emitter
LIC	Level indicator controller
LICV	Level indicator controller valve
LT	Level transmitter
MC	Monte Carlo
PC	Pressure controller
PCE	Polynomial chaos expansion
PCV	Pressure controller valve
<i>pdf</i>	Probability density function
QRA	Quantitative risk assessment
SV	Solenoid valve
<i>UC_s</i>	Sequence with undesired consequences

Major industrial accidents represent a considerable threat to not only the industrial community due to the possible immense human, material and economic losses, but also to the government and local authorities that are primarily responsible for safety. The names of several cities around the world have become associated with tragic industrial events, including Bhopal, India that witnessed in 1984 the worst industrial accident ever with a death toll that exceeded 8,000, to Tianjin, China where a series of gigantic explosions killed tens of thousands of innocents in 2015. Controlling the direct contact between the industrial facilities that deal with highly hazardous substances and humans represents a critical challenge.

In order to ensure that the risks that have potential to cause major damages are profoundly identified, analyzed, evaluated and controlled, several legislative and normative frameworks have been created and updated over the years, including the Seveso Directive for the control of major-accident hazards involving dangerous substances (Directive 2012/18/EU) and the Process Safety Management of Highly Hazardous Chemicals Standard (29 CFR 1910.119).

Quantitative risk assessment (QRA), which forms the backbone of such frameworks, aims to exhaustively reveal and identify all the sources of hazards associated with the studied installation, including materials and activities that can cause harm as well as determined vulnerable targets (safety and health of people, property, environment, etc.). Then, it creates all the possible scenarios that can lead to the recalcitrance of such sources in the presence of certain favorable conditions, quantify the accompanying risks that are conventionally characterized by the likelihood of occurrence of those undesired events, and determine the severity of the consequences. After, it evaluates those risks against specific criteria to weight and determine their acceptability. The main constituents of the conventional quantitative risk assessment are profoundly described in [1]. Nevertheless, such assessments predict and highlight several pivotal points, including the amount of the possible losses and performance level of the utilized safeguarding systems with respect to that of the needed safety.

Indeed, frequency analysis and consequence modeling form together the heart of QRA. However, the focus in this work is on the frequency analysis, which aims to measure the occurrence likelihood (represented by the occurrence frequency) of each potential major accident. This latter measure is employed to judge the acceptability of such events by comparing its value to certain predetermined thresholds. Accordingly, it provides direct and substantial support for the decision-making process in the context of safety and environment preservation. The genuine estimation of such measure is based on the inclusion of all the technical, human and natural causes that can contribute to the deviation of the processes from the normal operation as well as the inability of the employed safeguarding measures to detect and control such deviations. Several methods and tools can be used to perform such a task, such as Fault and Event Tree analyses, Markov models and Petri nets.

Bow-Tie diagrams have been widely used as a sort of combination of Fault Tree analysis and Event Tree analysis attached to each other at one central point, which represents the initiating event, to visualize the chronology of an accident in an arborous structure. In such models, the quantification of the average frequency (w^{avg}) of a given accident over a specific period of time that equals T can be performed using Equation (1), which assumes the independency between the involved events.

$$w^{avg} = \sum_{s=1}^S w_{UC_s} = \sum_{s=1}^S \left(\frac{1}{T} \int_0^T w_{IE}(t) \prod_{e=1}^E V_e(t) dt \right)_s \quad (1)$$

Where w_{UC_s} denotes the frequency relating to the s^{th} sequence that yields the studied undesired consequence, w_{IE} is the frequency of the initiating event that can be obtained from the quantitative treatment of the associated Fault Tree, and V_e denotes the probability of occurrence or non-occurrence of the e^{th} generic (pivotal) event involved in that specific sequence, which holds a total number of E different events. In the case where the generic events in the Event Tree are considered as safeguarding measures, V_e will represent the availability or the unavailability of the e^{th} measure, which can be estimated using supplemental Fault Tree analyses or any other reliability tool, such as Markov models.

However, as pointed out in [2], there are uncertainties associated with all elements in QRA, from the hazard identification to the models and probability calculations. Uncertainties are generally categorized into two classes: aleatory, which characterizes the inherent randomness that makes it irreducible, and epistemic, which represents the lack of knowledge that disappears as soon as the needed knowledge becomes available. The probabilistic framework is regarded as the suitable basis for treating the aleatory uncertainty, while many frameworks (e.g., fuzzy sets theory [3] and Dempster-Shafer theory [4-5]) have been supported for the epistemic class as alternatives to probability theory, which is often deemed inappropriate for this type of uncertainties. QRA, with its diverse elements, entails both kinds of uncertainty, which has been discussed and addressed in several references. For example, in [6] different kinds of uncertainties, Bow-Tie analysis are treated using fuzzy-based and evidence theory-based approaches. Also, in [7], a fuzzy logic approach is used to deal with uncertainties in the calculation of thermal hazard distances for consequences modeling, and recently, [8] focused on the choice of the appropriate approach to treat the uncertain assumptions in QRA.

