APPLICATION OF THE GENERALIZED POLYNOMIAL CHAOS EXPANSION TO THE SIMULATION OF AN INTERNAL COMBUSTION ENGINE FUELED WITH ETHANOL

Marcus Vinicius Costa de Souza, marcus.costa@gmail.com
Marcelo José Colaço, colaco@ufrj.br
Albino José Kalab Leiroz, leiroz@ufrj.br
Federal University of Rio de Janeiro, Department of Mechanical Engineering, Rio de Janeiro, Brazil.

Abstract. *The main subject of this paper consists in simulating the pressure curve of an internal combustion engine, with uncertainties in the mass fraction of burned fuel, when fueled with ethanol. For this purpose, the Wiener-Askey polynomial chaos was applied to a set of equations that represent the combustion process inside a single cylinder internal combustion engine modeled through a First Law analysis. The system of stochastic differential equation was numerically solved using the Mathematica® software. Two kinds of distribution were considered, Gaussian and uniform, to perform the stochastic solution. The results were compared against a deterministic solution.*

Keywords*: Internal combustion engines, thermodynamic model, Wiener-Askey polynomial chaos, uncertainty, stochastic differential equations system.*

1. INTRODUCTION

A description of a physical problem by means of deterministic mathematical models is subjected to uncertainties. In this context, a relatively new field called stochastic computation arises to study the influence of uncertainties on simulation results. Such research area has grown and developed in the past few years due the necessity to reach predictions provided by numerical simulation for physical systems with high accuracy.

The solution of partial or ordinary stochastic equations can be obtained by statistical or non-statistical methods. The first approach might include Monte Carlo simulation and stratified sampling, which have the disadvantage that the solution accuracy depends on the sample size and, consequently, the computational cost can be high. Non-statistical methods do not employ a sampling technique and, among such methods, the most widely used one is the Perturbation Method that has some restrictions regarding the degree of uncertainty, which cannot be high (Xiu e Karniadakis, 2004).

Among the non-statistical methods, the Generalized Polynomial Chaos (gPC) is a recent method and consists in a generalization of the Hermite Polynomial Chaos theory proposed by Wiener in 1938 (Wiener, 1938). This technique essentially represents the stochastic solution as a spectral expansion in a random space (Xiu, 2009). Furthermore, for solving the stochastic system of equations, orthogonal polynomials are employed, which must be chosen depending on the nature of the random distribution.

The gPC method was employed in various fields, e.g., in transient problems and/or non-linear, in fluid dynamics, flow-structure interactions, hyperbolic problems, deformation of materials, natural convection, Bayesian analysis for inverse problems, biological problems, etc (Xiu, 2009).

Orthogonal polynomials have an important class called Askey-scheme that associates the hypergeometric orthogonal polynomials with the differential equations being solved (Xiu e Karniadakis, 2002). Such scheme is applied in the present work.

In this paper, the Generalized Polynomial chaos together with Galerkin method is applied to a thermodynamic model of an internal combustion engine with uncertainties in some paremeters. In particular, since the random input is assumed with known distribution, a proper orthogonal polynomial is chosen through Askey-scheme. The results obtained are analyzed in order to investigate the influence of the uncertainty level in the pressure profile inside the combustion chamber.

2. PHYSICAL AND MATHEMATICAL PROBLEM

In this work we considered a Volkswagen (VW), 1.8 AP, FLEX, spark ignition engine, year 2005, with four cylinders, two valves at each cylinder (intake and exhaust), camshaft on cylinder head and whose technical data is reported on Tab. 1.

The physical problem takes place between the intake valve closing and the exhaust valve opening (combustion chamber closed), where the process of compression, combustion and expansion occurs. In this framework, a thermodynamic approach allows studying the air-fuel mixture behavior inside the combustion chamber and relates engine performance with fuel properties, mechanical parameters and engine operation (Melo, 2007).

