

Studies on the Effect of In-Cylinder Charge Stratifications on High Load HCCI Combustion

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ABSTRACT

The objective of this article is to clarify the effect of thermal and equivalence ratio stratification on Homogeneous Charge Compression Ignition (HCCI) combustion under several conditions with three-dimensional computational fluid dynamics (3D CFD). Reynolds Averaged Navier-Stokes (RANS) simulation was used to calculate in-cylinder fluid dynamics. The 3D CFD simulation is also coupled with detailed chemical reaction to calculate HCCI combustion. First, the study with a simple engine model reveals that thermal stratification is more effective for prolonged combustion duration, which is a key factor for a high load limit of HCCI combustion, than equivalence ratio stratification. Thermal stratification has two-stage combustion: the combustion propagates from hot region slowly at first and then ignites in the entire in-cylinder region. Owing to this phenomenon, thermal stratification is more effective to mitigate HCCI combustion. Furthermore, thermal stratification enables combustion efficiency to be maintained: combustion efficiency would be a problem to relieve HCCI combustion by intake charge stratification. Second, the study with a detailed engine model was conducted to evaluate the improvement of the high load limit and thermal efficiency under the constraint of the maximum in-cylinder pressure and the pressure rise rate. In the second study, mixture stratification was produced by inducing hot and cold intake mixture from respective intake ports. The result shows that the temperature of in-cylinder hot gas region plays an important role to extend the high load limit of HCCI combustion.

CITATION: Yoshimura, K., Mori, S., Nakama, K., and Kusaka, J., "Studies on the Effect of In-cylinder Charge Stratifications on High Load HCCI Combustion," *SAE Int. J. Engines* 9(4):2016, doi:10.4271/2016-32-0010.

INTRODUCTION

In recent years, global environmental issues have become urgent and important. Therefore, it is necessary to reduce the fuel consumption rate and emissions of internal combustion engines. HCCI combustion has the potential to improve them providing leaner and lower temperature combustion [1]. On the other hand, there is a high load limit of HCCI combustion due to a steep pressure rise rate. On high load combustion, the in-cylinder mixture can ignite at the same time because the initiation of HCCI combustion depends on chemical reaction. The fast combustion causes combustion noise and massive in-cylinder pressure which leads to engine damage. In addition, because the combustion temperature is lower than spark ignition (SI) combustion, it is likely that some part of the in-cylinder mixture can be misfired. This decreases combustion efficiency. Therefore, it is necessary to find a way to control high load HCCI combustion without decreasing of combustion efficiency.

Some previous papers focused on the control of HCCI combustion [2, 3, 4, 5]. The numerical study researched the effect of temperature stratification on HCCI combustion using large eddy simulation (LES) and 0-d multi-zone simulation [4]. It was found that the higher temperature stratification could be the longer combustion duration.

The length scale of the stratified temperature field plays an important role in the auto-ignition process. Another work investigated the potential of lowering the heat release rate of HCCI combustion by using partial fuel stratification to increase thermal stratification with numerical simulation and experiment [5]. The work showed that the combination of a premixed charge and injection of fuel in the compression stroke is effective for smoothing the heat release rate. Another numerical study with LES analyzed the interrelationships between mixture heterogeneity and reaction in a turbulent flow [6]. The result showed the equivalence ratio fluctuations with the large rms and the large length scale contributes to moderate a combustion process. In this way, several investigations have been conducted on the evaluation of the effect of thermal and equivalence ratio stratification. However, there have been few efforts to compare the effect of these manners of stratification on HCCI combustion. In order to extend a high load limit of HCCI combustion, it is therefore important to understand the characteristics of thermal and equivalence ratio stratification.

The objective of this article is to clarify the effect of thermal and equivalence ratio stratification on HCCI combustion under several conditions with 3D CFD. In the first study, the effect of the two types

of direction of in-cylinder mixture stratification on combustion was researched: the first shape of in-cylinder mixture stratification is parallel to bore axis and the second shape of that is parallel to cylinder axis. In addition, the effect of thermal stratification was compared to that of equivalence ratio stratification. These studies were undertaken using the simple engine model. In the second study, to evaluate the effect of thermal stratification under practical condition, the computation with the detailed engine model which had intake and exhaust ports was carried out. In the study, the thermal stratification was formed by induction of hot and cold intake mixture from respective intake ports: the method is called “dual intake ports stratification”. This manner makes a large hot region in combustion chamber. Moreover in the second study, the effects of “dual intake ports stratification” on combustion under the different engine speed.

