A Comparative Study of HCCI and ATAC Combustion Characteristics Based on Experimentation and Simulations - Influence of the Fuel Octane Number and Internal EGR on Combustion

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ABSTRACT

Controlled Autoignition (CAI) combustion processes can be broadly divided between a CAI process that is applied to four-stroke engines and a CAI process that is applied to two-stroke engines. The former process is generally referred to as Homogeneous Charge Compression Ignition (HCCI) combustion and the later process as Active Thermo-Atmosphere Combustion (ATAC). The region of stable engine operation differs greatly between these two processes, and it is thought that the elucidation of their differences and similarities could provide useful information for expanding the operation region of HCCI combustion. In this research, the same two-stroke engine was operated under both the ATAC and HCCI combustion processes to compare their respective combustion characteristics. The results indicated that the ignition timing was less likely to change in the ATAC process in relation to changes in the fuel octane number than it was in the HCCI combustion process. It was also observed that the combustion state and the operation range of HCCI combustion approached those of ATAC under the application of internal exhaust gas recirculation.

INTRODUCTION

Further improvement of the efficiency of internal combustion engines (i.e., reduction of specific fuel consumption) and the attainment of cleaner exhaust emissions are required today in order to make effective use of energy resources and preserve the global environment. Methods of improving the thermal efficiency (reducing the specific fuel consumption) of gasoline engines include raising the compression ratio to an optimum level of around 14:1~16:1, adopting lean-burn combustion to improve the specific heat capacity and reduce heat losses, and reducing pumping work [1-2]. Diesel engines already attain high thermal efficiency, but the difficulty of simultaneously reducing their nitrogen oxide (NOx) and soot levels remains a major issue to be addressed.

Against this backdrop, the Homogeneous Charge Compression Ignition (HCCI) [3-6] engine has attracted much interest because it achieves clean combustion with an ultra-low NOx level and no soot emission when operated under a non-throttled, lean-burn condition at an optimized compression ratio.

Examples of gasoline-fueled HCCI engines include four-stroke, high-compression-ratio engines that adopt a compression ignition combustion system [7] and two-stroke engines that operate under compression ignition combustion at partial load (part throttle). This type of combustion process is called by different names such as Active Thermo-Atmosphere Combustion (ATAC) or Activated Radicals (AR) combustion [8-10]. It is distinctly characterized by the ability to provide compression ignition combustion up to exceptionally high engine speeds. In this combustion process, high-temperature residual gas (internally recirculated exhaust gas, EGR) resulting from a gradual gas exchange is mixed with new air to induce autoignition. Meanwhile, methods of using internal EGR to induce and control ignition have also attracted attention for application to four-stroke HCCI engines [11-19]. However, the similarities and differences between the ATAC process of two-stroke engines and the HCCI combustion process of four-stroke engines are unclear in many respects, and it is desirable to have a comprehensive understanding of the autoignited combustion characteristics of the ATAC and HCCI processes.

Generally, combustion induced by autoignition is called by many different names, such as HCCI, PCCI (Premixed Charge Compression Ignition), CAI (Controlled Auto-ignition), ATAC, AR, and PCI...
(Premixed Compression Ignition), among others. While all of these combustion processes involve autoignition, there are some that differ only in their appellation and others that show slightly different combustion characteristics or whose names include a more specific meaning. The term HCCI is the general name that is used comprehensively to refer to these autoignited combustion processes. ATAC and AR can both be categorized as being one type of HCCI combustion process. Specifically, the ATAC and AR processes are aimed at improving unstable combustion and reducing unburned HC emissions of two-stroke engines under part-load operation. The simplest and most general form of HCCI is lean-burn combustion in a four-stroke engine operated at a high compression ratio and without throttling for the purpose of achieving high efficiency while simultaneously reducing NOx and soot emissions. In this study, we refer to this form of combustion simply as HCCI, and use ATAC to mean HCCI combustion in a two-stroke engine at part load. Both combustion processes were simulated in the same two-stroke engine in this research.

The definitions and major features of the ATAC and HCCI combustion processes examined in this study are outlined below.

(a) ATAC: Defined as autoignited combustion in a two-stroke engine at part throttle and accompanied by a large quantity of high-temperature residual gas, as shown in Fig. 1-(a)

(b) HCCI combustion: Defined as autoignited combustion at WOT that simulates the HCCI combustion process in a four-stroke engine and occurs in the presence of a small amount of residual gas, as shown in Fig. 1-(b).

(c) HCCI combustion + internal EGR: Defined as HCCI combustion with the application of internal EGR that is characteristic of the ATAC process. This process simulates HCCI combustion in a four-stroke engine with negative valve overlap.

In this study, a comparison was first made of (a) and (b) above, and combustion process (c) that combined the features of both was then created for the purpose of analyzing the combustion characteristics.

The typical engine operation regions of the ATAC and HCCI combustion processes are shown schematically in Fig. 2 in relation to the engine speed and mean effective pressure. Autoignited ATAC operation is possible in the low-load (part throttle), high-speed region, but engine operation is impossible at either high loads or low speeds because of misfiring. The reason for that is attributed to the reduced effect of the internal EGR (The reaction process deviated from the conditions leading to autoignition, owing to the change in scavenging accompanying the change in the engine speed and to the change in the temperature of the internal-EGR). On the other hand, autoignited HCCI operation is possible in the low-load region (with a large throttle valve opening but a low equivalence ratio) and low-speed region. Engine operation becomes impossible at high loads (high equivalence ratio) because of knocking and at high speeds and under low loads (low equivalence ratio) on account of misfiring.

