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A comprehensive investigation on the emissions of ethanol HCCI engines

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ABSTRACT

The environmental impact of automotive transport systems and the need for reducing petroleum dependence lead to the development of alternative combustion strategies and the use of renewable fuels. In this work, HCCI combustion mode, by using ethanol as fuel, is analysed in order to clarify the role of specific technical solutions, such as power boosting, downsizing, swirl motion, and of the thermo-physical properties of ethanol on emissions and performance of the engine. A multidimensional numerical approach, coupled with a kinetic reaction mechanism for ethanol oxidation and NO_x formation, is proposed and validated against experimental measurements. Specifically, CO emissions assessment is a major issue of this work, as this pollutant is strictly related to inhomogeneities in the combustion chamber near the walls and a multidimensional approach with an adequate grid resolution is mandatory for a correct simulation. CO, CO_2, UHC and NO_x emissions, specific fuel consumption, heat release rate and in-cylinder pressure are evaluated in order to give recommendations on the most suitable technological solutions.

1. Introduction

Among the new combustion strategies for Internal Combustion Engines (ICEs), the Homogeneous-Charge Compression-Ignition (HCCI) combustion mode is proposed as an interesting compromise between Spark Ignition (SI) and Compression Ignition (CI) strategies. In HCCI combustion mode, the charge is compressed until it auto-ignites and the chemical reactions take place in the combustion chamber without a well-distinguished flame front [1]. The high compression ratios of these engines guarantee high efficiency, as in CI engines. Besides, there is no need for the mixture to be stoichiometric and controlling can be obtained by changing the engine load, thus operating unthrottled with higher efficiency. On the other hand, since the HCCI combustion occurs relatively fast, the fuel–air mixture is relatively lean, eventually augmented by Exhaust Gas Recirculation (EGR) to slow down the chemistry and to result in a stable operation. The leanness of the charge ensures a low temperature combustion, with low NO_x production [2,3]. Furthermore, the high degree of homogeneity of the charge [4–6] guarantees the absence of fuel-rich regions, thus reducing particulate matter emissions with respect to CI engines. In order to fully exploit the potential of this combustion strategy, some challenging issues still remain to be untangled, i.e. the control of the combustion phasing, the extension of the operating range and the reduction of unburned hydrocarbon (UHC) and CO emissions [7].

To overcome these issues, both experimental and theoretical-numerical approaches have been addressed in the literature [8–12]. As regards the latter, different models with different levels of detail were developed and used, from zero-dimensional single zone models to three-dimensional CFD models with detailed kinetic reaction mechanisms [7]. Multizone models are often used for HCCI engines [13–16]; such models can correctly predict the HCCI engine performance in a reasonable computational time. However, the agreement between the numerical results and the experimental measurements in terms of carbon monoxide (CO) emissions is not so good as other parameters, such as the in-cylinder pressure and the heat release rate [17], since CO production is strongly influenced by the temperature inhomogeneities within the combustion chamber, especially near the walls. Bhave et al. [18] have shown that heat loss and wall temperature are important factors in determining CO emissions. Therefore, multidimensional models become essential to provide insights on pollutant emissions. In this work, the assessment of CO emissions is one of the major issues; this will be addressed by employing a reliable theoretical–numerical model.

The control of the ignition of the mixture and emissions and the extension of the operating range can be improved by varying the chemical–thermophysical properties of the reacting mixture, for example with the use of alternative fuels or blends of conventional hydrocarbons with novel fuels. Ethanol is an interesting candidate, because of its relatively high octane number and of the presence of oxygen in its molecule [19]. Several experimental studies on the use of ethanol in HCCI engines are available in the literature

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[20–29]. Specifically, in Ref. [20] the improvement in engine performance, with ethanol as an additive, is assessed in terms of maximum IMEP and indicated thermal efficiency. Many other contributions are available in the literature to control HCCI combustion [25], reduce the noise [24] and extend the operating range [23,26]. However, little work has been done from a numerical point of view. Some works concern with the development of reliable kinetic reaction mechanisms for the description of ethanol combustion [30–32], validated in zero- and one-dimensional configurations. A multidimensional simulation of an HCCI engine fueled by ethanol was performed by Kong et al. [22], but the results are limited to in-cylinder average pressure. Thus, the main contribution of this article is to provide a comprehensive investigation of emissions and performance of HCCI engines fueled by ethanol.

