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Numerical study of HCCI combustion fueled with diesel oil using a multizone model approach

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ABSTRACT

The main goal of this study is to analyze the potential of a *multi-zone combustion modeling* to simulate the homogeneous charge compression ignition (HCCI) in a process using mineral diesel fuel. The *multi-zone combustion modeling* consists of several volumes, named zones, that are located in fixed positions inside the combustion chamber and takes as homogeneous the composition and temperature for each volume being the pressure the same for all the zones. The start of combustion and its development were considered through specific formulations that were fitted to the model through a comparison between combustion chamber pressure measurements and model results. The model was applied to the HCCI combustion mode with both early and late injection, in the latter case with high turbulence intensity, and showed a very good capability for process simulation. The model also included the kinetics of NO_x and CO formation and gave data that were close to the experimental results.

1. Introduction

The HCCI has a big potential for NO_x, soot and smoke emissions [1] reduction. This technology is based on the auto-ignition [2] process of a homogenous air–fuel mixture without the need of an external device to achieve ignition. Being possible, at least theoretically, the combustion of almost any gaseous or liquid fuel as petrol [3], diesel, H_2 or biofuels, just to mention some of the most popular. The lack of an external device to achieve ignition involves the control of the ignition process by the chemical-kinetics oxidation mechanisms.

Diesel–fueled HCCI can be listed into three major categories depending on the fueling technique. The last two methodologies have been studied in this work:

1. Premixed HCCI, where the fuel is injected with the air at the intake [4]. This method is mainly used with petrol fuel.
2. Early direct-injection HCCI, in which fuel is injected in-cylinder in advance to TDC so that a homogeneous charge can be accomplished prior to auto-ignition [5].
3. Late direct-injection HCCI, in which fuel is injected later than in conventional diesel combustion, with high swirl levels and EGR [5] that allow mixture homogenization, rapid mixing and enough time delay for mixing.

Big efforts have been made in the last decade in different technical field [6] with computational fluid dynamics (CFD) and combustion multi-zone models also towards HCCI combustion [7]. CFD models are a powerful tool for analyzing fluid processes including combustion. However it is time consuming and the results are very sensitive to initial conditions. The multi-zone model is faster and it allows a deeper insight of the mechanisms that control this combustion process. Moreover, CFD combustion code has to use also the same sub-models used in multi-zone model. Heat transfer from combustion gases to cylinder walls, piston and head are also simulated with CFD using the same sub-models used in the multi-zone model. In this regard, you should have to consider that charge temperature is the most controlling variable of the HCCI combustion process and that heat losses can account for more than 30% of the energy liberated by fuel.

In the last decade, a considerable amount of research effort has been directed towards the investigation of HCCI combustion and,

Abbreviations: ATDC, after top dead center; BDC, bottom dead center; BTDC, before top dead center; CFD, computational fluid dynamics; DI, direct injection; EGR, exhaust gas recirculation; EVC, exhaust valve closing; EVO, exhaust valve opening; HCCI, homogeneous combustion compression ignition; HRR, heat release rate; IVO, inlet valve opening; IVC, inlet valve closing; N, number zones; RPM, revolutions per minute; S, chemical species; TDC, top dead center.

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Nomenclature

H_p	lower heating value (J/kg)	$\dot{Q}_i$	heat flux (W)
m	mass (kg)	L	characteristic length (m)
$\dot{m}$	mass flow (kg/s)	v	gas velocity (m/s)
C_V	specific heat capacity at constant volume (J/kg K)	α_{scaling}	scaling factor
C_P	specific heat capacity at constant pressure (J/kg K)	C_1, C_2	constant
T	temperature (K)	E_{ACT}	activation energy (J/kg)
t_{IG}	combustion start (s)	τ	delay ignition (s)
P	pressure (N/m^2)	ω	average angular speed (rad/s)
V	volume (m^3)	θ	crankshaft angle (rad)
R	ideal gas constant (J/kg K)		
Q_W	wall heat loss (kJ)		