In this study, the ATAC and HCCI combustion processes were compared using the same engine. Specifically, a two-stroke engine was operated under compression ignition combustion at partial load, corresponding to the ATAC process. The compression ratio and throttle valve opening of the same engine were then increased to achieve a combustion process equivalent to compression ignition combustion in a four-stroke engine under wide-open-throttle (WOT) operation. Under these conditions, two-stage ignition accompanied by the passage of a cool flame characteristic of a four-stroke HCCI engine was observed when a test fuel with a low octane number was used.

In addition, CHEMKIN software was used to perform numerical calculations of elementary reactions to investigate the behavior of intermediate products and the respective effect of the fuel octane number, scavenging temperature and internal EGR rate on compression ignition combustion in the different load regions of the ATAC and HCCI combustion processes. Based on the combustion characteristics thus found, the potential for expanding the HCCI operation region was investigated. Specifically, internal EGR was applied under HCCI operation in an effort to avoid knocking and expand the region of stable operation to the high equivalence ratio side (arrow 1 in Fig. 2). Simultaneously, an investigation was also made of the effect on expanding the operation region to the high-speed side and the lean-mixture side (arrows 2 and 3 in the Fig. 2) as a result of using the heat contained in the high-temperature internal EGR gas to prevent misfiring.

![Fig. 1 Image of residual gas rate of the ATAC and HCCI.](image)

![Fig. 2 Typical operation region of ATAC and HCCI.](image)
AUTOIGNITION PROCESS OF HYDROCARBON FUELS

Because both ATAC and HCCI combustion processes are characterized as autoignited combustion, the preflame reaction process leading to autoignition of the fuel is regarded as an important factor. Therefore, a brief explanation is given here of the autoignition process of hydrocarbon fuels [20-27].

Figure 3 shows the principal reaction paths of hydrocarbons. The combustion reactions of hydrocarbons begin with an equilibrium reaction that adds O₂ to the alkyl radical R. This first addition of O₂ can be written as

\[ R + O₂ \leftrightarrow RO₂ \] (1)

On the basis of this equilibrium reaction, low-temperature and high-temperature oxidation reactions can be distinguished as follows:

- \([R] > [RO₂]\): high-temperature oxidation reaction
- \([R] < [RO₂]\): low-temperature oxidation reaction

The resulting RO₂ undergoes internal isomerization of its ring structure by which internal H atoms are abstracted to produce QOOH. Subsequent reactions are divided depending on the temperature region. At low temperatures, a reaction takes place in which O₂ is again added to the alkyl radical (denoted as (1) in Fig. 3). A separate reaction takes place in which QOOH decomposes without O₂ being added again (denoted as (2) in Fig. 3). Reaction (1) in the low-temperature region is a chain branching step, and the reaction is accelerated in this temperature region (i.e., cool flame region). When the temperature rises further, the reaction changes to reaction (2). Because reaction (2) is a chain propagation step, acceleration of the reaction ceases in the negative temperature coefficient (NTC) region. Subsequently, the gradual reaction rate, compression by piston motion and other factors cause the temperature to rise to around 1100 K. At that temperature level, reaction (3) occurs, producing a large quantity of OH radicals (blue flame region) and leading to autoignition. In relation to the temperature rise, two-stage ignition occurs owing to the progression from reaction (1) to reaction (3), i.e., from a cool flame to NTC to autoignition.

With HCCI combustion, the premixed mixture begins to be compressed from a point below the cool flame temperature. Consequently, depending on the fuel used, HCCI combustion follows a low-temperature oxidation process in which a cool flame occurs, passes through the NTC region owing to the resultant temperature rise, and then proceeds to autoignition due to the occurrence of reaction (3) in the vicinity of 1100 K.

The degree to which reactions (1) and (2) occur depends not only on the temperature, but also differs greatly according to the molecular structure of the fuel. The reason is that the tendency for internal isomerization to occur varies depending on the molecular structure [28-29]. Consider, for example, the difference between n-heptane and iso-octane. Straight-chain n-heptane easily undergoes internal isomerization of its six- or seven-membered ring with low strain energy on account of its molecular structure. Owing to reaction (1) in Fig. 3, chain branching readily takes place. On the other hand, in the case of iso-octane with its side chains, internal isomerization of its five-membered ring with high strain energy is more apt to occur compared with the six- or seven-membered rings. Moreover, in the case that internal isomerization of the five-membered ring occurs, QOOH tends to decompose (QOOH => Q + HO₂) relatively stably to produce HO₂, and chain branching is not apt to occur. Consequently, n-heptane which passes through six- or seven-membered ring structures with low strain energy and results in chain branching is more likely to produce cool flame reactions. These observations explain why heat release due to a cool flame is clearly detected in HCCI combustion of n-heptane, but is nearly indiscernible in the case of iso-octane.

EXPERIMENTAL EQUIPMENT AND PROCEDURE

The test engine used in this study was a two-stroke air-cooled single-cylinder engine having the specifications shown in Table 1.

<table>
<thead>
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<th>Table 1 Specifications of test engine</th>
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<tr>
<td><strong>2-Stroke Air Cooled SI Engine</strong></td>
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<tr>
<td>Scavenging Type</td>
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<tr>
<td>Bore × Stroke</td>
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<tr>
<td>Displacement</td>
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<td>Effective Compression Ratio</td>
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The test engine was operated under the ATAC process at partial load at an effective compression ratio of 8.7:1 and under the HCCI process at WOT and effective compression ratios of 8.7:1 and 15:1. Cylinder pressure data, heat release rate and radical light emission behavior were recorded and analyzed under each set of operating conditions.

