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Application of the generalized Polynomial Chaos expansion to the simulation of an internal combustion engine with uncertainties

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HIGHLIGHTS

- Simulation of combustion under uncertainty.
- Stochastic simulation considering a First Law analysis.
- Uncertainties in the mass fraction of burned fuel.
- CPU time orders or magnitude lower than a Monte Carlo simulation.

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ABSTRACT

The study of combustion associated phenomena in internal combustion engines is important for reasons that include pollutant formation control, and the heat transfer between the hot gases, the piston and combustion chamber walls. Although there are several models for the chemically reacting turbulent flow inside the combustion chamber, such models always suffer from some level of uncertainties in their formulations or in the physical parameters used for their simulation. The main objective of the present paper consists in modeling the combustion phenomena in a combustion chamber of an internal combustion engine, using a model based on the First Law of Thermodynamics, considering uncertainties in the mass fraction of burned fuel. As a result, the curve describing the in-cylinder pressure as a function of the crank angle can be obtained for different uncertainties levels. For this purpose, the generalized Polynomial Chaos (gPC) and Monte Carlo techniques were applied to a set of ordinary differential equations obtained from a First Law analysis, and the stochastic moments of the solution were obtained. Uniform and Gaussian uncertainties distributions were considered in order to obtain the stochastic solution. Results show that the gPC is more computationally efficient than the Monte Carlo simulation for the considered application . Besides, experimental engine results were also used in order to validate the implemented numerical procedure.

1. Introduction

The accurate solution of physical problems in terms of mathematical models requires a fully understanding of all the basic phenomena involved and their detailed description, in general, in terms of ordinary or partial differential equations. Such models are formulated in terms of physical properties or constants that, in general, contain some level of uncertainties. In this context, a relatively new field called stochastic computation has arisen to study the influence of uncertainties on simulation results. Such research area has grown and developed in the past few years, due to the need of obtaining predictions provided by numerical simulation with corrupted or non-accurate data.

The solution of partial or ordinary differential stochastic equations can be obtained by statistical or non-statistical methods. Monte Carlo (MC) simulation and the stratified sampling method belong to the class of the statistical approaches for the solution of stochastic equations. However, a drawback of the statistical techniques is the fact that the solution accuracy depends on the sample size and, consequently, the computational cost can be very high. In the present paper the MC method is applied to a combustion problem modeled through a First Law analysis, and the results are compared with a non-statistical method, called the generalized Polynomial Chaos (gPC).

The gPC does not require the use of sampling techniques and thus can lead to low computational times. Among the so called

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Nomenclature

a_1	Wiebe's equation coefficient	T	temperature (°C)
a_2	Wiebe's equation coefficient	$\bar{T}$	mean temperature (°C)
AF	stoichiometric air–fuel ratio	T_p	constant wall temperature (°C)
D	cylinder diameter (mm)	V	instantaneous volume of the combustion chamber (cm^3)
d_ξ	random variable dimension	V_d	displaced volume (cm^3)
$\bar{k}$	Ratio between specific heats at constant pressure and constant volume	X	stochastic mass fraction of burned fuel
L	connecting rod length (mm)	x	mass fraction of burned fuel
N_p	higher degree of the orthogonal polynomial	w	probability density function
P	pressure (MPa)	θ	crank angle (degree)
$\bar{P}$	mean pressure (MPa)	θ_0	start of combustion (degree)
Q_{tot}	total amount of heat released by the fuel during the combustion (MJ/kg)	θ_f	exhaust valve opening angle (degree)
R	crankshaft radius (mm)	ξ	random variable
r	compression ratio	σ	uncertainty level
$\bar{S}$	support of the random variable	τ	torque (N m)
S_p	piston stroke (mm)	Ψ	polynomial functionals of random variables
S	distance between the crank axis and the piston axis (mm)	$\Delta\theta$	combustion duration (degree)

non-statistical methods, the most used is the Perturbation Method. However the Perturbation Method has a restriction regarding the degree of uncertainty, that cannot be very high [1].

