Comparison of different approaches to determine the effect of uncertainties in detailed chemistry on auto-ignition delay for air-hydrogen mixtures

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Abstract
The propagation of uncertainties in the chemical reaction rate constants onto the auto-ignition delay of an air-hydrogen mixture is studied with different approaches. An analysis of variance is carried out to reduce the number of stochastic dimensions of the problem to three reactions for the investigated case. Comparisons between Monte-Carlo method, adaptative cubature method and Polynomial Chaos expansion are then made, regarding both the accuracy and the computational cost.

1. Introduction

In self-igniting systems, the auto-ignition delay is an extensively used quantity in both low-order models and more advanced turbulent combustion models for Reynolds Averaged Numerical Simulations or Large Eddy Simulations. Its computation relies on detailed chemistry mechanisms in homogeneous reactors. However, the inherent uncertainty in the kinetic parameters of detailed chemistry mechanisms induces an uncertainty on the auto-ignition delay itself that must be evaluated in order to characterize some limitations in the aforementioned models.
Assuming small uncertainties, approaches based on sensitivity analysis [1] or variance propagation [2] have been used on chemical system. However, such approaches are not well suited for problems containing large uncertainties, where probabilistic methods are more adequate. Recent years have seen the development of spectral methods, which can be intrusive [3] or non intrusive [4]. Nonetheless, spectral methods suffer from the curse of dimensionality [5], and thus can not be used with detailed chemical mechanism.
The goal of this paper is to study the uncertainty on the auto-ignition delay of an air-hydrogen mixture due to uncertainties in the chemical reaction rate constants of a detailed mechanism. To do so, reference results using a Monte-Carlo method are first obtained on the full stochastic problem involving 33 uncertain chemical reaction rate parameters. Mean, variance and PDF of the auto-ignition delay are thus obtained. Then, the computation of Sobol indices allows to identify irrelevant uncertain reactions. This leads to reduced problems involving only three uncertain parameters at most. Monte-Carlo results are then compared to different methods affordable and more efficient in low dimensional problems, such as cubature methods, Polynomial Chaos [6].

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2. Uncertainty quantification of the auto-ignition delay: Reference results

2.1. Problem settings

Propagation of uncertainties in chemical reaction rates onto the auto-ignition delay of an air-hydrogen mixture is carried out by considering the detailed reaction mechanism from Konnov [7]. The mechanism involves 9 species and $n = 33$ reactions. For each reaction, uncertainty factors UF_i are given along with pre-exponential constants A_i, temperature exponents n_i and activation energies E_i. Uncertainties on the efficiencies of third body are also provided but are not taken into account in this study.
The prescribed uncertainty factors UF_i vary between the value 1.2 and 3.2 and characterize the full uncertainty in each reaction rate expression. Uncertain reaction rates are modeled as the deterministic ones multiplied by an uncertain coefficient. This is equivalent to consider that pre-exponential constants A_i are the only uncertain parameters. Thus, the constants A_i are assumed to be independent random variables with log-normal distributions. Those distributions are each characterized by their uncertainty factor UF_i, which defines a 3σ confidence interval (99.6% confidence interval):

$$Probability\left(A_i \in \left[\frac{A_i^0}{UF_i}, A_i^0\, UF_i\right]\right) = 0.996 \qquad (1)$$

The value A_i^0 is the nominal value of the pre-exponential constant as given by the detailed mechanism, and corresponds to the median value of the log-normal distribution.
The investigated mixture throughout this study is a stoichiometric air-hydrogen mixture with a temperature of 1100 K and a pressure of 1 atm.

2.2. Characteristics of the auto-ignition delay uncertainty

Once a chemical mechanism and initial thermodynamical conditions are prescribed, the auto-ignition delay

τ of the air-hydrogen mixture is determined from calculation of a homogeneous reactor at constant pressure. The auto-ignition delay is here defined as the instant where the mixture temperature is 200 K above the fresh gases initial temperature. Since only the pre-exponential constants A_i are considered uncertain, the mean auto-ignition delay $\overline{\tau}$ is given by computing the following integral:

$$\overline{\tau} = \int_{\mathbb{R}_+^n} \tau\left(A_1, ..., A_n\right) p\left(A_1, ..., A_n\right) \mathrm{d}A_1 ... \mathrm{d}A_n, \quad (2)$$

where $p\left(A_1, ..., A_n\right)$ is the joint Probability Density Function (PDF) of the pre-exponential constants. As shown in Eq. (2), the computation of the mean auto-ignition delay and of other moments such as the variance relies on the evaluation of multidimensional integrals. Various methods exist to approximate numerically such integrals. Given the high-dimensionality of the uncertain problem ($n = 33$), the only affordable approach for the full problem is the Monte-Carlo method.