The configuration of the test equipment used is outlined in Fig. 4, and the measurement positions are shown in Fig. 5. Light emission intensities of the radicals of interest were measured in the following way. Flame light in the combustion chamber was extracted by means of a quartz observation window installed in the top of the cylinder head and introduced into a polychromator via an optical fiber cable having a core diameter of 1 mm. The light was separated into wavelengths of 395.2 nm (corresponding to HCHO), 329.8 nm (HCO) and 306.4 nm (OH), and the light emission intensity at each wavelength was measured with a photomultiplier [30-36]. In order to investigate the overheated state of the engine and the operating conditions, measurements were made of the spark plug washer temperature (Tsp), scavenging temperature (Tsc) and exhaust gas temperature (Tex). The scavenging temperature was measured with a K-type thermocouple in the scavenging port at a point approximately 40 mm upstream of the cylinder scavenging port. And the exhaust gas temperature was measured with a K-type thermocouple in the exhaust port at a point approximately 40 mm downstream of the cylinder exhaust port.

The ignition timing used in the analysis of the heat release rate was defined as shown in Fig. 6.

Maximum cool flame value \( Q_{\text{Lmax}} \): maximum heat release rate of the cool flame

Maximum hot flame value \( Q_{\text{Hmax}} \): maximum heat release rate of the hot flame

Onset of ignition \( \theta_{\text{on}} \): the crank angle at which the heat release rate reaches 10% of the maximum heat release rate \( Q_{\text{Hmax}} \)

End of combustion \( \theta_{\text{off}} \): the crank angle at which the heat release rate falls below 10% of \( Q_{\text{Hmax}} \)

Combustion period \( \theta_{\text{comb}} \): \( \theta_{\text{off}} \) crank angle – \( \theta_{\text{on}} \) crank angle

Time of cool flame peak \( \theta_{\text{cool}} \): the crank angle of the peak heat release rate of the cool flame

Ignition delay after cool flame peak \( \tau \): the interval from the time of \( \theta_{\text{cool}} \) to the ignition timing \( \theta_{\text{on}} \)

Time of hot flame peak \( \theta_{\text{peak}} \): the crank angle of the peak heat release rate of the hot flame

Operation under autoignition combustion was accomplished in each case by stopping the electrical discharge from the spark plug.
CALCULATION METHOD

Numerical calculations of elementary reactions were performed using CHEMKIN 3.7 (AURORA Application) under dimensionless, adiabatic conditions and by applying the same volumetric change as that of the test engine. The following two types of reaction mechanisms were used, all of which were developed at the Lawrence Livermore National Laboratory (LLNL) [23-25].

1. n-heptane: 544 chemical species, 2,446 elementary reactions

2. primary reference fuels (PRF): 1,034 chemical species, 4,238 elementary reactions. (blended fuels of n-heptane and iso-octane)

RESULTS AND DISCUSSION

RADICAL LIGHT EMISSION BEHAVIOR AND MOLE FRACTION HISTORIES OF CHEMICAL SPECIES UNDER ATAC AND HCCI COMBUSTION

Autoignited combustion was induced in this study at partial load under an effective compression ratio of ε = 8.7:1 and an engine speed of approximately 2200 rpm. These conditions gave rise to autoignited combustion corresponding to ATAC at partial load in a two-stroke engine. As one example of ATAC characteristics, Fig. 7 shows the waveforms measured at an engine speed of N = 2500 rpm when n-heptane (0 RON) was used as the test fuel. The heat release rate (HRR) waveform for ATAC combustion indicates that autoignition was reached (region A in Fig. 7) without any discernable sign of heat release attributable to the passage of a cool flame prior to ignition. In general, increasing the throttle valve opening or reducing the engine speed causes misfiring in the ATAC process, making stable engine operation impossible. One reason for that in the case of a larger throttle valve opening is attributed to the resultant increase in scavenging efficiency which reduces the quantity of high-temperature combustion gas remaining in the cylinder (Internal-EGR). Reducing the engine speed, on the other hand, lowers the temperature of the residual gas, and the interaction of the two factors reduces the temperature at the onset of compression (Tepc), making it impossible to reach the temperature level needed to induce autoignition. However, when a fuel with a low octane number was used, it was observed that a region existed under WOT and low speed conditions where autoignited operation of the engine was possible.

Figure 8 shows the waveforms measured under WOT at N = 1000 rpm when n-heptane (0 RON) was used as the test fuel. Heat release presumably ascribable to the passage of a cool flame can be observed in the HRR waveform (region B) prior to ignition and a second heat release stage attributed to the hot flame is subsequently seen. This pattern indicates autoignited combustion corresponding to HCCI combustion in a four-stroke engine. Concurrent with the heat release attributed to the cool flame, the light emission intensity waveform of HCHO shows signs of faint light emission and degeneracy behavior (region C). It has been reported that light emission from a cool flame represents the luminescence of excited-state formaldehyde (HCHO) [37]. It is assumed that this faint HCHO light emission signifies such light emission from a cool flame. As these results indicate, the reaction path can lead to autoignition under conditions where a cool flame is manifested even in a low temperature region at the onset of compression. The combustion that occurs in such cases is thought to be the same as HCCI combustion in a four-stroke engine. As explained here, combustion resembling that of a four-stroke HCCI engine and accompanied by a cool flame occurred depending on the state of the residual gas. Therefore, estimates were made of the cylinder temperature (Tm) for ATAC and HCCI combustion, respectively, under the assumption of polytropic changes.

\[
T_m = T_{epc} \left( \frac{V_0}{V_{epc}} \right)^{n-1}
\]

\[
T_{epc} = \frac{\dot{M}_{epc} \cdot \eta_s \cdot T_{sc} \cdot C_p \cdot M_{epc} \cdot (1-\eta_s) \cdot T_{EGR} \cdot C_{p_{EGR}}}{\dot{M}_{epc} \cdot C_{p_{epc}}}
\]

Scavenging efficiency (\(\eta_s\)) is calculated on the basis of corrected delivery ratio (L), assuming perfect mixing scavenging [\(\eta_s = 1 - \exp(-L)\)].