The generalized Polynomial Chaos is a relatively recent method that consists in a generalization of the theory of Hermite Polynomial Chaos proposed by Wiener in 1938 [2]. The methodology uses the Polynomial Chaos Expansion and the Galerkin method, and is categorized as an intrusive method since it results in a distinct system compared with the original deterministic model. On the other hand, nonintrusive methods, such as the Collocation Method, allow the use of the original deterministic model as a "black box". This technique essentially represents the stochastic solution as a spectral expansion of orthogonal polynomials in a random space [3]. Furthermore, to solve the stochastic system of equations, the orthogonal polynomial must be chosen depending on the nature of the random distribution of the uncertainties being considered. Orthogonal polynomials have an important class called Askey-scheme that associates the hypergeometric orthogonal polynomials with the ordinary/partial differential equations being considered, establishing thus the range of their applications [4].

The use of the Polynomial Chaos approach to simulate nonlinear systems containing uncertainties became popular in the past decades, mainly due to the research carried out by Ghanem and Spanos since 1990 [5]. Although not the first researchers in this field, they introduced the polynomial chaos technique to engineering applications. In 1991 [6], Ghanem and Spanos solved structural mechanics problems involving material variability, which were modeled as stochastic processes using the Karhunem–Loève expansion. They also applied a Stochastic Galerkin technique to solve a nonlinear problem in vibrations with uncertainties [7]. Using the same methodology, they investigated the problem of a medium composed by two layers separated by an interface randomly fluctuating in space [8]. In 1998, Ghanem and Dham [9] used a two-dimensional multiphase model to investigate the movement of a NAPL (Non-Aqueous Phase Liquid) in heterogeneous aquifers. In this problem, the permeability of the porous media was modeled as a stochastic process using the Karhunen–Loève expansion and the Finite Element method [9]. Ghanem, in 1998 [10], modeled the hydraulic properties of a porous media as a spatial random process in order to investigate the mechanics of flow transport in a random porous medium. In 1999, Ghanem and Spanos used a Spectral formulation of the Stochastic Finite Element Method (SSFEM) to solve a heat conduction problem in a random medium [11]. More details about the Polynomial Chaos method can be found in [12].

In recent years, the research group of Xiu and Karniadakis has applied the gPC to several problems, including flow-structure interaction [13], steady-state diffusion problems [14], flow simulations [15], and transient heat conduction [16]. The gPC method was also used in various fields, e.g., in fluid dynamics, hyperbolic problems, deformation of materials, natural convection, Bayesian analysis for inverse problems, and biological problems, among others [3].

The present paper presents a new application of the generalized Polynomial Chaos to simulate in-cylinder processes in an internal combustion engine using a thermodynamic approach. Specifically, the thermodynamic states of an internal combustion engine are computationally predicted considering different levels of uncertainties by means of the generalized Polynomial Chaos (gPC) technique and the Monte Carlo Method (MC). The uncertainties are assumed to have known distribution and, by this reason, a proper orthogonal polynomial is chosen through the Askey's scheme. The results of both methodologies (gPC and MC) are compared in order to investigate the influence of the uncertainty levels in the final results, and to compare the efficiency of each technique in terms of computational time. A comparison against real experimental data is also presented in order to validate the numerical procedure.

2. Physical and mathematical models

In this paper, a simplified model for the combustion process in an internal combustion engine, modeled through a First Law analysis, is considered. Results are obtained for a spark ignition engine, with a total displaced volume of 1.8 l, 4 cylinders and eight valves. The engine being considered is capable of burn any blend of gasoline and hydrous ethanol (named "flex-fuel" engine in Brazil). Some general data about the engine are shown in Table 1.

Within the engine operational cycle, the physical model considers the time interval between the intake valve closing and the exhaust valve opening (combustion chamber closed), where the processes of compression, combustion and expansion occurs. In