SIMULATION METHOD

In this paper, RANS simulation was used to calculate in-cylinder fluid dynamics. The simulation is coupled with detailed chemical reaction to calculate HCCI combustion. The software and numerical models are shown in [table 1](#). CONVERGE v 2.2.0[7] was utilized to calculate fluid dynamics and HCCI combustion. The gasoline surrogate mechanism developed by Chalmers University [8] was used to calculate chemical reactions. Toluene reference fuel (TRF) 90 was used as a surrogate fuel. The blend ratio of three components: iso-octane, toluene and n-heptane, was adjusted to the ignition characteristics of 90 RON gasoline.

Table 1. Simulation software and numerical specifications.

Software	CONVERGE v2.2.0
Turbulent model	RNG k-ε model
Heat transfer model	Wall function
Combustion model	SAGE
Reaction mechanism	Chalmers gasoline surrogate(120species, 619 reactions)
Surrogate fuel	TRF90

ENGINE MODELS

In the first study, the engine model used is the single cylinder gasoline engine with the disc-shaped combustion chamber as shown in [Figure 1](#). This simple engine model was used to eliminate the effect of a combustion chamber shape from the nature of stratified HCCI combustion. The displacement of this model is 343 cc. For HCCI operation, compression ratio was set to 15:1. The bore and stroke of the engine is 73 mm and 82 mm respectively. The other specifications are shown in [table 2](#).

Table 2. Specification of the simple engine model

Displaced volume cc	343
Stroke mm	82
Bore mm	73
Compression ratio	15:1
Number of valves	0
Number of cells in combustion period	16100

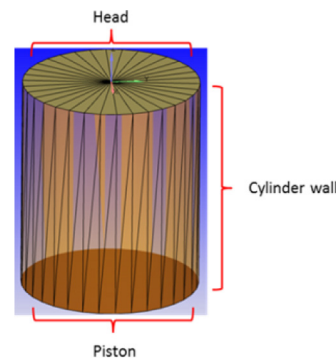


Figure 1. Overview of the simple engine model

In the second study, to evaluate the effect of thermal stratification under practical condition, the computation with the detailed engine model was carried out. The specification and overview of the detailed engine model are shown in [table 3](#) and [figure 2](#), respectively. The general dimensions are the same as the simple engine model shown in [table 2](#). The detailed engine model has a pent-roof combustion chamber. The model also has intake and exhaust valves and ports, which allow of dealing with gas exchange process. In this study, to eliminate the effect of evaporation and impingement to a wall of injected fuel, the detailed engine model has no fuel injector. Therefore, fresh air and fuel vapor are inducted from inlets of intake ports as mixture.

Table 3. Specification of the detailed engine model

Displaced volume cc	343
Stroke mm	82
Bore mm	73
Compression ratio	15:1
Number of valves	4
Number of cells in combustion period	300000

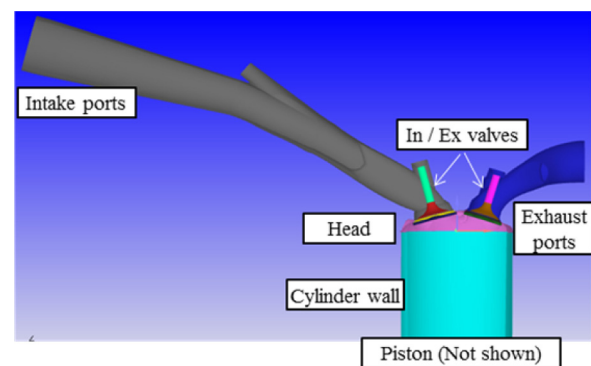


Figure 2. Overview of the detailed engine model

In the second study, “dual intake ports stratification” was calculated. As shown in [figure 3](#), hot mixture and cold mixture were inducted from each intake port. Because each port was separated with each other, the hot and cold mixture mixed only in the cylinder. Hot and cold mixture was inducted from the intake ports A and B, shown in [figure 3](#), separately. To measure in-cylinder gas temperature two probes were set, shown in [figure 4](#). The probe A and B was set near

the intake ports A and B, respectively. Therefore, the probe A is to measure temperature in hot region and the probe B is to measure temperature in cold region.