Table 1. Engine technical data. (Melo, 2007)

Symbol	Parameter		Value
D	Cylinder diameter (mm)		81.01
S_p	Piston stroke (mm)		86.4
L	Connecting rod length (mm)		144.0
V_d	Displacement (cm³)		1781
r	Compression ratio		11:1
θ_i	Intake valve closing angle[1]		-164°
θ_f	Exhaust valve opening angle[1]		+146°
		Gasoline	Ethanol
	Power	76 kW at 5250 rpm	78 kW at 5250 rpm
	Brake torque	153 Nm at 3000 rpm	157 Nm at 3000 rpm

[1]Top dead center corresponds to an angle of 0°

In order to model the phenomenon, some simplifying hypotheses have been adopted (Melo, 2007): (i) homogeneous mixture in combustion chamber; (ii) intake mixture formed by air and fuel; (iii) ideal gas behavior; (iv) no flame front propagation; (v) constant ratio between specific heats, $\overline{k}$; (vi) constant wall temperature, T_p; (vii) polytropic process between intake valve closing and start of combustion and (viii) stoichiometric air-fuel ratio, AF.

The mathematical formulation for the geometry of the engine follows the work of Melo (2007). The distance between the crank axis and the piston pin axis (S) as well as the cylinder volume (V) can be calculated as:

$$S(\theta) = Rcos(\theta) + \sqrt{L^2 - R^2 \sin(\theta)^2} \tag{1}$$

$$V(\theta) = \frac{\pi D^2}{4}\left(L + R - S(\theta) + \frac{2R}{r-1}\right) \tag{2}$$

In the above equations θ is the crank angle that rotates clockwise, L is the piston stroke, R is the crankshaft radius ($R = 0.5S_p$), r is the compression ratio, and D is cylinder diameter. Such values are shown in Tab. 1.

The mass fraction of the burned gases was modeled through a Wiebe's function (Heywood, 1988):

$$x(\theta) = 1 - exp\left[-a\left(\frac{\theta-\theta_0}{\Delta\theta}\right)^{m+1}\right] \tag{3}$$

where θ_0 is the start of combustion, $\Delta\theta$ is the combustion duration, and a and m are adjustable parameters. In this work we took such parameters as a = 5 and m = 2 (Heywood, 1988).

The total energy released by the fuel (Q_{tot}) can be calculated as follows (Heywood, 1988):

$$Q_{tot} = \eta_c m_F LHV \tag{4}$$

where η_c is the combustion efficiency, m_F is the mass fuel admitted and LHV is the lower heating value. Since air-fuel ratio (AF) is defined by the ratio between air mass (m_{air}) and fuel mass (m_F), Eq. (4) is rewritten as:

$$Q_{tot} = \eta_c \frac{m_m}{1+AF} LHV \tag{5}$$

where m_m is the mass of the mixture given by the sum of m_{air} and m_F. The value used for stoichiometric AF was 8.417 (Heywood, 1988).

The combustion efficiency was calculated according to Eq. (6), proposed by Alla (2002), where η_{max} is the maximum efficiency of a spark-ignited engine whose value was adopted as 90% (Heywood, 1988). The parameter λ is the ratio between real air-fuel ratio and stoichiometric one.

$$\eta_c = \eta_{max}\left(-1.6082 + 4.6509\lambda - 2.0764\lambda^2\right) \tag{6}$$

Since in this research a stoichiometric mixture was adopted, λ equals to unit and, applying it to Eq. (6), we obtain $\eta_c = 87\%$.

In intention of represent Eq. (5) in terms of the crank angle, Eq. (5) and Eq. (3) can be combined resulting in Eq. (7):

$$Q_{tot}(\theta) = Q_{tot}\, x(\theta) \tag{7}$$

A thermodynamic approach was chosen to represent the physical problem inside the combustion chamber. Specifically, a thermodynamic model called zero-dimensional (Heywood, 1988) was employed. Its deduction arises from First Law of Thermodynamics and reduces to:

$$\frac{1}{k-1}\frac{dT}{d\theta} = \frac{T}{PV}Q_{tot}\frac{dx}{d\theta} - \frac{T}{V}\frac{dV}{d\theta} \tag{8}$$

Other equation is needed to close the system of equations. Such equation is derived from ideal gas law in terms of crank angle and is given as:

$$\frac{1}{k-1}\left(V\frac{dP}{d\theta} + P\frac{dV}{d\theta}\right) = Q_{tot}\frac{dx}{d\theta} - P\frac{dV}{d\theta} \tag{9}$$

The ordinary differential equations system formed by Eqs. (8) and (9) predict the pressure and temperature profile inside the combustion chamber, e.g., the behaviour of the air-fuel mixture in the sense of thermodynamic states.

