

Large Eddy Simulation and Experiments of the Auto-Ignition Process of Lean Ethanol/Air Mixture in HCCI Engines

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ABSTRACT

Recent experiments and numerical studies have showed that piston geometry has a significant effect on the homogeneous charge compression ignition (HCCI) process. There are two effects generated by the combustor geometry: the geometry affects the flow/turbulence in the cylinder; the geometry also affects the temperature stratification. The temperature stratification is more directly responsible for the observed alteration of the auto-ignition process. To clarify this issue further we present in this paper a study of two engines with the same geometry but difference ways of cooling. Measurement of the two engines – a metal engine and quartz piston engine, both with the same piston bowl geometry – is carried out. Large eddy simulation (LES) is used to simulate the flow, the temperature field and the auto-ignition process in the two engines. The fuel is ethanol with a relative air/fuel ratio of 3.3. It is found that lower temperature stratification is established in the metal engine under similar conditions as the optical quartz engine due to the more effective cooling of the piston in the metal engine configuration. The combustion phasing in the two engines is the same by controlling the intake temperature. Both measurements and LES show a more rapid auto-ignition in the metal engine than in the optical engine with the same piston geometry. This confirms the conclusion that large temperature stratification can decrease the pressure-rise-rate and thereby increase the load of HCCI engines. The dependence of temperature stratification on the wall temperature and intake temperature is systematically studied using LES.

INTRODUCTION

Recent experiments [1-4] on homogeneous charge compression ignition (HCCI) engines with different piston geometry have revealed that HCCI combustion is rather sensitive to the piston geometry. Several possible

reasons may be responsible for this high sensitivity; one is that in the square bowl piston engine reported in [1-4] the turbulence intensity is higher when the piston is near the top dead center (TDC) [1,2], which might affect the ignition process. Recent chemiluminescence and acetone fuel tracer laser induced fluorescence (LIF) experiments revealed that due to the high convective flow motion between the bowl and squish room the ignition front in the bowl engine resembles that of a flame propagation front with sharp finger-like structure [3,4]. This combustion process has been studied using large eddy simulation (LES) with a progress-variable equation to trace the heat release [5]. It was shown that indeed the turbulent flow in the bowl piston case is higher when the piston is near the top dead center and the finger-like reaction front structure was predicted by LES. However, in the intake and most compression stroke, the turbulent flow field is not affected greatly by the bowl since the flow is more directly dependent on the intake manifolds. A major finding of the LES study reported in [5] is that the temperature stratification in the bowl piston and the flat disc piston engine is fairly different. The reason is that the bowl piston has a larger area-to-volume ratio which enhances the heat transfer from the hot piston wall to the bulk flow during the intake phase. A 30-40K temperature stratification can be obtained in the bowl engine whereas the stratification in the flat disc engine is about half of that in the square bowl engine. This can trigger an earlier ignition process in the bowl. When the combustion phasing (characterized by CA50, the crank angle at which 50% of heat has released) is kept the same for the bowl engine and the disc engine, it was found that the pressure-rise-rate in the bowl engine is lower. This finding is consistent with the numerical simulation of Sjöberg et al. [6], who used a multi-zone model coupled with detailed chemistry to simulate the influence of temperature stratification on HCCI combustion with the flow being neglected. Their results also showed that with high temperature stratification and low wall temperature

the ignition timing the same, higher temperature stratification can cause slower pressure-rise-rate.

To scrutinize the effect of turbulence and the strong squish flow motion from the effect of temperature stratification, new engine experiment is carried out and some of the results are reported here whereas more detailed engine performance data are presented in [7]. In the experiments, a metal piston is used with a square bowl identical to that of the quartz piston [3, 4]. This is expected to generate similar turbulent flow field in the two engines but different temperature field due to the different heat capacity, conductivity and cooling in the metal piston engine and the quartz piston engine. LES is used in this study to explore the development of temperature stratification in both the metal and the quartz piston engine, with respect to the variation of intake temperature, compression ratio and wall temperature. Finally, LES is used to predict the ignition process and the in-cylinder pressure. Comparison between the LES results and experiments are satisfactory which allow us to explain the experimentally observed differences in the in-cylinder pressure-rise-rate and combustion efficiency in the two engines.