Within the probabilistic framework for the treatment of uncertainty, the Monte Carlo simulation showed a high ability to deal with complex problems. It has been used for several decades to create the probability distribution of the output of interest by directly evaluating the relating model using a set of realizations that are sampled from the probability distributions of the involved uncertain input quantities. One of the biggest limitations of such an approach is the computational time can be very expensive for the practical complex problems. Thus, the hub in this paper is the so-called "generalized polynomial chaos expansion" that is used to simplify the model of interest by substituting it with an approximated truncated series so it can be treated easily and inexpensively with reasonable accuracy. Thus, the intended objective is the reduction of the computation cost of treating the parameter uncertainties involved in the frequency analysis of industrial risks.

Recently, many contributions have been made in this context to treat several engineering problems. For instance, a new algorithm is proposed in [9] for the design of nonlinear dynamical systems with dependent uncertain parameters. A polynomial-chaos-Legendre-meta model is presented in [10] to evaluate the time responses of engineering structures with interval and/or random parameters. In dependability, polynomial chaos expansion is employed, as seen in [11] for time-variant reliability problems and [12] for evidence theory-based reliability optimization design.

The remainder of this paper is organized as follows: Section 2 provides a theoretical description of the generalized polynomial chaos expansion with a focus on a non-intrusive regression based approach. Section 3 holds an application of such an approach to analyze the parametric uncertainties involved in the estimation of the average frequency of a potential accident that can occur in a selected steam boiler system. Finally, some concluding points are given in Section 4.

2. Polynomial Chaos Expansion

The generalized polynomial chaos expansion (also known as Wiener-Askey polynomial chaos expansion) [13] extends the original Wiener polynomial chaos expansion, which was introduced in [14] through the direct inclusion of non-Gaussian random variables with an optimal convergence rate by considering the Askey scheme polynomials [15].

Its basic idea is representing any second order random process (with finite variance), characterized here by the "scalar" output of interest $Y(Y \in L_2(\Omega, \mathcal{F}, P))$, which depends on the N -dimensional random vector $X = (X_1, X_2, \dots, X_N)$ (with elements that are considered here to be continuous and independent, so its joint pdf $\pi_X = \prod_{r=1}^N \pi_{X_r}$), that can be written as shown in Equation (2):

$$Y = f(X) = \sum_{j=0}^{\infty} \alpha_j \Psi_j(X) \quad (2)$$

Where α_j represents the "unknown" deterministic coefficients to be computed, and $\Psi_j(X)$ is a multivariate polynomial basis function that can be expressed as the product of the univariate orthogonal basis functions: $\Psi_j = \prod_{r=1}^N \psi_{j_r}(X_r)$ for the multi-index: $j = \{j_1, j_2, \dots, j_N\}$ with $|j| = \sum_{r=1}^N j_r$, which in turn represents a set of mutually orthogonal polynomials that belong to the Askey scheme (which is not the case in the original Wiener expansion where only the Hermite polynomials are considered) that of course satisfies the property of orthogonality represented in Equation (3):

$$\langle \psi_a, \psi_b \rangle = \int_{D_X} \psi_a(X) \psi_b(X) w(X) dX = h_a^2 \delta_{ab} \quad (3)$$

Where D_X is the support of X , $\langle \cdot, \cdot \rangle$ denotes the inner product, $w(X)$ is the weighting function, h is a nonzero constant with a value that equals 1 if the polynomials are orthonormal, and δ is the Kronecker delta that equals 0 for $a \neq b$ and 1 otherwise $\forall(a, b) \in \mathbb{N}^2$.

In fact, the choice of the orthogonal polynomial basis is based on the correspondence between the probability distribution function of the involved parameter and the weighting function associated with that specific sequence in order to ensure an optimal convergence rate. Taken from [13], Table 1 shows the relationship between the Wiener-Askey polynomials and their matching continuous and discrete probability distributions.

However, in the situations where other distribution families are involved, probabilistic transformations can be applied to take them into consideration.