2.3. Monte-Carlo method

2.3.1. Presentation of the method

Monte-Carlo method [8] is a stochastic method to compute integrals from probability theory. The convergence rate is quite slow as it is inversely proportional to $\sqrt{N_{eval}}$ where N_{eval} is the number of evaluation of the function to integrate. Nonetheless, a key advantage of the Monte-Carlo method is that the asymptotical convergence rate is independent of the dimension of the problem, avoiding the "curse of dimensionality" that affects other methods. Thus, the Monte-Carlo method becomes the most efficient numerical integration method for problems with a large dimensionality, typically more than 4 or 5 [9]. Besides, the accuracy of the results can be estimated and therefore controled.

By generating independent random pre-exponential constants $A_i^{(j)}$ following their prescribed lognormal distribution, the mean auto-ignition delay is estimated by

$$\overline{\tau} \approx \frac{1}{N_{eval}} \sum_{j=1}^{N_{eval}} \tau\left(A_1^{(j)}, ..., A_n^{(j)}\right). \quad (3)$$

In practice, the random parameters $A_i^{(j)}$ are generated from random number generators of uniform distribution. Thus, $A_i^{(j)} = F(v_i^{(j)})$ where the variables v_i follow a uniform distribution on an interval $[a, b]$. The integral in Eq. (2) can then be written equivalently as the following one:

$$\overline{\tau} = \frac{1}{(b-a)^n} \int_{[a,b]^n} \tau\left(F(v_1), ..., F(v_n)\right) \mathrm{d}v_1 ... \mathrm{d}v_n \quad (4)$$

This expression of the integral on an hypercube will be useful for cubature methods introduced in Sec. 4.2.

2.3.2. Monte-Carlo results

The Monte-Carlo method is carried with all 33 uncertain reactions taken into account. The required accuracy for the mean and standard deviation of the auto-ignition delay is set to 1%. The results are presented in Tab. 1. The mean value $\overline{\tau}$ differs slightly from the deterministic value of the auto-ignition delay $\tau^0 = 109.90\,\mu$s. The standard deviation σ_τ is roughly 8% of the mean auto-ignition delay, showing that the uncertainties in the detailed mechanism result in a moderate uncertainty in τ for the investigated case.

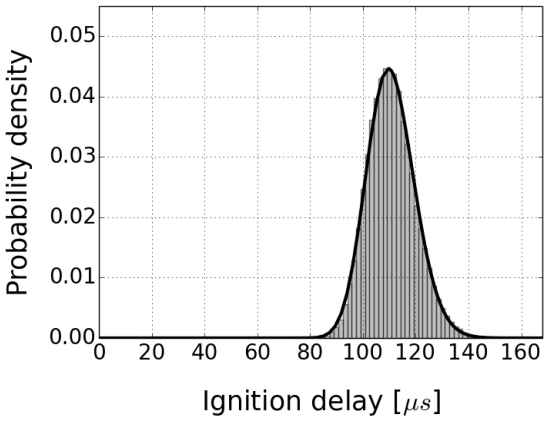

Figure 1: Histogram of the PDF of the auto-ignition delay taking into account all 33 uncertain chemical parameters A_i. Plain black line: fitted lognormal distribution profile.

$\overline{\tau}$ (μs)	σ_τ (μs)	N_{eval}	T_{cpu}	UF_τ
110.76 ± 0.11	9.07 ± 0.09	11,559	$6h40m$	1.266

Table 1: Mean ($\overline{\tau}$), standard deviation (σ_τ) and uncertainty factor UF_τ of auto-ignition delay, number of evaluations (N_{eval}), computational time (T_{cpu}) using the Monte-Carlo method for the full mechanism. Standard deviations of the estimated value of $\overline{\tau}$ and σ_τ are given.

An histogram of the PDF of the auto-ignition delay is presented in Fig. 1 along with a lognormal distribution with the same mean and standard deviation. The good agreement demonstrates that the distribution of τ can here be molded by a lognormal.