3. SOLUTION METHODOLOGY

In this section it is explained how to solve the stochastic and deterministic approach of the problem.

3.1 Deterministic solution

Initially a deterministic solution was found, were no uncertainties in the parameters were considered. In this case, a numerical solution can be obtained by using known methods to solve the ordinary differential equations system. A fourth order Runge-Kutta method was applied to Eq. (8)-(9) together with the initial conditions given by Eqs. (10)-(11):

$$T(\theta_i) = T_0 \tag{10}$$
$$T(\theta_i) = P_0 \tag{11}$$

where θ_i is crank angle at the beginning of compression process or the intake valve closing angle.

3.2 Stochastic solution

The present paper considers uncertainties in the mass fraction of burned fuel (x) because it is an empirical equation and has relevant influence in temperature and pressure field inside the cylinder (Melo, 2007). Due to its empirical character, Eq. (3) does not represent the released energy with high fidelity and, for this reason, uncertainties must be taking into account. The technique chosen to numerically solve the problem by this approach was the generalized polynomial chaos (gPC) together with Galerkin method.

3.2.1 Generalized Polynomial Chaos (gPC)

The solution of stochastic partial/ordinary differential equations can be obtained by statistical or non-statistical methods. The first one includes, for example, Monte Carlo simulation and stratified sampling, but the accuracy depends on the sample size and thus the computational cost can be undesirable. Among the non-statistical techniques, the Perturbation method is often employed. However, such technique cannot deal with problems with very large uncertainties (Xiu e Karniadakis, 2004).

Another non-statistical approach, that is recent and was applied in different kinds of research, is the generalized polynomial chaos. This method consists in a generalization of the Hermite polynomial chaos theory, proposed by Wiener in 1938 (Wiener, 1938). In this case the stochastic solution of the system is given by a spectral expansion of a random space (Xiu, 2009). The methodology that represents a random field by means of an orthogonal polynomial function expansion is called generalized polynomial chaos.

Xiu and Karniadakis, in 2002, presented a method based on Galerkin projections together with an extension of Wiener's polynomial chaos that represent stochastic processes using an optimal trial basis from the Askey family of orthogonal polynomials. The advantage of such technique is the exponential convergence of the error and the lower dimensionality of the system (Xiu e Karniadakis, 2002).

Briefly, the Askey-scheme classifies the hypergeometric orthogonal polynomials that satisfy some type of differential equation and establishes a limit to this relation (Xiu, 2010). An important role in the scheme of Askey is that some types of orthogonal polynomials have weighting functions identical to the probability function of certain types of random distributions (Xiu e Karniadakis, 2002). Table 2 shows the random variable associated to the respective Weiner-Askey polynomial chaos and the support to conduct the projection.

Table 2. Correspondence between the Wiener-Askey polynomial chaos and the random variable. (Xiu e Karniadakis, 2002)

	Random Variable (ξ)	Weiner-Askey chaos $\{\Psi(\xi)\}$	Support ($\bar{S}$)
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, …}
	Binomial	Krawtchouk-chaos	{0, 1, 2, …, N[1]}
	Negative Binomial	Meixner-chaos	{0, 1, 2, …}
	Hypergeometric	Hahn-chaos	{0, 1, 2, …, N[1]}

[1]$N \geq 0$ is a finite integer.

The gPC was employed in a variety of areas, in transient and/or non-linear problems, for example, fluid dynamic, interactions between structure and flow, hyperbolic problems, material deformations, natural convection, Bayesian analysis for inverse problem, biological problems, etc (Xiu, 2009).

3.2.2 Numerical solution with uncertainty by gPC Galerkin method

In this paper, the fraction of mass burned was considered to be the uncertainty variable. Thus, the uncertainty is added to Eq. (3) as

$$X(\theta,\xi) = x(\theta) + \mu\xi x(\theta) \tag{12}$$

where μ is the percentage of uncertainty which range from 0 to 1 and ξ is a single random variable with known distribution. As the random variable is continuous, there is a properly probability density function $w(\xi)$.