Table 1. The correspondence of the types of Wiener-Askey polynomial chaos and their underlying random variables ($N \geq 0$ is a finite integer) [13]

	Random variables	Weiner-Askey chaos	Support
Continuous	Gaussian	Hermite-chaos	$(-\infty, \infty)$
	Gamma	Laguerre-chaos	$[0, \infty)$
	Beta	Jacobi-chaos	$[a, b]$
	Uniform	Legendre-chaos	$[a, b]$
Discrete	Poisson	Charlier-chaos	$\{0, 1, 2, \dots\}$
	Binomial	Krawtchouk-chaos	$\{0, 1, \dots, N\}$
	Negative binomial	Meixner-chaos	$\{0, 1, 2, \dots\}$
	Hypergeometric	Hahn-chaos	$\{0, 1, \dots, N\}$

In spite of the nature of the chosen polynomial bases, the expected value (E) and variance (V) of Y with orthonormal polynomials can be expressed as shown in Equations (4) and (5) respectively:

$$\begin{aligned} E(Y) &= \int_{\Omega} y \pi_y dy = \int_{\Omega} \left(\sum_{j=0}^{\infty} \alpha_j \Psi_j(x) \right) \pi_x dx \\ &= \alpha_0 \int_{\Omega} \Psi_0(x) \pi_x dx + \sum_{j=1}^{\infty} \alpha_j \int_{\Omega} \Psi_j(x) \pi_x dx = \alpha_0 \end{aligned} \quad (4)$$

$$\begin{aligned} V(Y) &= \int_{\Omega} (y - E(Y))^2 \pi_y dy = \int_{\Omega} y^2 \pi_y dy - (E(Y))^2 \\ &= \sum_{j=0}^{\infty} (\alpha_j)^2 \int_{\Omega} \Psi_j^2(x) \pi(x) dx - \alpha_0^2 = \sum_{j=1}^{\infty} (\alpha_j)^2 \langle \Psi_j^2(x) \rangle \\ &= \sum_{j=1}^{\infty} (\alpha_j)^2 \end{aligned} \quad (5)$$

Practically, the infinity in Equation (2) is truncated to a certain finite number M as shows Equation (6):

$$Y \approx f_M(X) = \sum_{j=0}^M \alpha_j \Psi_j(X) \quad (6)$$

Where M can be expressed in terms of N and the highest order p of the polynomials within Ψ_j using Equation (7):

$$M + 1 = \frac{(N + p)!}{N! p!} \quad (7)$$

The estimation of the deterministic coefficients can be conducted by means of several alternative approaches that can be broadly classified into intrusive (mainly, Galerkin projection) and non-intrusive (e.g., spectral projection) methods. Typically, the intrusive methods are based on the injection of the polynomial expansions into the original governing model to obtain a set of $M + 1$ new equations that need be solved "generally" in a different way. However, such reformulation of the original model is considered unpractical in many applications. On the other hand, the non-intrusive methods treat the model as a black-box, where it is employed to propagate a certain number of input realizations through it in order to obtain a set of evaluations of the output of interest. According to [16], in which a comparison is performed between these two classes for the dynamic system uncertainty propagation, intrusive and non-intrusive methods can produce almost the same results, with an obvious superiority of the non-intrusive methods for complex problems. Additional comparisons between the two classes of approaches can be found in [17-18].

The Galerkin method that is used in [19] relies upon forcing the residual error between $f(X)$ and $f_M(X)$ to be orthogonal with respect to the space spanned by $\{\Psi_j\}_{j=0}^M$.

$$\langle f(X) - f_M(X), \Psi_j(X) \rangle = 0 \quad (8)$$

An interesting non-intrusive regression approach that gained much attention is detailed in [20-21]. This approach is based on the least-squares regression method to minimize the residual sum of squared errors between the exact and approximated solutions:

$$\begin{aligned} \arg \min_{\alpha} \left\{ \sum_{i=1}^n \left(f(x^{(i)}) - f_M(x^{(i)}) \right)^2 \right\} = \\ \arg \min_{\alpha} \left\{ \sum_{i=1}^n \left(f(x^{(i)}) - \sum_{j=0}^M \alpha_j \Psi_j(x^{(i)}) \right)^2 \right\} \end{aligned} \quad (9)$$

Where $f(x^{(i)})$ yields the i^{th} evaluation of $f(X)$ that results from the i^{th} realization $(x^{(i)})$ of X for a total number of n realizations, which must be greater than M .

As it is shown in [21], the estimation of the unknown coefficients based on the solution of such an optimization problem can be formulated as follows:

$$\hat{\alpha} = \left\{ \left(\frac{1}{n} \sum_{i=1}^n \Psi(x^{(i)}) \Psi^T(x^{(i)}) \right)^{-1} \left(\frac{1}{n} \sum_{i=1}^n \Psi(x^{(i)}) f(x^{(i)}) \right) \right\} \quad (10)$$

3. Implementation for Accident Frequency Analysis

Fully described in [22], the steam boiler system represents a kind of widely utilized systems to transfer energy from fuel sources to water for the purpose of generating steam to supply a variety of equipment and applications. In addition to its common utilization, this system is considered for the case study due to its combination of simplicity and inclusion of many representative information and elements (e.g., different kinds of safety barriers).