EXPERIMENTAL SETUP

ENGINE SETUP

The engine used in this study is a six cylinder Scania D12 truck sized diesel engine converted to HCCI operation by the use of port fuel injection (PFI). Combustion was maintained in one of the cylinder whereas the rest of the cylinders were motored. This was possible when the five motored cylinders heads were removed and replaced with steel plates. To decrease the compression work holes were drilled into the pistons and counter weights were mounted, resulting in a fully balanced engine. A piezoelectric water-cooled Kistler 7061B pressure transducer was used to monitor the in-cylinder pressure and this information was used to control the phasing of combustion by changing the intake air temperature with an electrical heater. Some key data can be found in Table 1.

COMBUSTION CHAMBERS AND OPTICAL ACCESS

A square bowl combustion chamber was tested in this study both in a normal metal engine with metal pistons and in an optical engine with quartz glass pistons. The quartz glass engine configurations were modified for optical access measurements; information about the optical measurements and corresponding results can be found in [3,4]. The focus in this study is to compare how the material of the piston influences the ignition. The comparison will be between the metal piston and the quartz glass piston. It is known that in the square bowl combustion chamber with a narrow squish region a strong squish motion forces the swirling motion of the charge into the bowl during the compression stroke, thereby creating a stronger turbulence, especially in the corners of the bowl [1-5].

As shown in Table 2, the two studied engines have the same bowl geometry and nearly the same compression ratio. The top-land distance for the optical engine is nearly double of that of the metal engine, but the squish volume is less than that of metal engine. This difference might cause a difference in the combustion efficiency as shown in Table 3 where the optical engine has shown a lower efficiency of 82.9% with respect to the 89.3% in the metal engine case. As we will show later, this difference in combustion efficiency is also strongly related to the combustion process in the main part of the combustor.

Table 1 Operating conditions and geometrical data of the Scania D12 Engine.

Displaced volume	1951 cc
Stroke	154 mm
Bore	127 mm
Connecting rod	255 mm
Exhaust valve open	34° BBDC @ 0.15 mm lift
Exhaust valve close	6° BTDC @ 0.15 mm lift
Inlet valve open	2° BTDC @ 0.15 mm lift
Inlet valve close	29° ABDC @ 0.15 mm lift
Valve lift inlet	14 mm
Valve lift exhaust	14 mm
Fuel Injection	PFI
Fuel	Ethanol
Relative Air/Fuel Ratio	3.3
Engine Speed	1200 rpm
Intake Pressure	0.9-1 Bar Absolute
Intake Temperature	75-125°C

Table 2 Geometrical data of the combustion chambers in both optical and metal engine configuration. Squish distance, wall area, squish area, squish volume and squish area to volume ratio were all calculated at TDC. The bowl dimensions are expressed as width times depth in the square bowl cases (SQ_Q-square bowl quartz piston and SQ_M-square bowl metal piston).

	Optical Engine	Metal Engine
Geometry	SQ_Q	SQ_M
CR	17.2:1	17.0:1
Squish Distance[mm]	1.75	2.00
Topland Height [mm]	44.5	24.7
Spacer height [mm]	30	14
Bowl Dimensions [mm]	47 x 37	47 x 37
Wall Area [cm²]	333	332
Squish Area [%]	65.6	65.0
Squish Volume [%]	15.3	17.1
Squish Area/Volume ratio	11.8	10.4
Piston Crown Material	Quartz	Steel

The combustion phasing in the two engines is controlled by intake gas temperature. As listed in Table 3, it was

found that to have 50% heat release crank angle (CA50) at about 6 CAD ATDC, the intake gas temperature was set to 388K for the metal engine, and 354K for the quartz piston engine.

The main difference in these two engines is the material of the piston and in the way that the pistons are cooled. The metal piston is cooled with an oil spray form beneath. The quartz glass piston is cooled with an air jet. Therefore, the quartz piston is hotter than the metal piston. The influence of the wall/piston temperature on the temperature field is studied in detail below using LES.