Under this assumption, the solution $T(\theta)$ and $P(\theta)$ of the Eqs. (8)-(9) will be a stochastic process $T(\theta,\xi)$ and $P(\theta,\xi)$, respectively. The solution T and P together with the variable with uncertainty can be expanded by the generalized polynomial chaos (spectral expansion in the random dimension ξ) as

$$T(\theta,\xi) = \sum_{i=0}^{N_P} T_i(\theta)\,\Psi_i(\xi) \tag{13}$$
$$P(\theta,\xi) = \sum_{j=0}^{N_P} P_j(\theta)\,\Psi_j(\xi) \tag{14}$$
$$X(\theta,\xi) = \sum_{k=0}^{N_P} X_k(\theta)\,\Psi_k(\xi) \tag{15}$$

Note that the above series were truncated at the finite term ($\boldsymbol{N_P + 1}$). Furthermore, $\{\boldsymbol{\Psi_i}\}_{\boldsymbol{i=0}}^{\boldsymbol{n}}$ is a random trial basis based on the Askey-scheme and the total number of expansion terms $\boldsymbol{N_P + 1}$ were determined by the random variable dimension (taken as one in this paper) and the highest order of the polynomials ($\boldsymbol{n}$) as follows:

$$N_P = \frac{(1+n)!}{1!n!} - 1 \tag{16}$$

Upon substituting Eqs. (13)-(15) into Eqs. (8)-(9), the following stochastic ordinary differential equations can be obtained:

$$\frac{1}{k-1}\sum_{i=0}^{N_P}\sum_{j=0}^{N_P}\frac{dT_i}{d\theta}P_j\Psi_i\Psi_j = \frac{Q_{Tot}}{V}\sum_{i=0}^{N_P}\sum_{k=0}^{N_P}T_i\frac{dx_k}{d\theta}\Psi_i\Psi_k - \frac{1}{V}\frac{dV}{d\theta}\sum_{i=0}^{N_P}\sum_{j=0}^{N_P}T_iP_j\,\Psi_i\Psi_j \tag{17}$$
$$V\sum_{j=0}^{N_P}\frac{dP_j}{d\theta}\Psi_j + k\frac{dV}{d\theta}\sum_{j=0}^{N_P}P_j\,\Psi_j = (k-1)Q_{Tot}\sum_{k=0}^{N_P}\frac{dx_k}{d\theta}\Psi_k \tag{18}$$

A Galerkin projection of Eqs. (17)-(18) into the polynomial basis $\{\Psi_i\}$ is then conducted in order to ensure that the error is orthogonal to the functional space spanned by the finite dimensional orthogonal polynomial basis. The projection is realized by the Hilbert space inner product,

$$\langle(\cdot),\Psi_m\rangle \coloneqq \int_{\bar{S}}(\cdot)w(\xi)\Psi_m(\xi)d\xi \tag{19}$$

where $\boldsymbol{\bar{S}}$ is the support of the random variable as reported on Tab. 2.

Applying Eq. (19) in Eqs. (17)-(18) and using the fact that the inner product in Hilbert space is a linear transformation, Eqs, (20)-(21) are obtained:

$$\frac{1}{\bar{k}-1}\sum_{i=0}^{N_P}\sum_{j=0}^{N_P}\frac{dT_i}{d\theta}P_j\,e_{ijm}=\frac{Q_{Tot}}{V}\sum_{i=0}^{N_P}\sum_{k=0}^{N_P}T_i\frac{dx_k}{d\theta}e_{ikm}-\frac{1}{V}\frac{dV}{d\theta}\sum_{i=0}^{N_P}\sum_{j=0}^{N_P}T_iP_j\,e_{ijm} \tag{20}$$

$$V\frac{dP_m}{d\theta}\langle\Psi_m^2\rangle+\bar{k}\frac{dV}{d\theta}P_m\langle\Psi_m^2\rangle=(\bar{k}-1)Q_{Tot}\frac{dx_m}{d\theta}\langle\Psi_m^2\rangle \tag{21}$$

where $e_{ijk}=\langle\Psi_i\Psi_j,\Psi_k\rangle$, $\langle\Psi_i^2\rangle=\langle\Psi_i,\Psi_i\rangle$ and m varies from 0 to N_P.

