Analysis of Combustion Processes in HCCI Engine using LES

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Abstract

The Homogeneous Charge Compression Ignition (HCCI) is still a promising concept to optimize internal combustion (IC) engines with respect to emissions and particulate matter. However in HCCI combustion processes the cycle-to-cycle variations of in-cylinder flow play an important role and can lead to combustion instability due to the lean as well as knock combustion conditions. In this paper, multi-cycle Large-Eddy Simulation (LES) based analysis is carried out on a single cylinder, four-stroke IC-engine with two vertical valves in order to characterize the unsteady effects of HCCI combustion processes. For this purpose, LES simulation of HCCI combustion based on fully premixed iso-octane and early-direct spray injection has been carried out for 40 and 25 engine cycles obtained on coarse and fine grid, respectively. In order to reach the sufficient number of statistically independent samples a parallelization strategy has been used allowing perform LES of cyclic fluctuations in HCCI IC-engine with reasonable statistical accuracy. The effects of cycle-to-cycle velocity fluctuations on the resulting HCCI combustion processes are pointed out. In particular, a qualitative analysis of the intensity of cyclic fluctuations of in-cylinder velocity, temperature and pressure is provided in terms of mean and standard deviation.

Introduction

While gasoline direct injection appears to be the most attractive path to improve fuel efficiency of spark ignition (SI) engines, Homogeneous Charge Compression Ignition (HCCI) strategy has becoming a promising combustion process for SI and compression ignited engines. Having the potential of both providing high efficiency that is similar to diesel engine combustion and also producing ultra-low emission characteristics of NOx and particulate matters [1-6] it features combustion properties different from the two well-known, namely the premixed combustion mode in SI gasoline engines and diffusion flames in diesel engines. So, HCCI combustion represents a third mode of combustion in which the process essentially involves a premixed fuel-air mixture that is induced into the cylinder at equivalence ratios that can vary from lean to stoichiometric. Once within the cylinder, the fuel-air charge is then compressed until ignition commences. The ignition leads to a very rapid combustion phase where all heat is released [1-8].

Even though ignition is expected to occur homogeneously in the entire combustor and thus combustion to be governed by chemical kinetics, observations rather demonstrate inhomogeneity in terms of temperature or thermal stratification, concentration stratification and species stratification (exhaust gas recirculation) or wall effects [9, 10]. Thus, it faces the challenges of ignition and combustion timing control as well as operating range extension, since it better runs at low load. It is reported that the maximum Indicated Mean Effective Pressure (IMEP) is no more than half of the full load for natural aspirated HCCI engines. Its correlation to maximum rate pressure rise and to NOx emission has been investigated in [11].

It is worth noting that inhomogeneity of the fuel-air-exhaust gas mixture would cause inhomogeneous ignition and this should affect the overall combustion process [1, 6-14]. Previous work was mainly based on the assumption that the process is controlled by chemical kinetics. Simulations of HCCI combustion based on only the chemical kinetics have failed to reproduce the experimental data [2-7]. Incorporating detailed chemistry in single zone models, simulations greatly overestimated the rates of heat release and showed poor agreement with the experimentally obtained in-cylinder pressure development history [15]. The deficiencies of the single zone models are due to their inability to account for the temperature gradient within the mixture [3, 6, 7, 15]. Multiple zone models allowing spatial variations have been applied and reported by Aceves et al. in [4]. However, these studies showed that a great number of zones (at least ten) are required to resolve the detailed emissions using k-epsilon turbulence closure. Kraft et al. [5] used a stochastic reactor model to account for the spatial temperature gradient while the flow field was still modeled as single zone, the diffusion induced by turbulence mixing being described by the IEM (interaction by exchange with the mean) model within the Reynolds averaged Navier-Stokes (RANS) approach. Even though the prediction of CO and unburned hydrocarbons were shown to be bet-

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ter than the single-zone model, the stochastic model that needs the input information of turbulence suffers from the limitation of the turbulence RANS based input.