3. Dimension reduction

3.1. Sensitivity analysis based on Sobol indices

Among all parameters in the full problem, several of them might not contribute noticeably to the resulting uncertainty in the auto-ignition delay. Identifying irrelevant dimensions help decreasing significantly the dimensionality of the problem. If the number of remaining dimensions is not too large, other approaches more efficient than the Monte-Carlo method can be considered.

An analysis of variance is carried out where Sobol indices for each reaction are computed using Polynomial Chaos (PC) [10]. The Sobol index of a chemical reaction rate is the ratio between the variance due to the corresponding uncertain pre-exponential constant on the total variance.

It varies then between 0 and 1 and quantifies the global sensitivity of the uncertainty in the auto-ignition delay for each reaction.

3.2. Relevant reactions

In the condition prescribed for the initial mixture, only 3 Sobol indices, reported in Tab. 2 have been found greater than 1%. The sum of the Sobol indices associated to these 3 reactions is 97%, which shows that they account for most of the variance in the auto-ignition delay. The influence of the uncertainty in other reactions is negligible.
Although the uncertainty factors of the three reactions are quite low compared to others, the impact of those reactions on the uncertainty is the more important. This is not surprising given that the identified reactions are well-known for their key role in auto-ignition at high temperature. For the investigated mixture, reducing the uncertainty in the auto-ignition delay requires mainly to increase the accuracy of $H + O_2 = OH + H$.

Reaction	UF_i	S_i
$H + O_2 = OH + H$	1.5	88%
$O + H_2 = OH + H$	1.3	5%
$H_2 + OH = H_2O + H$	2.0	4%

Table 2: Chemical reaction, uncertainty factor (UF_i) and Sobol indices (S_i) for the 3 reactions with an associated Sobol indice greater than 1%.

As only three reactions have a significant impact, the dimensionality of the problem is strongly reduced by considering only these three reactions to be uncertain. Other chemical reaction rate constants are set to their nominal value. The impact of the reduced dimensionality is studied by considering one, two or three uncertain reactions. The corresponding 1D, 2D and 3D problems are given in Tab. 3.

	Uncertain reactions
1D	$H + O_2 = OH + H$
2D	$H + O_2 = OH + H$ $O + H_2 = OH + H$
3D	$H + O_2 = OH + H$ $O + H_2 = OH + H$ $H_2 + OH = H_2O + H$

Table 3: Uncertain chemical reactions taken into account in the 1D, 2D and 3D problems.

4. Uncertainty quantification of the auto-ignition delay: Reduced problems

The aforementioned reduced problems are hereafter considered with different approaches.

4.1. Monte Carlo results

The Monte-Carlo method has been applied to the $1D$, $2D$ and $3D$ problems. Results are presented in Tab. 4. The mean and standard deviation of the auto-ignition delay are determined with an accuracy of 1%, providing reference results of the resulting uncertainty in these reduced problems.

	$\overline{\tau}$ (μs)	σ_τ (μs)	N_{eval}	T_{cpu}	UF_τ
$1D$	110.64 ± 0.17	8.56 ± 0.08	2,508	$1h26m$	1.251
$2D$	110.68 ± 0.13	8.70 ± 0.09	6,220	$3h34m$	1.256
$3D$	110.84 ± 0.12	8.90 ± 0.08	5,006	$2h51m$	1.261

Table 4: Mean ($\overline{\tau}$), standard deviation (σ_τ) and uncertainty factor UF_τ of auto-ignition delay, number of evaluations (N_{eval}), computational time (T_{cpu}) using the Monte-Carlo method for the reduced problems. Standard deviations of the estimated value of $\overline{\tau}$ and σ_τ are given.

On the one hand, the reduction of dimension has no impact on the mean auto-ignition delay compared to the value obtained by taking into account all reactions as uncertain. On the other hand, the resulting standard deviation σ_τ decreases slightly. This reduction is linked to the Sobol indices of the retained uncertain reactions as shown in Tab. 5 where the relative variation of σ_τ compared to the value σ_τ^{ref} in Sec. 2.3.2 on the full problem is given.

Case	$\left(\sigma_\tau/\sigma_\tau^{ref}\right)^2$	$\sum S_i$
$1D$	89%	88%
$2D$	92%	93%
$3D$	96%	97%

Table 5: Comparison between the ratio of variances $\left(\sigma_\tau/\sigma_\tau^{ref}\right)^2$ and the sum of Sobol indices associated to the reactions involved ($\sum S_i$) for the different studied cases.