The same procedure must be applied to the dependent variable $X(\theta,\xi)$ and, for this purpose, Eqs. (12) and (15) must be combined. Then the Galerkin projection together with the inner product properties result in:

$$X_m(\theta)=\langle\Psi_m^2\rangle^{-1}x(\theta)\{\langle1,\Psi_m\rangle+\mu\langle\xi,\Psi_m\rangle\} \tag{22}$$

The initial condition given by Eqs. (10)-(11) must also be projected onto polynomial basis $\{\Psi_i\}$ and the spectral representation of temperatures, Eq. (13), and pressure, Eq. (14), used to achieve Eqs. (23)-(24):

$$T_m(\theta_i)=T_b\langle\Psi_m^2\rangle^{-1}\langle1,\Psi_m\rangle \tag{23}$$

$$P_m(\theta_i)=P_b\langle\Psi_m^2\rangle^{-1}\langle1,\Psi_m\rangle \tag{24}$$

where $\boldsymbol{T_b}$ and $\boldsymbol{P_b}$ are the temperature and pressure at the beginning of the engine compression stroke, respectively. It is important to note that in the deterministic approach, such initial conditions are constant.

The stochastic ordinary differential system of N_P+1 equations is then formed by Eqs. (20)-(21) together with Eqs. (23)-(24). The numerical solution as well as the parameters is reported in section 4.

4. RESULTS AND DISCUSSION

Some engine parameters were reported on Tab. 1. Table 3 shows others input data necessary to proceed with the computational simulation.

Table 3. Input data for the numerical solution . (Melo, 2007)

Description	Parameter	Value	Unit
Start of compression	θ_0	-10.0	°
Combustion duration	$\Delta\theta$	33.8	°
Initial temperature	T_b	35	°C
Initial pressure	P_b	54.63	kPa
Speed	Rot	1500	rpm
Lower Heat Value	LHV	24.804	MJ kg^{-1}
Engine air flow	V_{air}	37.61	kg h^{-1}

The set of equations obtained joining Eqs. (10)-(11) and Eqs. (17)-(18) was solved by the software Mathematica® using the function NDSolve. This function solves a differential equation system numerically and returns the solution in terms of interpolating function. The result of function is based on numerical sampling, error estimates, and use many different methods for solving, like predictor-corrector Adams method with orders 1 through 12, implicit backward differentiation formulas with orders 1 through 5, forward Euler method, etc. The software can also choose the solution method automatically as it was done in this research.

To carry out the numerical solution, the random variable dimension was adopted as unit and the higher polynomial degree was chosen as 4.

For post processing purposes, the mean (first term of the sum) and the variance were calculated as follows:

$$\bar{T}(\theta)=T_0(\theta) \tag{25}$$

$$\bar{P}(\theta)=P_0(\theta) \tag{26}$$

$$T_{\sigma^2}(\theta)=\sum_{i=1}^{N_P}T_i(\theta)\,\langle\Psi_m^2\rangle \tag{27}$$

$$P_{\sigma^2}(\theta)=\sum_{i=1}^{N_P}P_i(\theta)\,\langle\Psi_m^2\rangle \tag{28}$$

The Uniform (at the interval [-1,1]) and Gaussian (zero mean and unit standard deviation) distribution were selected together with the respective generalized orthogonal polynomial presented in Tab. 2. The polynomial degree as was fixed as 4, and 4 levels of uncertainties (0%, 1%, 10% and 20%) were adopted for each distribution. Table 4 reports the monic polynomials of Hermite-Chaos and Legendre-Chaos from zero-th to fourth degree.