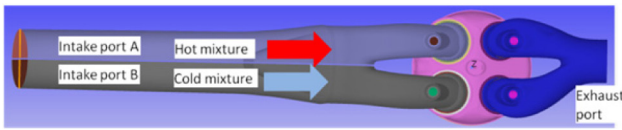


Figure 3. Overview of the intake ports of "dual intake ports stratification"

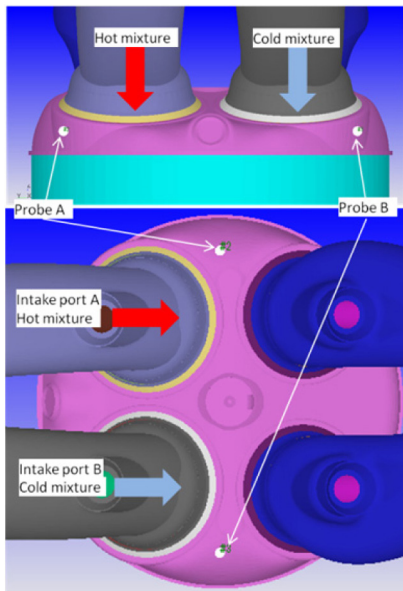


Figure 4. Overview of probes in the combustion chamber

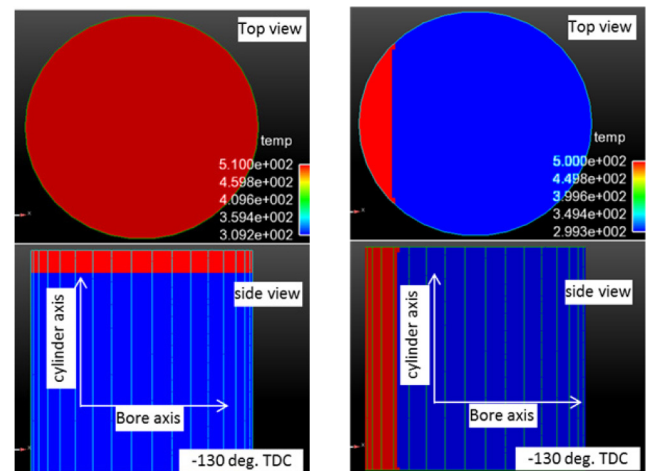
CALCULATION CONDITIONS

The First Study: the Effect of Thermal and Equivalence Ratio Stratification

The calculation conditions of the first study are presented in [table 4](#) and [figure 5](#). Firstly, the two shapes of initial thermal distribution were set to research the effect of the direction of in-cylinder mixture stratification. As shown in [figure 5](#), the first shape of thermal distribution is parallel to bore axis and the second shape of that is parallel to cylinder axis. The difference in initial in-cylinder temperature of hot zone and cold zone was set to 200 K in both shapes. The volume of hot region was set to 10 % in both shapes. The start timing of the calculation is -130 deg.aTDC: the crank angle is the partway of the compression stroke. The engine speed was fixed at 1200 rpm. In order to calculate under high load condition, in-cylinder fuel mass was set to 25.35 mg/cycle/cylinder, which corresponds to BMEP:1200 kPa. Initial average in-cylinder temperature was adjusted to set CA50 at just before and after 5 deg.aTDC, respectively. To evaluate a maximum in-cylinder pressure rise rate and combustion duration at the same CA50, these values then were interpolated at CA50: 5 deg.aTDC. To sustain the initial mixture stratification until the combustion initiation, the initial in-cylinder flow velocity was set to zero.

Table 4. Calculation Condition of the first study

Start timing of calculation	-130 deg.aTDC
Engine speed rpm	1200
Spatial average equivalence ratio	0.667
In-cylinder fuel mass mg/cyc./cyl.	25.35
Initial spatial average in-cylinder temperature	Adjusted to set CA50 at just before 5 deg.aTDC Adjusted to set CA50 at just after 5 deg.aTDC
Initial in-cylinder pressure	Adjusted along to initial in-cylinder temperature to maintain fuel mass
External EGR ratio %	0
Initial in-cylinder flow m/s	0
Initial turbulent kinetic energy m^2/s^2	1
Initial turbulent dissipation m^2/s^3	10
Wall temperature on Piston K	410.7
Wall temperature on cylinder head K	416.9
Wall temperature on cylinder liner K	385.5



a. Thermal stratification parallel to bore axis b. Thermal stratification parallel to cylinder axis

Figure 5. Overview of the thermal distributions. The volume of hot region: 10 %

Besides the research of the effect of the direction of in-cylinder mixture stratification, the simulation in comparison of thermal stratification with equivalence ratio stratification is conducted in the shape of stratification in [Figure 5 \(b\)](#); we define a high-ignitable and low-ignitable zone are in the left (red) and right (blue) zone of the cylinder, respectively. Those conditions are listed in [table 4](#) and [5](#). In [table 5](#), 2 values of initial temperature were set to simulate with CA50 at just before and after 5 deg.aTDC, respectively. In the cases 1 - 6, the simulations of equivalence ratio stratification were conducted. The high-ignitable and low-ignitable zone is defined as rich and lean zone, respectively. In these cases, the initial temperatures of 2 zone are different with each other by 3 - 13 K since in-cylinder fuel mass is fixed at a certain value. We regard the small difference in initial temperature as negligible for evaluation of the effect of equivalence ratio. In the cases 7 - 12, the simulation of thermal stratification was

conducted. In the cases 11 and 12, the initial temperature of low-ignitable zone is low, since the amount of in-cylinder fuel mass is so large that it is easy to ignite without cooling of in-cylinder mixture. In the real engine tests, the amount of in-cylinder fuel mass has to be adjusted. In the case 13, the simulation of homogeneous case was conducted for comparison with the stratification case.