An histogram of the probability density function of the auto-ignition delay is presented on figure 2 only for the $3D$ case. The agreement with the previously fitted lognormal distribution is remarkable, demonstrating the adequacy of the dimension reduction.

4.2. Cubature methods

Contrary to the Monte-Carlo method which is stochastic, cubature methods are deterministic, which means that they use predefined points and weights, specific to the chosen method to calculate an approximation of the integral. When the number of dimensions is small, such methods significantly outperform the Monte-Carlo method. Multidimensional integral approximations rely on quadrature rules in one dimension which are first briefly detailed.

4.2.1. 1D quadrature rule

Among classical quadrature rules, one can cite trapezoidal and Simpson's rule. Other quadrature rules like Gauss-Legendre [11], Clenshaw-Curtis and Fèjer [12] quadrature rules are much more interesting because of their very high convergence rate (spectral like) under some assumptions on the regularity of the function.
All quadrature rules considered throughout this study will

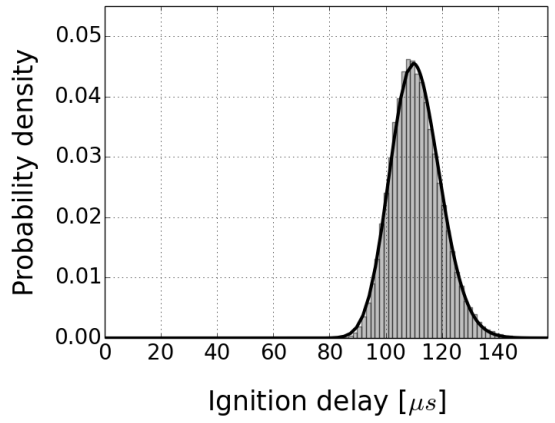

Figure 2: Histogram of the PDF of the auto-ignition delay of the $3D$ case. Plain black line: fitted lognormal distribution profile of the full problem.

be quadrature rules on the $[-1, 1]$ interval, which remains general as seen in obtaining Eq. (4). Thus, if only one uncertain reaction is considered, the mean auto-ignition delay can be expressed as:

$$\overline{\tau} = \frac{1}{2}\int_{[-1,1]} \tau\left(F\left(v\right)\right) dv \approx \sum_{i=1}^{N} w_i \tau\left(F\left(v_i\right)\right) \qquad (5)$$

In this expression, the v_i are points of $[-1, 1]$ where the function has to be evaluated, and the w_i are weights characteristic of the quadrature rule considered. The convergence rate with the number of evaluations N_{eval} is an important criterion for choosing a quadrature rule, but some other criteria have also to be taken into account.
In our case, the extremity of the interval (i.e. -1 and 1) correspond to a forward chemical rate constant equal to 0 or to a forward chemical rate constant equal to ∞. Those extreme values for the chemical rate constant can lead to an absence of auto-ignition, which corresponds to an infinite auto-ignition delay. Those situation have normally a zero-probability for a lognormal distribution, but the use of a quadrature rule that relies on those extreme values gives them a non-zero probability due to the corresponding weight which can be non-zero there. As a consequence, quadrature rules such as Clenshaw-Curtis that use the points -1 and 1 in their estimation are not retained.
Another desirable property is to use nested quadrature rules. A nested quadrature rule allows to reuse the previous evaluations when increasing the number of points to gain in accuracy. This is not the case of the Gauss-Legendre quadrature rule.
All those reasons led us to choose using the second Fèjer quadrature rule: it is a nested quadrature rule that does not rely on the extreme values of the interval.

4.2.2. Multidimensional cubature

Cubature methods are extensions of mono-dimensional quadrature rules in multidimensional integration problems. Cubature methods are obtained by tensorization of quadrature rules that are used on each dimension. This tensorization gives a grid of points with weights where the integrated function is evaluated.
One big problem of the cubature methods is that, for a given accuracy of the estimator of the integrals, the number of evaluations grows exponentially with the number of dimensions. This phenomena, called the "curse of dimensionality", is the reason why in practice, the Monte-Carlo method remain better than all cubature methods for multidimensional problems involving more than 4 or 5 dimensions [9].
It is possible to moderate the "curse of dimensionality" by using a sparse grid instead of the full grid obtained by a simple tensorization. Sparse grids can be obtained using the method first proposed by Smolyak [13]. However, only nested quadratures rules can be used to build sparse grids.