As shown in Fig. 9, the temperature at the onset of compression in the ATAC process is considerably higher owing to the presence of a large quantity of high-temperature residual gas and exceeds 1100 K near TDC. It is presumed that a hot flame is induced by autoignition in the vicinity of 1100 K, so in the case of ATAC, compression by piston motion alone can lead to autoignition. Under HCCI operation, on the other hand, the temperature at the onset of compression is lower, and it is clear that compression alone does not lead to autoignition. Looking at a temperature of 750 K in the cool flame region, it is seen that this temperature level is reached in the ATAC process at a crank angle of 60 deg. BTDC and in the HCCI combustion process at about 20 deg. BTDC.

These results suggest that the difference between ATAC and HCCI combustion is attributed to variation in the low-temperature oxidation reaction characteristics of a hydrocarbon fuel resulting from changes in the cylinder temperature and pressure and in their time histories. That variation corresponds to changes in the degree of influence of the passage of a cool flame and NTC. It suggests that a good understanding of these characteristics can be useful in suppressing or promoting autoignition.
Next, we will discuss the respective calculated results for ATAC and HCCI combustion. It is presumed that a large quantity of internal EGR gas is present in the ATAC process. Accordingly, the calculations were performed under the following hypotheses in order to take account of internal EGR.

(1) The internal EGR composition is assumed to contain the components produced by burning the mixture having the equivalence ratio of interest. The components include N2, O2, CO2, H2O, OH, CO, H2, H.

(2) The temperature of the internal EGR (T_{EGR}) is the mean value of the exhaust gas temperature (T_{ex}) and the blowdown gas temperature (T_{epo}) (see the APPENDIX[a]).

(3) The internal EGR rate is found under the assumption of perfect mixing scavenging.

As for assumption (1) above, calculations were run at the equivalence ratio of interest, and the internal EGR gas was assumed to have the composition of the exhaust gas at 106 deg. ATDC (the opening timing of the exhaust valve). There are reports in the literature that OH radicals and other radicals are contained in the residual gas. Therefore, two types of ATAC calculations were performed. One type considered only the stable components (N2, O2, CO2 and H2O) of the residual gas composition. The second type considered the other components. It should be noted that the mole fractions of the stable components (N2, O2, CO2 and H2O) accounted for 99.7% of the gas composition at 106 deg. ATDC, and the mole fractions of the other components represented the remaining 0.3%.

Based on the assumptions above, ATAC calculations were run at a scavenging efficiency Șs=0.43 (internal EGR rate of 57%). Figure 10 shows the results of the calculation that considered only the stable components (N2, O2, CO2 and H2O). In this case, N2 was substituted for the remaining 0.3% to make 100% in total.
As for assumption (3) above, the internal EGR rate was found with the following specific procedure:

Step 1: The corrected delivery ratio (L) is found from the intake air flow rate.

Step 2: Scavenging efficiency (\( \eta_s \)) is calculated on the basis of L, assuming perfect mixing scavenging[38].

\[
\eta_s = 1 - \exp(-L)
\]

Step 3: Because \( \eta_s \) represents the new air, the internal EGR rate is calculated on the assumption that the remainder is residual gas.

\[
\text{In-EGR} = (1 - \eta_s) \times 100\%
\]

The internal EGR rate was determined in this way and used in the calculations. In the actual gas exchange process, perfect mixing scavenging does not occur. In this study, though, the internal EGR rate was used for the purpose of evaluating the relative effect of internal EGR on autoignited combustion. For that reason, the internal EGR rate was defined on the assumption of perfect mixing scavenging (see the APPENDIX [b]).

Based on these hypotheses, the ATAC calculations were performed at a scavenging efficiency of \( \eta_s = 0.43 \) and under the assumption that residual gas, having the composition and temperature noted above, was perfectly mixed with the new intake air. In the ATAC simulation results in Fig. 10, neither the cylinder pressure waveform nor the HRR waveform shows any sign of a temperature rise attributable to a cool flame in region A' prior to the development of the hot flame. However, looking at the mole fraction histories of the chemical species, weak peaks are observed in the vicinity of 50 deg. BTDC (region D in Fig. 10). These peaks are believed to indicate the position where reactions corresponding to the passage of a cool flame occurred (i.e., reaction (1) in Fig. 3). Because their level is extremely low, however, the passage of a cool flame is not discernable in the HRR waveform.

Figure 11 presents the results of calculations that simulated the experimental HCCI characteristics in Fig. 8. In this case, heat release attributable to the passage of a cool flame can be observed. Concurrently, sharp peaks also appear in the mole fraction waveforms of the chemical species, and a notable increase is seen in HCHO (line B') among the OH, HCHO and HCO radicals. The reason for that can be understood as follows. In the HCCI combustion process, chain branching reactions (reaction (1) in Fig. 3) take place at low temperature, causing the fuel to decompose and resulting in the formation of a large quantity of HCHO as an intermediate product.