Table 3 Performance comparison between the optical and metal engine configuration at an engine speed of 1200 rpm and $\lambda=3.3$.

	Optical Engine	Metal Engine
Geometry	SQ Q	SQ M
CA10 [CAD]	-1.2	2.5
CA50 [CAD]	6.8	5.8
CA90 [CAD]	18	11.0
CA90-CA10 [CAD]	19.2	8.5
η_{comb} [%]	82.9	89.3
Residual gas [K]	500	500
Intake temperature [K]	354	388
Intake pressure [bar]	0.9	0.9

LES MODEL AND NUMERICAL METHODS

The present LES model has been presented in [5,8,9]. Here only a brief description is given. The spatially filtered continuity equation, and transport equations for momentum, enthalpy, and a reaction progress variable are employed in the LES. Since the fuel is injected to the intake manifolds and auto-ignition takes place mostly around the end of compression stage, the inhomogeneity in the fuel concentration field can be neglected. The local ignition process can be modeled by the reaction progress variable c that is a normalized cumulative heat release [8,10]. $c=0$ corresponds to the state of initially fresh fuel/air mixture, whereas $c=1$ represents the state that all the chemical energy has been released to heat. Therefore, c at the end of the combustion stroke is comparable with the combustion efficiency η_{comb} in the experiments (Table 3).

The progress of the combustion process, as described by the transport equation of the reaction progress variable, depends on two events, turbulent transport of mass and heat, and chemical reactions. The chemical reactions are taken into account in the source term in the c -equation. Detailed ethanol/air chemical kinetic mechanism [11] is used to simulate the auto-ignition process of the mixture with different initial temperature and pressure. The normalized heat release rate is the source term of the progress variable transport equation

(dc/dt) , thus it is stored in a data-library as a function of the total enthalpy, pressure and the progress variable itself. The auto-ignition history (i.e. the evolution of all species mass fractions, temperature, etc.) is also stored as a function of initial total enthalpy (or initial temperature), pressure and reaction progress variable.

The low Mach flow assumption has been used to simplify the governing equations. With this assumption, the pressure is treated as the sum of a hydrodynamic pressure and a thermodynamic pressure. The thermodynamic pressure is uniform in space and it is used with the equation of state to calculate density and temperature. This pressure is comparable with the in-cylinder pressure from the measurements. The hydrodynamic pressure is used in the momentum equation to drive the flow motion.

Following the low Mach number assumption, the inflow mass flux is determined by the piston velocity by assuming global mass conservation in the cylinder. This is likely appropriate in the current low engine speed conditions (1200 rpm), however, not accurate under high load conditions. The manifolds of the intake ports are not resolved; therefore a model of the flow at the exit of the intake ports is used. Details about the inflow treatment are given in [9].

The wall boundary condition involves the treatment of wall heat transfer and determination of wall temperature. Due to the lack of measurement, the wall temperature has been assumed a constant value. Heat transfer near the walls is a complex process requiring considerable care. In LES, the grid resolution is not sufficient to resolve the fine scales. It is therefore necessary to employ wall models. This can be done by using a 'wall-function' which models the heat flux at the wall by using flow quantities at the first cell near the wall [12,13]. Comprehensive survey of wall models for LES has been given by several authors for example Piomelli & Balaras [14].

The governing equations are solved numerically on a staggered moving Cartesian grid system. The spatial discretization is done using a 5th order WENO scheme for the convective terms and 4th order central difference for the diffusive terms [15]. The discretized system of equations is integrated in time with a 2nd order Adam-Bashforth scheme. An additional corrector step is used to maintain numerical stability during the late compression stage when high density gradients are formed in the flow field. The corrector step is performed using a 2nd order Crank-Nicholson method. At each step, a variable-coefficient Poisson equation is numerically solved to determine the hydrodynamic pressure. The discrete pressure equation is solved using Gauss-Seidel iterative method, together with a multi-grid method to accelerate the convergence [16]. The simulation has been parallelized based on domain decomposition.