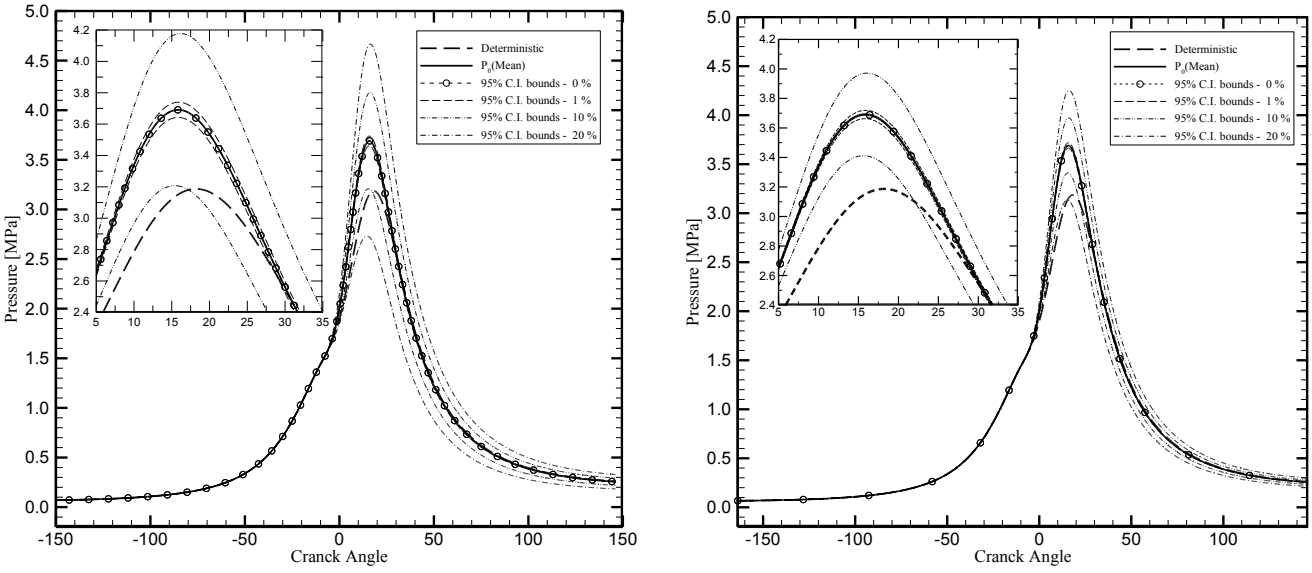
Table 4. Legendre-chaos and Hermite-chaos from 0th to 4th degree

Degree	Hermite-chaos	Legendre-chaos
0	1	1
1	ξ	ξ
2	$\xi^2 - 1$	$\xi^2 - \frac{1}{3}$
3	$\xi^3 - 3\xi$	$\xi^3 - \frac{3}{5}\xi$
4	$\xi^4 - 6\xi^2 + 3$	$\xi^4 - \frac{6}{7}\xi^2 + \frac{3}{35}$

Figure 1 shows the deterministic and stochastic solutions for the pressure inside the combustion chamber. The solution without uncertainties was obtained by means of the function NDSolve applying the same input data used for the stochastic version of the problem, but with no uncertainties in the model. Also, the problem with no uncertainties was verified through results available in literature (Melo, 2007). The confidence interval (C.I.) was considered with 95% of confidence level. The purpose of the present figure was to study the influence of the uncertainty level in the solution. For both distributions (Gaussian and uniform) it can be seen that the mean pressure achieved was the same, but the confidence interval was different for each distribution as the level of uncertainties changed.

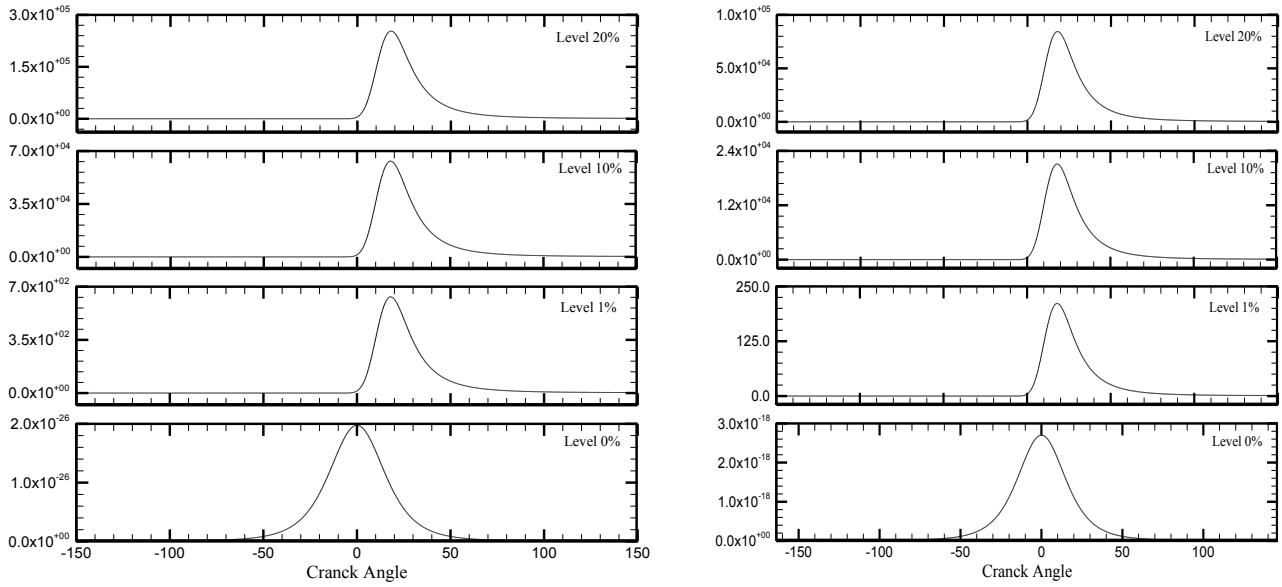
The confidence interval behavior can be justified by Fig. 2, where the percentage of uncertainty ranges from 0 to 20%. For example, comparing the distributions for the level 20%, the shapes are similar but the values associated to the Uniform distribution are smaller. Similar behavior can be noticed until the level 1%. For a 0% of uncertainty, the variance is less than 10^{-16} and thus is numerically negligible.