These results suggest that compression-induced ignition is strongly influenced by the cylinder temperature and pressure paths resulting from compression by piston motion and by their time-related changes.

Figure 12 presents the results of calculations that include unstable components, in addition to the stable ones, using the calculation conditions in Fig. 10. In this case, the ignition timing was advanced to an earlier crank angle than that for Fig. 10. It is seen in Fig. 12 that reactions corresponding to the passage of a cool flame (reaction (2) in Fig. 3) occur at 60 deg. BTDC (line D' in fig. 12), and evidence of a slight heat release can be observed at that point in the HRR waveform. This implies that the timing of the low-temperature oxidation reactions and the ignition timing are influenced depending on the composition of the residual gas. However, in both cases, the effect of the cool flame is extremely slight when compared with the HCCI conditions discussed below.

The results suggest that the characteristics of the low-temperature oxidation reactions change depending on the EGR composition, when a large quantity of residual gas is applied in the ATAC process. In any case, however, the low-temperature oxidation reactions are more moderate in comparison with HCCI combustion.
In addition, HCCI and ATAC engines appear to have uniform ignition and combustion without much cycle-to-cycle variation compared with SI engines, and both are regarded as having a bulk combustion process. In actuality, however, inhomogeneities occur due to uneven mixture concentrations and temperatures. Our calculations, on the other hand, assume that combustion occurs uniformly in dimensionless space and heat losses are ignored on the assumption of an adiabatic condition.

For those reasons, the calculations produce markedly larger values than the experimental data recorded with the test engine. In order to discuss the absolute pressures and heat release rates, it would be necessary to conduct 3-D analyses of the in-cylinder conditions. However, the calculations involved are difficult to run when using a detailed chemical kinetics model. The objective of our numerical analysis in this study was to examine qualitatively from a chemical kinetics standpoint differences in the combustion tendencies attributable to changes in temperature or internal EGR rate.

In other words, we wanted to ascertain the behavior of chemical species in low-temperature oxidation reactions and whether ignition timing was advanced or delayed in relation to changes in the EGR rate and temperature regions. Consequently, we did not make any numerical predictions of the ignition timing or combustion period.

The experimental and calculated maximum HRR values ($Q_{Hmax}$) differ by tenfold, although the area of the heat release zone differs only by about twofold. In other words, because the calculations assume dimensionless space, the mixture throughout the entire cylinder burns all at once in the computation, resulting in a needle-like spike in the HRR waveform.
INFLUENCE OF FUEL OCTANE NUMBER ON IGNITION TIMING IN ATAC AND HCCI COMBUSTION

The results presented in the preceding subsection revealed a significant difference between ATAC and HCCI combustion in that a cool flame was not manifested in the former process, whereas it was in the latter process. That difference was attributed to a difference in temperature at the onset of compression, among other factors. As the next step, the octane number of the fuel was varied and an investigation was made of the resultant effect on the autoignition tendency of the ATAC and HCCI combustion processes.

The influence of the octane number (RON) on the HRR waveforms is shown in Figs. 13 and 14 for ATAC and HCCI combustion, respectively. All of the waveforms are plotted in relation to a constant scavenging temperature (Tsc). However, when 80 RON fuel and gasoline were used, the engine could not be operated under HCCI combustion because of misfiring, so the corresponding waveforms are for a higher scavenging temperature where ignition was possible. It is presumed that a large quantity of internal EGR gas is present in the ATAC process. And the temperature at the onset of compression is influenced by the residual gas, and that effect increases when a larger quantity of residual gas is present. When the exhaust gas temperature differs, the effect of the residual gas temperature changes the temperature at the onset of compression. To avoid that, both Tex and Tsc were kept constant. Moreover, in the discussion in the preceding section, a compression ratio of 8.7:1 was also used as one of HCCI operating conditions. The reason for using the same compression ratio was to show the differences between the ATAC and HCCI combustion processes in terms of the state of the residual gas. However, four-stroke HCCI engines are generally operated at a higher compression ratio of around 15:1. Consequently, the following discussion concerns a compression ratio of 15:1 for both the experiments and calculations in order to reproduce the operating conditions of four-stroke HCCI engines more closely.

As seen in Fig. 13, varying the octane number of the test fuel did not change the ignition timing appreciably in the ATAC process (arrow E). In contrast, the results for HCCI combustion in Fig. 14 indicate that varying the fuel octane number reduced the amount of heat released by the passage of a cool flame (arrow F) and substantially retarded the ignition timing (arrow G) compared with that seen for ATAC. In other words, the octane number of the fuel had a marked effect on the ignition timing under HCCI operation, whereas its effect was small under ATAC operation. As the reason for that difference, we can consider the differences in the respective temperature histories followed by the ATAC and HCCI combustion processes. With HCCI combustion, increasing the fuel octane number retarded ignition, which presumably can be attributed to the low-temperature reaction rate stemming from the molecular structure, or in other words, the influence of a cool flame.

In ATAC, a cool flame was not manifested even when a fuel with a low octane number was used, which is why little correlation is seen between the octane number and the change in ignition timing.
Next, we will discuss the respective calculated results for ATAC and HCCI combustion. Figures 15 and 16 show the calculated results for ATAC and HCCI operating conditions, respectively. As is evident in both figures, the calculated results show nearly the same tendencies as the experimental data. It is clear that varying the fuel octane number had much less effect on the ignition timing in the ATAC process compared with HCCI combustion.