To improve the turbulence prediction, the Large Eddy Simulation (LES) model was developed and used in [6, 7] to investigate the development of in-cylinder turbulence, temperature stratification, onset of auto-ignition, and development of the reaction fronts in HCCI engines. Note that LES has already been used for better capturing fine spatial and temporal structures in Internal Combustion (IC) engines. Cycle-to-cycle variation effects on mixing and combustion processes have been investigated in [12, 13, 16, 17]. In [12, 13, 16, 18, 19] the KIVA-3V code extended to LES has been used to perform up to 40 full consecutive engine cycles on a realistic IC-engine configuration. Especially a coupling of a detailed auto-ignition chemical kinetic to the flow field simulations has been reported in [14] in which the KIVA-3V code has been applied. A recent review of LES in IC-engines is provided by Rutland in [20].

The objective of this work is to investigate HCCI combustion processes along with coupled effects of pre-mixing and cycle-to-cycle variations on the flow, mixing and combustion process under early-direct spray injection and homogeneous conditions. For this purpose both a premixed iso-octane and an early-spray injected HCCI are studied and compared to a non-reacting single-phase flow case. In contrast to [21] in which numerical simulations of premixed HCCI engines have been reported based on RANS models, the present work applies LES with the KIVA-3V code integrating an autoignition model. Dealing with motored engine, the validation based on experimental data is always difficult issue since a very limited number of available experimental results due to the high costs of experiment or confidentially policy, see references [6, 7]. Nevertheless, the models used in this paper were separately validated by a number of test-cases as reported in references throughout the paper. A verification based on mesh refinement study has been done in the present paper.

The paper is organized as follows. The numerical method, engine configuration and parameters of injection are given in the following section. The results and their discussion are given further. The main findings are summarized in the final section.

**Numerical approach**

The KIVA-3V code [22] widely applied in the automotive community for the simulations of IC-engine fluid dynamics is used in this work. In order to account for the highly unsteady and complex processes of in-cylinder flow a LES subgrid-scale model based on classical Smagorinsky model [23] has been implemented into the code [18, 19]. A square duct configuration was used to validate the modified KIVA-3V code and results were found to be in a good agreement with available DNS and LES data [18]. Numerous applications of the KIVA-3V code for investigation of the unsteady dynamics of turbulent flows in the context of LES are documented in the literature [24, 25]. Discussion about controlling the numerical, modelling as well as statistical errors is provided in [19, 26]. As the analysis of transient phenomena requires a large number of statistically independent samples in order to obtain qualitatively good statistics, a parallelization technique has been developed and applied in [12, 13, 16, 18].

The KIVA-3V code uses a quasi-second-order upwind differencing for spatial discretization and the first order Euler scheme for calculating time derivatives. The conservation equations are discretized using the finite volume method on an arbitrary hexahedral mesh applying the arbitrary Langrangian Eulerian method [27]. The spray module used for the early-spray injection case is based on the discrete droplet model of Dukowicz [28] with Lagrangian, computational particles that represent parcels of spray droplets with uniform properties. The spray and fluid interactions are thereby accounted for by means of a number of sub-models including aerodynamic drag, dispersion, evaporation, secondary break-up models. Modelling details and validation are provided in [16, 19, 22, 26, 29, 30]. A standard Arrhenius-based combustion model with single step mechanism corresponding to [22] was used as first step for simulation of HCCI combustion.