From a safety perspective, lack of water inside the steam boiler, which is monitored and controlled by a regulation loop (consists of two parallel level emitters (LE), a level indicator controller (LIC) and a level indicator controller valve (LICV)), with the continuous operation of the burner can lead to an excessive augmentation of pressure inside the container, which can lead to an explosion of the system. Even with the failure of the regulation loop to maintain a certain level of water, the fuel that supplies the burner is supposed to be cut off by another loop composed of the previously mentioned LE and LIC in addition to a level transmitter (LT), a solenoid valve (SV) and a pressure controller valve (PCV). The malfunctioning of this

latter loop will inevitably cause pressure augmentation inside the container. This critical situation can be overcome by means of an additional loop that consists of a pressure controller (PC), SV and PCV. Otherwise, the pressure will increase until it is freed by exploding the container.

Such scenarios are treated in [23] by employing a Bow-Tie model to show the relationship between the various involved events and their escalation to generate such accidents. Actually, the previously described components (i.e., LE, LIC, LICV, LT, SV, PCV and PC) are considered periodically tested and instantaneously repaired; therefore, only their relating failure rates (λ) and test intervals (T) are taken into account in the analysis. This latter parameter is assumed to be identical for all the components with a value that equals one year (8760 hours). Furthermore, as mentioned earlier, LE is composed of two "identical" parallel components, so the contribution of common cause failures (CCF) is taken into consideration using the Beta factor model with the parameter (β).

The quantitative treatment of the corresponding model yields Equation (11) as an approximated formula for the estimation of the average frequency of the accident:

$$w^{avg} = (\lambda_{LIC} + \beta_{LE} \lambda_{LE}) \left(\lambda_{SV} \frac{T}{2} + \lambda_{PCV} \frac{T}{2} + \lambda_{PC} \frac{T}{2} \right) + \lambda_{LICV} \left(\lambda_{SV} \frac{T}{2} + \lambda_{PCV} \frac{T}{2} + \lambda_{LT} \lambda_{PC} \frac{T^2}{3} \right) + 2(1 - \beta_{LE})^2 \lambda_{LE}^2 (\lambda_{SV} + \lambda_{PCV} + \lambda_{PC}) \frac{T^2}{3} \quad (11)$$

Data relating to the involved input parameters is given in Table 2, which was adopted from [23].

Table 2. Reliability data of the steam boiler system

Parameters	Data
λ_{LE}	$\ln N (-13.78, (0.668)^2)$
λ_{LIC}	$\ln N (-12.56, (0.843)^2)$
λ_{LICV}	$\ln N (-13.18, (0.843)^2)$
λ_{LT}	$\ln N (-14.80, (0.978)^2)$
λ_{PC}	$T (1.6E-6, 2E-6, 2.5E-6)$
λ_{SV}	$U (0.9E-6, 1.5E-6)$
λ_{PCV}	$U (2E-6, 5E-6)$
β	$U (0.1, 0.3)$

An approximated surrogate model (w_M^{avg}) is created using the discussed approach of PCE to replace the model given in Equation (11) for the purpose of analyzing the propagation of those uncertain quantities. To show the correspondence between the original model and the surrogate model, a set of 120 samples were propagated through both of them to get the results depicted in Figure 1.

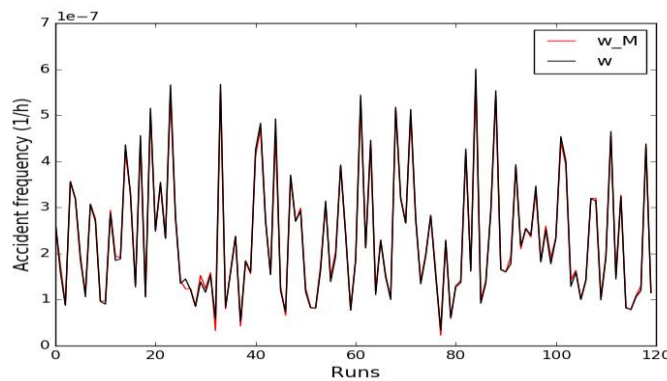


Figure 1. Simulation results of w^{avg} and w_M^{avg}

Furthermore, the created model was employed to estimate the mean and standard deviation relating to accident frequency. The obtained results are given in Table 3, which are compared to those attained by directly applying MC simulation to the original model.