4.2.3. Cubature method results

Sparse grids coupled to the second Fèjer quadrature rule have been used to compute the mean and the standard deviation of the auto-ignition delay in the $1D$, $2D$ and $3D$ reduced problems. The implementation of the algorithm used to construct sparse grid is based on the one presented in [14]. This algorithm iteratively construct an adaptative sparse grid to estimate the value of the integral. It stops when the difference of the estimator's value between two successive steps of the computation is below a prescribed accuracy. Here, this criterion has been taken equal to 1% of the value of the estimator, for both the mean and the standard deviation. This is identical with the previous results obtained with the Monte-Carlo method. The results for the different cases are presented in the Tab. 6.

	$\overline{\tau}\ (\mu s)$	$\sigma_\tau\ (\mu s)$	N_{eval}	T_{cpu}	UF_τ
$1D$	110.56 ± 0.01	8.51 ± 0.09	31	$13s$	1.249
$2D$	110.53±0.008	8.75 ± 0.05	33	$48s$	1.257
$3D$	110.83 ± 0.34	8.86 ± 0.05	383	$115s$	1.260

Table 6: Mean ($\overline{\tau}$), standard deviation (σ_τ) and uncertainty factor UF_τ of auto-ignition delay, number of evaluations (N_{eval}), computational time (T_{cpu}) using cubature method based on second Féjer quadrature rule.

The indicated errors correspond to the value of the stop criterion between the two last steps. Results are similar to the ones obtained with the Monte Carlo method in Tab. 5. The CPU time is much less than the CPU time for the Monte-Carlo for the same cases, which confirm the fact that cubature methods are much more advantageous in low dimension problems. However, an histogram of the PDF of the auto-ignition delay is not accessible directly with cubature method. This drawback that is not

present in methods such as polynomial chaos expansion which provide a surface response for $\tau A_1, ..., A_n$ along with an estimation of the mean and variance of τ.

4.3. Polynomial Chaos

4.3.1. Presentation of Polynomial Chaos

The auto-ignition delay, as a multidimensional function, can be approximated by Polynomial Chaos (PC) expansion [15], introduced for the first time in [6]. Those Polynomial have the property to form an orthonormal basis as explained in [14]. This expansion of the auto-ignition delay in terms of PC can be expressed as:

$$\tau\left(F\left(v_1, ..., v_n\right)\right) \approx \sum_{i=0}^{N_p} \alpha_i P\left(v_1, ..., v_n\right) \tag{6}$$

Due to the orthonormal character of the PC basis, the mean and the variance of the auto-ignition delay have simple expression in function of the coefficient α_i:

$$\bar{\tau} = \alpha_0 \tag{7}$$

$$Var\left(\tau\right) \approx \sum_{i=1}^{N_p} \alpha_i^2 \tag{8}$$

Furthermore, the PC expansion gives an approximation of the auto-ignition delay, which can be used as a response surface. Therefore, the knowledge of the α_i is necessary. In this study, the substitution of the equation 4 has been done, and the corresponding PC considered are the generalized PC of Legendre polynomial [16], and the expression of the corresponding coefficients α_i is given by the following integral:

$$\alpha_i = \frac{1}{2^n} \int_{[-1,1]^n} \tau\left(F\left(v_1, ..., v_n\right)\right) P_i\left(v_1, ..., v_n\right) dv_1 ... dv_n \tag{9}$$

This integration can be done using Monte-Carlo or cubature methods. An interest of this expansion is that an evaluation onto this surface response is significantly less expensive than a direct evaluation of the auto-ignition delay, and a Monte-Carlo simulation on this surface response can rapidly give approximate CDF or PDF of the auto-ignition delay. Thus, even if a cubature method has been used to compute the projection coefficient α_i, one can access to the PDF or the CDF of the function indirectly thanks to the response surface given by the PC expansion.

Unfortunately, the PC suffer also from a curse of dimensionality. Indeed, for a PC basis in a multidimensional case involving n variables, and with a maximum degree d for the polynomials of the basis, the number N_p of polynomials in the basis is given by :

$$N_p = \frac{(n+d)!}{n!d!} \tag{10}$$

Depending on the function, one can need to use polynome of high degree to approximate correctly the function, and thus have a good response surface. Due to the dependance of the number of polynome in the basis with the dimension and the degree, it is not possible in high dimensional problem to have high degree for polynomials for computational cost. The use of PC to obtain a response surface is thus often restricted to low dimensional problems.