**Engine configuration**

In order to investigate the unsteady effects on HCCI combustion processes the four-stroke IC-engine with two vertical valves shown in Figure 1 has been used. The main parameters of the IC-engine are collected in Table 1. Engine speed is set equal to 1600 rpm, compression ratio is 23.0. The definition of valve-lift curves is given in Figure 2. The free following cases have been considered: 1). LES simulation of single-phase flow has been performed in order to estimate magnitudes and locations of velocity cycle-to-cycle fluctuations; 2). LES of fully premixed mixture has been carried out to investigate autoignition and HCCI combustion processes under homogeneous conditions. Iso-octane was used as a fuel, initial fuel-air ratio was set equal to 0.02. 3). Autoignition process and HCCI combustion were also simulated at early-direct spray injection. The injector is located in the middle of the cylinder head with an installation angle of 90°. A hollow spray profile shown in Figure 4 has been used for the spray simulation. The injection parameters for the spray are given in Table 2. A fuel is injected within the CONE angle with the fuel thickness equals to parameter DCONE, see Figure 4. The total number of injected droplets was equal to 5000.
Geometry and computational meshes were created by standard preprocessor program. A coarse computational grid with 152,000 control volumes provides a grid resolution of the order of 2.0 mm. In order to perform a mesh refinement study in HCCI IC-engine a relatively fine grid with the total number of control volumes equals to 380,000 providing a grid resolution of the order of 0.6 mm has also been used. A discussion about the grid sensitivity in motored engine operating under single-phase non-reacting flow conditions was reported in previous works of authors, where authors made contribution to control not only statistical errors, but also modeling and numerical errors have been estimated using the systematic grid and model variation [19, 26]. The relatively coarse grid was used due to the very high computation costs in order to provide 3 series of 40 engine cycles. As it was reported in [19], the mesh with a grid size of the order 1.0 mm seems to be the minimum requirement to represent the flow field with reasonable accuracy. Nevertheless, the results obtained on the coarse grid allow to perform a qualitative comparative analysis for considered cases. Initial and boundary conditions for LES calculations were formulated as follows. The temperature of piston, cylinder wall and cylinder head was set equal to 420 K. No-slip velocity boundary conditions at the walls were applied. The pressure is specified as constant atmospheric mean total pressure at the intake and static mean pressure at the exhaust port. Marginal cycle-to-cycle differences of the order of 2 mbar in the intake pressure traces inside the intake port were obtained with LES. In order to minimize the effects of initial and boundary conditions on LES predictions, the first three engine cycles were excluded from consideration.

<table>
<thead>
<tr>
<th>Parameters</th>
<th>Values</th>
</tr>
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<tr>
<td>Bore</td>
<td>82.55 mm</td>
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<tr>
<td>Stroke</td>
<td>142.1 mm</td>
</tr>
<tr>
<td>Clearance height</td>
<td>5.7 mm</td>
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<tr>
<td>Engine speed</td>
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</tr>
<tr>
<td>Compression ratio</td>
<td>23.0</td>
</tr>
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<td>Inlet valve open</td>
<td>15° BTDC</td>
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<tr>
<td>Intake valve close</td>
<td>180° ATDC</td>
</tr>
<tr>
<td>Exhaust valve open</td>
<td>140° ATDC</td>
</tr>
<tr>
<td>Exhaust valve close</td>
<td>15° BTDC</td>
</tr>
</tbody>
</table>

Results and Discussion

The main results discussed in this section were obtained using LES for the three mentioned cases, namely the non-reacting single-phase flow, the premixed HCCI and early-spray injected HCCI. The aim of these calculations was to show the effect of velocity cyclic variations on processes of autoignition and HCCI combustion under considered conditions and to retrieve the area with high intensity of cycle-to-cycle fluctuations of combus-
tion properties. For this purpose 40 and 25 consecutive engine cycles have been performed for each considered cases on coarse and fine grids, respectively. It should be noted that the presented calculations of HCCI combustion involve the fuel history effects from the previous engine cycle, i.e. effect of gas residual.

Single-phase flow: intensity of velocity cyclic variations

Figure 5 shows the typical in-cylinder flow field pattern and averaged velocity flow filed during the intake stroke at CA = 65° after top dead centre (ATDC). There are two pronounced intake jets which form three regions with a circular motion within the combustion chamber. Due to the specific engine configuration there is no in-cylinder charge motion that mainly rises during the intake stroke. Figure 6.a illustrates the mean velocity flow field structure at the end of compression stroke at CA = 15° before top dead centre (BTDC) while Figure 6.b depicts instantaneous, mean and rms velocity profiles obtained on fine grid. Velocity magnitude during the compression stroke is considerable smaller compared to the intake stroke. A rather uniform velocity flow field has established revealing homogenous cycle-to-cycle fluctuations (see Figure 6.b) with up to 5.4 m/s deviation from the mean velocity. At the same time the standard velocity deviation normalized with the local mean velocity ($u_{rms} / u_{mean}$) reaches the values with a peak intensity of 0.35 m/s along the whole combustion chamber.