Table 3. Mean and standard deviation of the accident frequency

Measure (h^{-1})	PCE	MC	MC[23]
Mean	2.11E-7	2.11E-7	2.97E-7
Standard deviation	1.64E-7	1.63E-7	2.19E-9

As illustrated in Table 3, the values of both the mean and standard deviation of w^{avg} obtained using PCE (with 170 evaluations) are almost identical to the those of MC simulation (with $5E+5$ runs). The matter that shows the important benefit in terms of computational cost can be gained by employing PCE. However, the MC results given in [23] look a little different especially for the standard deviation. The matter that can be referred to the dissimilarity of the used codes including the utilized sampling technique.

To further study those two measures, their values are estimated using a set of model evaluations by using the PCE and MC methods. Figures 2 and 3 show the obtained results, which represent the convergence of the values of the mean and standard deviation respectively with regard to the number of simulations obtained using the two methods. Obviously, the mean value stagnates starting from 120 runs in the case of PCE, while $3E+4$ for the MC simulation. On the other hand, the value of the standard deviation stagnates almost from 150 runs for PCE and from more than $1E+5$ for the MC simulation.

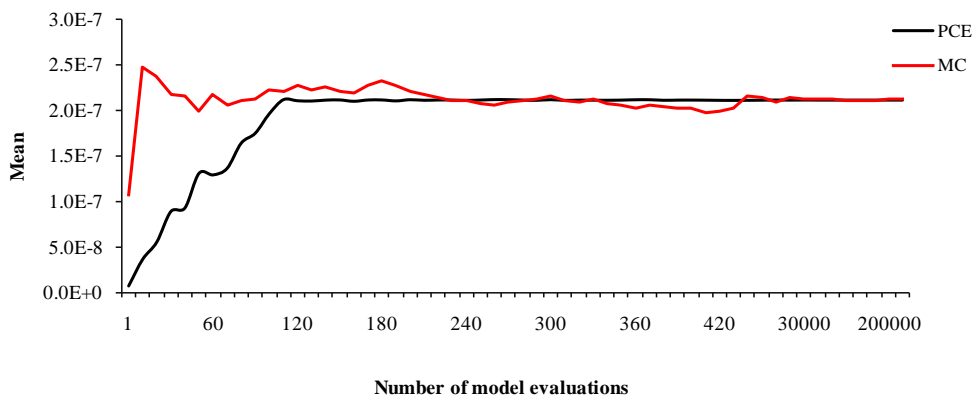


Figure 2. Mean values obtained from PCE and MC methods

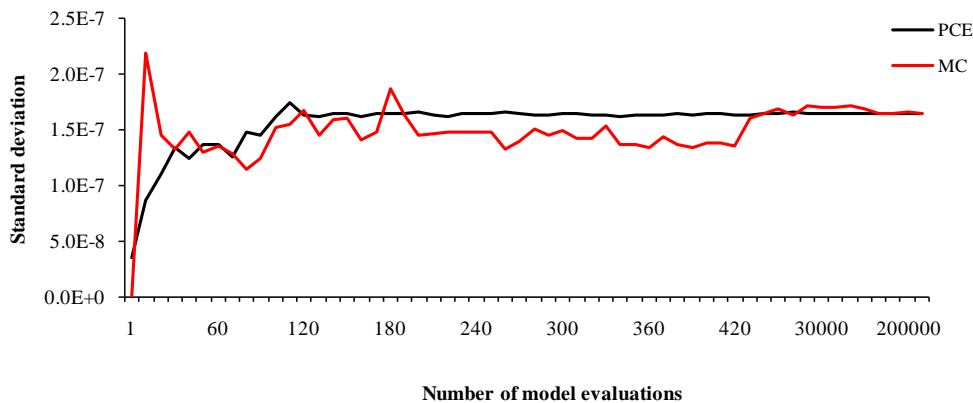


Figure 3. Standard deviation values obtained from PCE and MC methods

4. Conclusions

This paper aimed to treat the parametric uncertainty related to the estimation of the frequency of major industrial accidents, which form the prime basis upon which several decisions should be taken that have direct impacts on human safety, the environment, etc. The main contribution of this work lies in the utilization of a non-intrusive polynomial chaos approach to build a surrogate model that can effectively substitute the original model with extra flexibility.

The application of such an approach in the estimation of explosion frequency of a steam boiler system showed an important superiority of the method in comparison with the classical application of the Monte Carlo simulation in terms of the required number of simulations. Indeed, such superiority can be extremely beneficial for highly complex practical systems that encompass large numbers of highly uncertain parameters.

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