Table 5. Initial condition of the first study

Case	Volume ratio of the high-ignitable zone %	Equivalence ratio			initial temperature K		
		high-ignitable zone	low-ignitable zone	difference between 2 zones	high-ignitable zone	low-ignitable zone	difference between 2 zones
1	2.55	1.15	0.65	0.5	329 339	332 342	3
2	2.55	2.62	0.62	2.0	320 330	332 342	12
3	8.85	1.12	0.62	0.5	319 339	322 342	3
4	8.85	2.50	0.50	2.0	311 331	323 343	12
5	29.45	1.02	0.52	0.5	320 340	323 343	3
6	29.45	2.08	0.08	2.0	333 353	346 366	13
7	8.85	0.67	0.67	0	368 408	318 358	50
8	8.85	0.67	0.67	0	415 455	315 355	100
9	8.85	0.67	0.67	0	500 510	300 310	200
10	29.45	0.67	0.67	0	359 399	309 349	50
11	29.45	0.67	0.67	0	378 388	278 288	100
12	29.45	0.67	0.67	0	463 473	263 273	200
13	0	-	0.67	-	- 335	340 335	-

The Second Study: the Analysis of Thermal Stratification with "Dual Intake Ports Stratification"

The calculation conditions of the second study are shown in [table 6](#). Two levels of engine speed were set to calculate under different turbulent intensity and flow velocity condition. A/F is changed to calculate under the different engine load condition. The spatial average intake air temperature is changed to adjust CA50. The calculation is started just before exhaust valve open (EVO) timing. The wall temperatures were obtained by GT-POWER. The inlet boundary conditions of intake ports are listed in [table 7](#). Three levels of boundary conditions were set. In the moderate stratification case and the strong stratification case, the differences in intake mixture temperature between intake port A and B were set to 100 K and 200 K respectively, shown in [table 7](#) and [figure 3](#). In the homogeneous case, there is no temperature difference between intake port A and B. Intake

mixture temperature was changed to make the maximum in-cylinder pressure and the pressure rise rate under certain limits. In some cases of strong stratification case, the intake temperature is too low because of the same reason of the initial condition of the first study.

Table 6. Calculation condition of the second study

Engine speed rpm	1200, 3000
A/F	25 - 48
Temporal average intake air pressure kPa(abs)	200
External EGR ratio %	0
Initial in-cylinder flow m/s	0
Initial turbulent intensity m^2/s^2	1
Initial turbulent dispersion m^2/s^3	10
Wall temperature on Piston K	386
Wall temperature on cylinder head K	396
Wall temperature on cylinder liner K	371

Table 7. Intake boundary condition of the second study

	Case		
	Homogeneous	Moderate stratification	Strong stratification
Difference in intake mixture temperature between intake port A and B K	0	100	200
Intake mixture temperature of intake port A K	345-405(1200rpm) 415-445(3000rpm)	395-455(1200rpm) 465-525(3000rpm)	445-505(1200rpm) 515-565(3000rpm)
Intake mixture temperature of intake port B K	345-405(1200rpm) 415-445(3000rpm)	295-355(1200rpm) 365-425(3000rpm)	245-305(1200rpm) 315-365(3000rpm)

RESULTS AND DISCUSSIONS

The First Study: the Effect of the Direction of In-Cylinder Mixture Stratification

The effect of the direction of in-cylinder mixture stratification was simulated in accordance with [table 4](#) and [figure 5](#). Result is shown in [table 8](#) and [figure 6](#) and [7](#). The result shown in [table 8](#) is the data which was interpolated at 5 deg.aTDC. The results shown in [figure 6](#) and [7](#) are the data which CA50 is near 5 deg.aTDC. As is obvious from [table 8](#), the stratification parallel to cylinder axis has longer combustion duration and lower maximum in-cylinder pressure rise rate compared to the stratification parallel to bore axis. Therefore, the stratification parallel to cylinder axis is more effective to slow the combustion and mitigate the in-cylinder pressure rise rate. The comparisons of in-cylinder pressure and heat release rate are presented in [figure 6](#). In the case of thermal stratification parallel to cylinder axis, combustion initiates earlier than that of thermal