The effect of temperature stratification due to the velocity cyclic variations is shown in Figure 6.c. Directly before autoignition the intensity of temperature cycle-to-cycle fluctuations is not exceeded 70 K while the mean value of in-cylinder temperature is the order of 1070 K. Thereby the initialization of combustion occurs under relatively high intensity of velocity and rather low intensity of temperature cyclic variations.

![Figure 5 Streamlines and mean velocity flow field in the cross section of the combustion chamber at CA = 65° ATDC.](image)

![Figure 6 Streamlines and mean velocity flow field (a), instantaneous, mean and rms of velocity (b) and temperature (c) profiles at z = 0.095 m in the cross section of the combustion chamber for 25 consecutive engine cycles at CA = 15° BTDC, fine grid.](image)

Premixed HCCI combustion

Figure 7 shows contour plots for the cycle-to-cycle fluctuations and standard deviation of in-cylinder velocity (top) and temperature (bottom) at the end of the compression stroke at CA = 15° BTDC. The profiles were obtained along the line marked “A” shown in Figure 7.c, top. The results demonstrate a high correlation between velocity and cyclic variations of temperature and fuel-air ratio (not shown here) as depicted in Figure 7.b. A homogeneous autoignition is initialized at CA = 15° BTDC as depicted through the temperature field in the cross section of the combustion chamber in Figure 7.a, bottom.

Figure 8 depicts the velocity (top) and temperature (bottom) profiles obtained at top dead centre (TDC) of compression stroke on coarse (a) and fine (b) grids. Both velocity and temperature fluctuations are rather homogenous. Velocity magnitude and intensity of velocity cyclic fluctuations decrease towards TDC. Due to the
lack of in-cylinder charge motion the velocity flow field has no pronounced structure and can be characterized as rather uniform. Magnitudes and standard deviation of velocity are comparable with corresponding values obtained for the single-phase flow.

Figure 7 Contour plots (a), instantaneous profiles at \( z = 0.095 \) m (b) and standard deviation (c) of velocity (top) and temperature (bottom) in the cross section of the combustion chamber. Data obtained for 25 engine cycles at top dead centre for homogeneous autoignition at \( CA = 15^\circ \) BTDC, fine grid.

Figure 8 Instantaneous, mean and rms profiles of velocity (top) and temperature (bottom) at \( z = 0.095 \) m, \( CA = 0^\circ \) (TDC). a) fine grid, 25 engine cycle; b) coarse grid, 40 engine cycles; c) comparison of mean and standard deviation profiles between coarse and fine grids.

Figure 8.c demonstrates comparison of the mean and rms velocity and temperature profiles at TDC obtained on fine (red lines) and coarse (green lines) computational meshes. From the above results it can be concluded that distinctions in velocity prediction between fine and coarse grids are visible. At the same time LES predicts rather similar in-cylinder temperature on both grids. Also the intensity of velocity and temperature fluctuations is comparable for both cases. Although the results obtained on coarse grid can be used for qualitative analysis of
location and origin of cycle-to-cycle fluctuations, quantitative analysis of intensity and peak values of cyclic variations requires consideration of fine grid. However, the computational costs for LES calculations in the case of the fine grid are too high so that a compromise in grid resolution is required. Based on the previous publications of the authors [19, 26] a mesh with grid size the order of 1.0 mm can be recommended as the minimum requirement to represent the engine flow field with reasonable accuracy.

**Early-spray injected HCCI combustion**

In order to provide a proper conditions for HCCI combustion fuel spray injection takes place during the intake stroke according to parameters in Table 2. Figure 9.a shows the in-cylinder velocity flow field structure together with injected fuel droplets at CA = 65° ATDC. The injected fuel spray spreads into the combustion chamber but does not affect the structure of in-cylinder flow. The interaction of fuel spray with much stronger intake jet leads to shifting the fuel jet to the left side of the combustion chamber. At the same time the process of fuel-air mixing, shown in Figure 9.b by means of the fuel-air ratio, takes place.