In this work a multidimensional CFD in-house Reciprocating and Rotary Engine Combustion (REC-2000) code [33] is employed to study the ethanol combustion in an HCCI combustion mode engine. In order to account both for kinetics and fluid dynamics [34,35], the REC code is coupled with a skeletal kinetic reaction mechanism for ethanol oxidation, which involves 43 chemical species in 235 reactions [30]. The numerical results are compared with available measurements, in terms of in-cylinder average pressure, heat release rate and emissions [21]. Several computational grid resolutions are used to get results that are grid-independent and the influence of the grid spacing, especially near the walls, is addressed and discussed. Simulations are also performed in order to quantify the advantages of supercharging and of downsizing the engine. Supercharging advantages can be exploited by avoiding knock occurrence, due to the relatively high octane number of ethanol, while power boosting can be coupled with downsizing technique to enhance engine efficiency. Specifically, emissions are analysed by using different values of the boost pressure and of the displaced volume (V_d).

The work is organized as follows: the next section describes the mathematical and numerical model, then the computational set-up is shown and the results are discussed. The paper ends with conclusions and specific recommendations.

2. The multidimensional model

An accurate and reliable multidimensional computational model has been chosen in order to capture the relevant features of the HCCI strategy. This model is able to take into account the role of inhomogeneities in the combustion chamber, specifically on emissions. Moreover, it includes a comprehensive kinetic combustion model in order to predict the ignition delay time and to account for the thermo-chemical properties of fuel and intermediate chemical species and for their role on engine performance and emissions.

Due to mixture inhomogeneities in HCCI operation mode, the oxidation process may be partly controlled by the turbulent mixing, whereas, in the case of fast mixing, the combustion is simply controlled by the Arrhenius conversion rate. The model evaluates the new species concentrations, by including the influence of the turbulent timescale τ_t on the kinetic timescale τ_k. The turbulent timescale is computed as $\tau_t = C_{m2}k/\epsilon$, where C_{m2} is the turbulent mixing model constant proposed by Magnussen and Hjertager [36], whereas the kinetic timescale is computed as the maximum value between the fuel and the CO kinetic timescales. Hence, following Kong and Reitz [37], the new species concentrations are computed by modifying the species reaction rates with the correction factor $\tau_k/(\tau_k + r\tau_t)$, where r is a progress variable, given by $r = (1 - exp^{-g})/(1 - exp^{-1})$, with g the ratio of the current products concentrations to the products concentrations in the case of complete combustion. The effect of this correction has already been explored by Viggiano and Magi [38].

The REC-2000 code solves the three-dimensional Reynolds-Averaged Navier–Stokes (RANS) equations for transient, two-phase, turbulent, chemically reactive flows with sprays [33]. Turbulence is modeled by a two-equations $k - \epsilon$ model [39], and wall heat transfer and shear stresses are computed by wall functions, as originally proposed by Launder and Spalding [39]. The wall functions account for the effect of the turbulence boundary layer near the wall. The wall boundary layer is divided into a viscous laminar sublayer, where velocity profile is assumed to be linear, and a fully turbulent layer, where velocity profile follows the well-known log-law.

The code uses an implicit finite volume numerical method to solve the system of the governing equations, with an overall second order spatial accuracy and a first-order temporal discretization. The pressure equation, obtained by manipulating the continuity and momentum equations using the equation of state, is solved by Stone's strongly implicit iterative method [40] for multidimensional partial differential equations.

The skeletal kinetic reaction mechanism is made up of 235 reaction steps and requires the solution of the transport equations of 43 chemical species [30]. This mechanism was validated in Ref. [30] by comparing numerical results with experiments in terms of ignition delay time, laminar burning velocities and structures of counterflow flames at near-atmospheric pressure. The use of this mechanism at higher pressure conditions, as those encountered in standard engine operations, was assessed in Ref. [38]. Moreover, the NO_x sub-mechanism proposed in Ref. [30], made up of 53 reaction steps among 14 chemical species, is also used for the assessment of emissions.

The source terms due to chemical reactions, corrected to account for the effect of turbulent mixing, are explicitly solved by means of a variable-coefficient ODEs solver [41].

3. The computational set-up

In order to compare the numerical results with measurements, the engine specifications and the operating conditions fully match those used by Christensen et al. [21], as summarized in Table 1, where T_{air} and p_{air} are the air intake temperature and pressure, respectively. The high value of the compression ratio, set to 21:1, is justified by the high octane number of the specific fuel adopted. EGR is not included and the engine runs lean due to the extra-amount of inlet fresh air with respect to stoichiometric condition. Similar to the experimental tests, several lean mixture equivalence ratios are considered. The inlet air is preheated, in order to reach

Table 1
Specifications of the engine and operating conditions.

Engine specifications	
V_d	1600 cm^3
Bore	12.065 cm
Stroke	14 cm
Connecting rod	26 cm
Compression ratio	21:1
Operating conditions	
Engine speed	1000 rpm
Equivalence ratio	0.16 – 0.26
T_{air}	353 – 393 K
p_{air}	0.1 MPa
T_{wall}	450 – 500 K
Turbulent diffusivity	57 cm^2/s
Intake valve close	13° ABDC
Exhaust valve open	39° BBDC
EGR	0%