4.3.2. Polynomial Chaos results

The cubature method of Sec. 4.2.3 was used to compute coefficients α_i of PC expansions of maximum degree varying from one to four for $1D$, $2D$ and $3D$ cases. The mean value and the standard deviation of the auto-ignition delay were computed using Eq. (7) and (8). Results are reported in Tab.. 7, 8 and 9.

d	$\overline{\tau}\,(\mu s)$	$\sigma_\tau\,(\mu s)$	N_{eval}	T_{cpu}	UF_τ
1	110.56	8.25	31	$151s$	1.241
2	110.56	8.28	127	$164s$	1.242
3	110.56	8.44	127	$138s$	1.247
4	110.56	8.44	511	$288s$	1.247

Table 7: Maximum degree of the PC expansion basis (d), Mean ($\overline{\tau}$), Standard deviation (σ_τ), and uncertainty factor UF_τ of auto-ignition delay, number of evaluations (N_{eval}), computational time (T_{cpu}) using a PC expansion in the $1D$ case computed using a cubature method based on second Féjer quadrature rule.

d	$\overline{\tau}\,(\mu s)$	$\sigma_\tau\,(\mu s)$	N_{eval}	T_{cpu}	UF_τ
1	110.53	8.45	225	$578s$	1.247
2	110.53	8.46	705	$320s$	1.248
3	110.53	8.63	961	$688s$	1.253
4	110.53	8.64	961	$911s$	1.253

Table 8: Maximum degree of the PC expansion basis (d), Mean ($\overline{\tau}$), Standard deviation (σ_τ), and uncertainty factor UF_τ of auto-ignition delay, number of evaluations (N_{eval}), computational time (T_{cpu}) using a PC expansion in the $2D$ case computed using a cubature method based on second Féjer quadrature rule.

d	$\overline{\tau}\,(\mu s)$	$\sigma_\tau\,(\mu s)$	N_{eval}	T_{cpu}	UF_τ
1	110.83	8.67	239	$154s$	1.253
2	110.83	8.70	13663	$3514s$	1.254
3	110.83	8.86	13663	$3457s$	1.260
4	110.83	8.87	25695	$6656s$	1.260

Table 9: Maximum degree of the PC expansion basis (d), Mean ($\overline{\tau}$), Standard deviation (σ_τ), and uncertainty factor UF_τ of auto-ignition delay, number of evaluations (N_{eval}), computational time (T_{cpu}) using a PC expansion in the $1D$ case computed using a cubature method based on second Féjer quadrature rule.

As the polynomial P_0 is equal to 1, the computed value of the coefficient α_0 is equal to the mean value of the auto-ignition delay computed in Sec. 4.2. The values

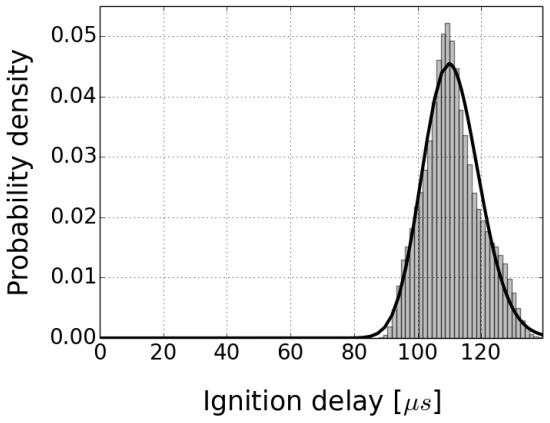

Figure 3: PDF of the PC expansion of degree 3 for the $3D$ case, and its corresponding lognormal

for the standard deviation differ slightly from the ones obtained with the Monte-Carlo method, but get closer as the maximal degree of the polynomial basis increases. The chosen PC basis might not be suited to approximate accurately the auto-ignition delay, as shown by the PDF of the response surface given by the polynomial chaos expansion presented on Fig. 3, that does not coincide with the PDF of the corresponding lognormal as the Monte-Carlo does.

5. Conclusions

In this paper, the impact of the uncertainties in chemical reaction rate constants of the detailed mechanism from Konnov[7] onto the auto-ignition delay has been investigated. Reference results of the full problem involving the 33 uncertain chemical reaction rates were obtained using a Monte-Carlo method. Then, a sensitivity study based on Sobol indices was done, allowing to reduce the number of retained uncertain reactions to three. A comparative study was finally done between methods such as Monte-Carlo, cubature methods, and Polynomial Chaos expansion in terms of accuracy and computational cost.

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