Sequences of instantaneous temperature field in the perpendicular section of the combustion chamber are shown in Figure 10 for illustration of the development of the ignition processes in case of early-direct spray injection for different crank angles. At the proper conditions initialization of autoignition processes takes place at CA = 13° BTDC, where the ignition occurs at several places through the combustion chamber. The range of the temperature field shown in Figure 10 corresponds to 2000 – 2100 K. Instantaneous temperature fields have pronounced asymmetrical shapes in the X-Y plane for consecutive cycles.

![Figure 9 Streamlines, velocity flow field together with injected droplets (a) and fuel-air ratio (b) in the cross section of the combustion chamber at CA = 65° ATDC during fuel spray injection.](image)

Figure 11 provides information about intensity and distribution of velocity and temperature cycle-to-cycle variations at TDC along the combustion chamber at z = 0.095 m obtained on coarse grid. The flow field structure and temperature behaviour obtained for non-premixed HCCI combustion are similar to results that were observed in the case of premixed HCCI combustion as can be seen from comparison of Figure 8.b and Figure 11. The results reveal the same location of regions with high intensity of velocity and temperature cyclic-to-cyclic fluctuations for both cases. The amplitudes of velocity and temperature in the early-spray injected case are approximately 33% and 40%, respectively, higher compared with those of the homogeneous HCCI combustion. Taking into account that the initial and boundary conditions were set identical for all considered consecutive engine cycles, we can conclude that the velocity cyclic variations can be considered as the possible source of in-cylinder temperature stratification. It should be noted that the presented calculations of HCCI combustion involve the fuel history effects from the previous engine cycles. The residual gas from the previous engine cycle can be also considered as a possible source of temperature cycle-to-cycle fluctuations at the beginning of the intake engine stroke.

![Figure 10 Initialization of combustion processes in early-direct spray injection case, Temperature field in the perpendicular section (z = 0.095 m) of the combustion chamber at different crank angles, fine grid.](image)
Instantaneous, mean and rms profiles of velocity (a) and temperature (b) at z = 0.095 m, CA = 0° (TDC). Data obtained on coarse grid for 40 engine cycles in early-direct spray HCCI combustion case.

Direct comparison of in-cylinder mean pressure and temperature near TDC obtained on coarse grid for three considered cases is presented in Figure 12. LES predicts rather similar in-cylinder mean pressure for both premixed and early-direct spray HCCI combustion cases. The results for non-reacting single-phase flow are shown here for the reference. The pressure reaches maximal value of 92.0 bar and 94.0 bar at TDC for premixed and early-direct injected cases, respectively. Visible distinctions in the values of temperature between two considered HCCI combustion cases close TDC can be explained by high sensitivity of simulation of fuel spray injection to the grid resolution.

The effects of grid sensitivity on LES prediction of mean in-cylinder pressure and temperature is depicted in Figure 12 for fully premixed HCCI combustion (i.e. case B). The examination of the results reveals that the mean pressure and temperature is qualitatively and quantitatively well captured on both used computational grids.

Summary and Conclusions

A qualitative comparative analysis of cycle-to-cycle phenomena of in-cylinder flow in a HCCI engine has been carried out using LES. LES is required to provide well resolved turbulence inputs needed to better capture and understand the cycle-to-cycle variation effects of velocity fluctuations on HCCI combustion processes. Thereby, non-reacting single-phase, homogeneous and inhomogeneous auto-ignition cases have been considered. Multi-cycle analysis is required to gain valuable statistical analysis. Hence, three series of 40 and 25 consecutive engine cycles performed on coarse and fine grids, respectively allow to characterize the intensity and locations of velocity, temperature and pressure cycle-to-cycle fluctuations during intake and compression engine strokes. The authors believe that the cycle-to-cycle phenomena are firstly directly linked to the turbulence, and the random nature of turbulence is the most likely origin of the in-cylinder velocity cyclic variations. It was also shown that the velocity cycle-to-cycle fluctuations result in temperature stratification. In spite of the fact that some data discussed in this work were obtained on relatively coarse grid, the results can be used as a basis for further systematical analysis of the effect of cycle-to-cycle fluctuations on auto-ignition and HCCI combustion processes along with detailed characterization of combustion variability using detailed chemistry. The influence of cyclic variations on soot formation and emissions can be then be well addressed.
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References