in particular, diesel HCCI [8–10] where the difficulty in achieving diesel HCCI combustion has been highlighted. The absence of an ignition mechanism has led researchers to explore a range of control strategies. However, to carry out this research solely in the laboratory would be inefficient, expensive and impractical since there are numerous variables that have complex interactions. Fundamental tools, such as CFD or combustion multi-zone models, need to be applied in order to provide an insight into the combustion process. Codes of this nature are computationally very intensive and usually require some simplifications to expedite the solution while attempting to maintain accuracy. Fully coupled CFD/kinetic models have employed a number of different combustion methodologies. Kusaka and Daisho [11] made no explicit modification to the reaction rate due to mixing; the only mixing considered to occur during combustion was that normally calculated by the CFD code. Results with a detailed kinetic scheme showed a more rapid combustion event than in the experiment. However, the relatively coarse grid that was used meant that the mass in colder zones could have been underestimated. Kong et al. [12] coupled the KIVA-3V CFD code with kinetics modified for turbulence effects and found a similar effect; i.e., when a turbulence effect was not used, a higher energy release rate was predicted than was found experimentally. All of these models suffer from a major drawback: the huge computational load, which precludes the efficient and rapid analysis of the HCCI process.

In the present study an aforementioned multi-zone model is used for the simulation of the closed part of the cycle of an HCCI engine and validated with experimental results [13,14]. Changes in the mixture composition in each zone due to combustion are determined using the governing equations. The global HRR is evaluated from the instantaneous release of energy during combustion for each zone.

For the heat release rate (HRR) a law to model the HCCI process was used. The parameters concerning this law were suited by an optimization process to allow the combustion chamber pressure given by the model to be fitted to the experimental data.

Since the CFD models are able to predict the fluid motion in a detailed way, these and their hybrids are of a high interest for supplementary investigations in exchange of a higher computational load [15]. CFD results could be compared to those resulting from the multi-zone approach presented in this work. These issues are the goals of oncoming researches.

2. Experimental methodology

The experimental results of this work are based on a test set up to run the naturally aspirated [16], four stroke, single cylinder DI diesel engine DEUTZ FL1 906, modified to operate in HCCI mode. In DI combustion mode, the original engine fueled with diesel fuel had a rated power of 11 kW at 3000 rpm and maximum torque of 45 Nm at 2100 rpm. The original engine configuration was modified with the following subsystems/adjustments: independent control of EGR [17], intake air pre-heating (not used in this work), start of injection 45° BTDC for early injection and 10° BTDC for late injection with high swirl through the bowl in piston and an increase of the maximum injection pressure up to 650 bar. This change in the injection pressure improves mixture homogeneity increasing the surface to volume ratio of the fuel drops and thus promoting faster fuel evaporation. In addition, reduction in the injection period was achieved. The main characteristics of the modified engine to run in HCCI combustion mode are shown in Table 1 and the experimental installation is represented in Fig. 1. In order to control the HCCI combustion process, exhaust gases were cooled down close to ambient temperature before mixing with inlet air. EGR was calculated as follows:

$$EGR(\%mass) = \frac{\dot{m}_{EGR}}{\dot{m}_{EGR} + \dot{m}_{Air}} \times 100 \tag{1}$$

For the experimental tests the engine started from initial load condition without EGR and with fixed injected fuel as well as engine speed. The experimental procedure then involved increasing the EGR percentage while keeping the intake temperature constant.

3. Model description

In this study, a thermodynamic multi-zone model has been developed in order to analyze and evaluate the parameters associated with an analytical HRR law. The combustion chamber is divided into N zones, being each zone contemplated as a reactor with perfect mixture and variable volume, free temperature, mass and chemical composition distributions (see Fig. 2) and with the same pressure in all zones. The model considers heat losses through the cylinder liner and engine head. The volume for each zone changes through all the engine as the cycle evolves according to a user-defined criteria.

In the developed multi-zone model, the combustion chamber is considered as a group of N zones and S chemical species where each zone is defined by $(4 + S)\cdot N$ independent parameters. The model uses eight chemical species and it has $12\cdot N$ independent variables.

The variables considered in the model with N independent zones are shown in Table 2.

The variables outlined above are related through a system of linear differential equations, although some simplifications are required since it is well known to exist interactions of great complexity between the physical and the chemical phenomena throughout the combustion process. The aforementioned equations are shown in Table 3.