The difference of magnitude caused by the distribution in the variance explains why, starting from the top dead center of the engine, the values of the C.I. bounds are lower for the Uniform distribution than for the Gaussian distribution.



(a) (b)

Figure 1. Stochastic and deterministic solution for (a) Gaussian and (b) Uniform distribution for 0%, 1%, 10% and 20% of uncertainty in the mass fraction burned



(a) (b)

Figure 2. Pressure variance for (a) Gaussian and (b) Uniform distribution for 0%, 1%, 10% and 20% of uncertainty in the mass fraction burned

4. CONCLUSION

The physical problem consists of predicting the thermodynamic states inside of an internal combustion engine fuelled with ethanol. The problem was modeled thermodynamically and such mathematical formulation was written in a stochastic and a deterministic version. The stochastic problem was proposed in order to consider uncertainties in the model of the combustion process whose nature is empirical. Gaussian and Uniform distributions were considered in order to perform the numerical solution. The numerical solution was analyzed to investigate the influence of the level of uncertainty. Finally, the gPC Galerkin method has the advantage of not using sampling and, for the case studied, presented low computational cost. Furthermore, the methodology seems to be feasible to a mathematical model of an internal combustion engine in order to turn it more realistic.

5. ACKNOWLEDGEMENTS

The authors would like to thank the Brazilian agencies for the fostering of science, *Agência Nacional do Petróleo, Gás Natural e Biocombustíveis* (ANP), *Conselho Nacional de Desenvolvimento Científico e Tecnológico* (CNPq), *Coordenação de Aperfeiçoamento de Pessoal de Nível Superior* (CAPES) and *Fundação Carlos Chagas Filho de Amparo à Pesquisa do Estado do Rio de Janeiro* (FAPERJ), for the financial support for this work. Mr. Souza is also greateful to the PRH37-ANP/MCT doctoral scholarship.

6. REFERENCES

Alla, G.H.A., 2002. "Computer Simulation of a Four Stroke Spark Ignition Engine". Energy Conversion and Management, Vol.43, No. 8, pp. 1043-1061.

Heywood, J.B., 1988. Internal Combustion Engine Fundamentals. McGraw-Hill, New York.

Melo, T.C.C., 2007. Modelagem Termodinâmica de Um Motor do Ciclo Otto Tipo Flex-Fuel, Funcionando com Gasolina, Álcool e Gás Natural. Master thesis, Universidade Federal do Rio de Janeiro, Rio de Janeiro, RJ.

Wiener, N., 1938. "The Homogeneous Chaos". American Journal of Mathematics, Vol. 60, pp. 897–936.

Xiu, D e Karniadakis, G. E., 2002. "The Wiener–Askey Polynomial Chaos for Stochastic Differential Equations". SIAM J. Sci. Comput., Vol. 24, No. 2, pp. 619–644.

Xiu, D. and G.E. Karniadakis, G. E., 2004. "Supersensitivity Due To Uncertain Boundary Conditions". Int. J. Num. Meth. Eng.,Vol. 61, pp. 2114-2138.

Xiu, D., 2009. "Fast Numerical Methods For Stochastic Computations: A Review". Comm. Comput. Phys., Vol. 5, pp. 242-272.

Xiu, D., 2010. Numerical Methods for Stochastic Computations: A Spectral Method Approach. Princeton University Press, New Jersey.

7. RESPONSIBILITY NOTICE

The authors are the only responsible for the printed material included in this paper.