A further comparison is made here of the behavior of the chemical species during the low-temperature oxidation reactions under HCCI and ATAC operation, focusing specifically on the results for the PRF of 50 RON. Figure 17 shows the results calculated for ATAC and HCCI combustion with this test fuel. The notations i-OOQOOH and n-OOQOOH in the figure indicate OOQOOH produced from iso-octane and n-heptane, respectively.

As seen in the figure 17, evidence of the passage of a cool flame can be observed in the HRR waveform under HCCI operation but not in the HRR waveform for ATAC operation. Looking at the behavior of the chemical species, it is seen that n-heptane and iso-octane were partially consumed in the HCCI process when a cool flame occurred, with notably large consumption of n-heptane (arrow $\alpha$ in Fig. 17). In that connection, OOQOOH was formed in a reaction corresponding to the passage of a cool flame. In the case of ATAC, a reaction corresponding to the passage of a cool flame occurred near 60 deg. BTDC on account of the high temperature at the onset of compression (Tepc). However, the HRR waveform does not show any sign of a cool flame, nor is there any evidence of fuel consumption during reactions that would correspond to the passage of a cool flame. The amount of OOQOOH produced was also very slight compared with that for HCCI operation.

The peak mole fractions of OOQOOH during the cool flame reaction period are shown in Figs.18 and 19. The results for HCCI and ATAC are shown in Fig.18, while Fig.19 shows an enlarged representation of the results for ATAC. The peak mole fraction of OOQOOH is indicated as the maximum value of the species during the cool flame reactions (line $\beta$ in Fig.17) in the case of HCCI and as the value at 60 deg. BTDC (line $\gamma$ in Fig.17) in the case of ATAC because there was no maximum value during the cool flame period.

It is seen in the graph in Fig.18 that a large quantity of OOQOOH was produced from n-heptane during HCCI operation (approximately tenfold more than was produced from iso-octane). The reason for that is attributed to the molecular structure of iso-octane, which made it difficult for the reactions to accelerate at low temperature. A comparison of the OOQOOH values indicates that very little OOQOOH was produced in ATAC compared with HCCI combustion. The amount of OOQOOH produced from n-heptane in ATAC was only 1/8,000,000 of the quantity that formed under HCCI operation. That difference is attributed to the fact that the reactions were not likely to accelerate at low temperature in ATAC owing to the difference in the temperature regimes between the two processes.

The amount of OOQOOH produced from n-heptane in ATAC was around eightfold greater than the quantity that formed from iso-octane, as seen in Fig. 19. Because of the effect of the temperature regime, the amount of OOQOOH that formed under ATAC operation was incommensurably smaller in comparison with HCCI.
operation (on the order of one millionth to one ten-millionth less). For that reason, the reactions were presumably not accelerated at low temperatures even when n-heptane was used, with the result that there was less change in the ignition timing due to the different octane numbers (i.e., molecular structure of the fuel).

By way of summary, the relationship found experimentally between the fuel octane number and ignition timing in ATAC and HCCI combustion is shown in Fig. 20, and the corresponding calculated relationship is shown in Fig. 21. The plots in Fig. 20 represent the average values obtained in 25 cycles under each set of conditions. It is clear from both the experimental and calculated results that the octane number had less influence on the ignition timing under ATAC than it did under HCCI combustion. The fact that the ATAC process allows autoignition of fuels over a wide range of octane numbers also correlates with these results.
EFFECT OF SCAVENGING TEMPERATURE ON HCCI COMBUSTION

Figures 22 and 23 show the experimental and calculated results for the effect of varying the scavenging temperature on the HRR waveforms under HCCI combustion using n-heptane (0 RON) as the test fuel. In the HCCI process with a low octane number fuel, the passage of a cool flame occurred at an earlier crank angle and the maximum HRR of the cool flame decreased as the scavenging temperature increased (arrow H in Fig. 22). A difference was seen between the extent to which the passage of the cool flame was advanced and the development of the hot flame was advanced (interval τ in Fig. 22). The same tendencies are seen in the calculated results obtained by simulation in Fig. 23.

Figure 24 shows the time at which the cool flame peak occurred (tcool), the ignition timing (ton) and the ignition delay after the cool flame peak (τ). Compared with the decrease in tcool, the slope of the decline seen for ton is more gradual. The reason for this difference is thought to be attributable to the effect of heat release by the cool flame. As the scavenging temperature increases, the temperature at the onset of compression rises, so the temperature for the passage of a cool flame is reached at an earlier crank angle. Although this causes a cool flame to occur earlier, it also reduces the amount of heat produced by the cool flame. That presumably accounts for the longer ignition delay (τ) after the cool flame peak.

Moreover, the calculated results disagreed with experimental results. The calculations assume the reactions occur uniformly in dimensionless space, and heat losses are ignored under the assumption of an adiabatic condition. In addition, the operating conditions of the test engine include various aspects that are not considered in the calculations. For these and various other reasons, the ignition timing and combustion period cannot be predicted numerically. In order to predict them, it is necessary to consider all the parameters that affect ignition and combustion, which would require 3-D simulations.
EFFECT OF INTERNAL EGR ON HCCI COMBUSTION

Application of internal EGR by means of negative valve overlap (NVO) is one technique that can be used to expand the operation region and control the ignition timing in four-stroke HCCI engines. This can be understood as the application of high-temperature residual gas, which is a characteristic of two-stroke HCCI (ATAC) operation, to the HCCI combustion process in a four-stroke engine. Experiments were conducted to investigate how the relationship between the combustion characteristics of the two processes would change in this case. The resultant combustion characteristics that were obtained when internal EGR was applied to HCCI combustion (i.e., HCCI + internal EGR) at WOT and a compression ratio of 15:1 were investigated and a comparison was made with the results obtained for ATAC.

Figures 25 and 26 present the experimental and calculated results for the influence of the internal EGR rate (In-EGR) on the HRR waveforms. Figure 27 shows both the experimental and calculated results for the corresponding effect on ignition characteristics. In the experiments, an EGR valve installed in the exhaust gas outlet was throttled to lower the corrected delivery ratio \( L \) and increase internal EGR. Assuming a state of perfect mixing \[38\], the internal EGR rate was defined as

\[
\text{In-EGR} = (1 - \eta_s) \times 100% \\
\eta_s = 1 - \exp(-L)
\]

The quantity of fuel supplied, \( Q_{in} \) (mg/cycle), was kept constant in the experiments. The calculations were performed by running simulations on the basis of the same three assumptions made earlier for ATAC. As indicated in Fig. 25, throttling the EGR valve to change the internal EGR rate from 35% to 42% under HCCI combustion at WOT using n-heptane (0 RON) as the test fuel with a corrected delivery ratio of \( L = 1.1 \) advanced the passage of a cool flame and also the development of the hot flame (arrows J and K in Fig. 25). When the internal EGR rate was then increased to 46%, the passage of the cool flame was further advanced, but the hot flame occurred at a later crank angle compared with In-EGR of 42%. Increasing In-EGR further to 54% extinguished the heat release of the cool flame and further retarded the ignition timing substantially. In short, internal EGR initially advanced the ignition timing, but that trend was reversed before long and the ignition timing was delayed. The same tendencies are seen in the calculated results obtained by simulation in Fig. 26. It is presumed that this behavior resulted from the particular effects of internal EGR. Internal EGR is thought to have the following main effects on the ignition timing.

1. Heat contained in the internal EGR gas has the effect of quickening the ignition timing.
2. By lowering the specific heat ratio, it has the effect of retarding the ignition timing.
3. By reducing the cool flame, it has the effect of retarding ignition.

The combined effect of these three factors is thought to largely determine the ignition timing. In other words, the ignition timing is advanced if the effect of (1) above is large, but it is retarded if the reduction of the specific heat ratio produces a large effect.

\( n = 15:1 \)
\( N = 1000 \text{ rpm} \)

![Fig. 25 Influence of internal EGR on combustion (Experimental).](image1)

![Fig. 26 Influence of internal EGR on combustion (Calculated).](image2)
With an internal EGR rate of 54% or higher, it is seen in Fig. 27-(a) that the combustion interval ($\phi_{\text{comb}}$) became longer. One presumed reason for that increase is that the inactive nature of the internal EGR gas suppressed the combustion reaction rate of autoignition. Another reason that can be considered, though, is that $\phi_{\text{comb}}$ was also influenced by the ignition timing inasmuch as the ignition timing was substantially retarded as well. Figure 27-(b) plots the calculated results for the time of the cool flame peak ($\phi_{\text{cool}}$), ignition timing ($\phi_{\text{on}}$) and the ignition delay after the cool flame peak ($\phi$). Similar to the experimental data, the calculated results show that the time of the cool flame peak advances as the internal EGR rate is increased; the ignition timing advances until an internal EGR rate of 45%, but above 50% it reverses direction and is retarded.

Therefore, a comparison was made of the cylinder pressure, HRR and pressure rise rate ($\frac{dP}{dT}$) waveforms under conditions where the ignition timing was virtually identical, though the internal EGR rate differed. Figure 28 shows the waveforms obtained for internal EGR rates of 33% and 46% when 30 RON fuel was supplied at a constant quantity of 6.4 mg/cycle. As is evident from this figure, changing the internal EGR rate did not cause combustion to become sluggish. In other words, if sluggish combustion results from internal EGR, it can be attributed to retarded ignition timing. The waveforms obtained, however, when gasoline was supplied at a constant quantity of 9.6 mg/cycle are shown in Fig. 29. It is clear from this figure that increasing the internal EGR rate had the effect of moderating the waveform in which knock-like pressure oscillations occurred. The reason for this difference is thought to lie in the different composition of the internal EGR gas owing to the supply of a larger quantity of gasoline to prevent misfire. Because the internal EGR gas contained the combustion gas from a mixture having a higher equivalence ratio, it is presumed that there were larger quantities of inactive and low specific heat ratio constituents such as CO2 and H2O. However, when such a large volume of internal EGR was applied to avoid knocking, not enough new air could be drawn into the cylinder, and the load could not be increased as a result. Supercharging or some other means will have to be used to achieve engine operation at higher loads [39].
The results in the figure indicate that the ignition timing differed substantially in relation to the different octave numbers of the fuel under a condition of a small internal EGR rate. The difference in ignition timing between the 0 RON fuel and 60 RON was around 18 CA deg. (region X) in Fig. 30. However, as the internal EGR rate was increased, the ignition timings of the test fuels converged. At an internal EGR rate of around 55%, the difference between the 0 RON fuel and the 60 RON fuel closed to approximately 8 CA deg. (region Y). Although data were not obtained at higher internal EGR rates for the high-octane number fuel because of misfiring, the results in the figure show a tendency for the ignition timing to converge (arrow Z) as a result of increasing the internal EGR rate. This suggests that increasing the internal EGR rate under HCCI operation at WOT and a compression ratio of 15:1 resulted in a state of ATAC-like combustion. The combustion state obtained under four-stroke HCCI operation when internal EGR was applied by means of NVO presumably resembled that ATAC-like combustion.

The waveforms for HCCI combustion with internal EGR in Fig. 25 are superimposed with those for ATAC in Fig. 31. Looking at the HRR waveforms, HCCI combustion with an internal EGR rate of 35% (WOT with the internal EGR valve fully open), shows a peak HRR of around 60 J/deg. At higher internal EGR rates, however, the peak HRR values decline and are on the same order of the HRR waveforms for ATAC at internal EGR rates of 60% and 65%. These heat release results also imply that the application of internal EGR to HCCI operation resulted in a state of ATAC-like combustion.

The results in the figure show a tendency for the ignition timing to converge (arrow Z) as a result of increasing the internal EGR rate. This suggests that increasing the internal EGR rate under HCCI operation at WOT and a compression ratio of 15:1 resulted in a state of ATAC-like combustion. The combustion state obtained under four-stroke HCCI operation when internal EGR was applied by means of NVO presumably resembled that ATAC-like combustion.
Based on the calculated results in Fig. 26, an investigation was made of how the combustion reactions changed when internal EGR was increased. The results obtained are shown in Fig. 32. It is seen in the graphs in the figure that increasing the internal EGR rate advanced the passage of a cool flame to an earlier crank angle; the magnitude of the cool flame decreased and it was eventually extinguished. Looking at the behavior of the chemical species, it is observed that the quantities of species produced by the cool flame reactions decreased as the internal EGR rate was increased and the waveforms come to resemble the calculated results for ATAC in Fig. 10.

Kalghatgi and Angstrom [19] showed that combustion phasing was little affected by fuel autoignition quality under the application of heavy EGR, though it was affected under light EGR. Similarly, Kalghatgi and Head [40] reported that combustion phasing was not influenced by fuel autoignition quality when the intake charge was heated and in the case of exceptionally high intake pressures. The differences seen in combustion characteristics between the ATAC and HCCI processes in this study coincide with the findings reported by the researchers mentioned here.

POTENTIAL FOR EXPANDING THE HCCI OPERATION REGION

In the ATAC process, an engine may misfire when the throttle valve is opened because ignition is apt to occur under a light load in a relatively high operating speed range. With HCCI combustion, on the other hand, an engine may misfire when the speed is raised because ignition tends to occur at a low engine speed with a large throttle valve opening. The operation region characteristics of these two combustion processes are contradictory with respect to the engine speed. The primary factor driving ignition in each combustion process can be considered as follows:

ATAC: elevation of the temperature at the onset of compression due to internal EGR
HCCI: elevation of the temperature due to heat release from a cool flame and high compression pressure

An investigation was made of the potential for expanding the stable engine operation region by combining these two combustion processes. Figure 33 shows the region of an ignitable mixture under the conditions of $\varepsilon=15:1$, n-heptane, WOT and a fully open EGR valve, and Fig. 34 shows the operable region of the test engine under the conditions of $\varepsilon=15:1$, gasoline, WOT and a fully open EGR valve. The vertical axis of each figure shows the quantity of fuel supplied in relation to the engine speed along the horizontal axis.

The region above the x-plots is where the test engine did not operate stably because of knocking or backfiring. The region below the closed triangle plots is where the test engine did not operate stably because of misfiring. The region in between is where stable ignition was possible.

Using n-heptane (0 RON) and a compression ratio of $\varepsilon=15:1$, actual power output was not obtained because the ignition timing was too early. In the experiments, the set engine speed was maintained by motoring the engine even under a condition of negative torque, so the engine continued to run, but no torque was obtained. Accordingly, the term “ignitable region” is used in the case of the 0 RON fuel instead of using “operable region.” With the 0 RON fuel, ignition was possible to an engine speed of $N = 3000$ rpm even with the EGR valve fully open. In contrast, when gasoline was used, the engine could not be operated in the vicinity of $N = 1500$ rpm due to misfiring. It is thought that the higher octane number lengthened the ignition delay, resulting in insufficient time for ignition.

An attempt was therefore made to expand the engine operation region by applying internal EGR as in the case of ATAC. Figure 35 shows the region of an ignitable mixture under the conditions of $\varepsilon=15:1$, n-heptane, WOT and the application of internal EGR by setting the EGR valve opening at 1/16. Figure 36 shows the operable region of the test engine under the conditions of $\varepsilon=15:1$, gasoline, WOT and the application of internal EGR with the EGR valve 1/16 open. The ignitable and operable regions without the application of internal EGR (EGR valve fully open) are also indicated in each figure respectively by the hatched area.

When internal EGR was applied, the ignitable and operable regions were expanded on the lean mixture side for both n-heptane (0 RON) and gasoline (arrows in Figs. 35 and 36). It is thought that the elevated temperature at the onset of compression enabled the process to proceed to autoignition without being dependent on heat release from low-temperature oxidation reactions. With gasoline as the test fuel, the ignitable and operable regions also expanded on the high-speed side in relation to the engine speed, enabling the test engine to operate stably in the vicinity of $N = 3000$ rpm. Measurements were not made above 3000 rpm because of the allowable operating speed of the electric regenerative dynamometer used in the experiments.

Representative measured waveforms obtained without internal EGR at $N = 1500$ rpm with n-heptane (0 RON) are shown in Fig. 37, and typical examples of those measured with n-heptane at $N = 1500$ rpm with internal EGR are shown in Fig. 38. Each figure shows the measured waveforms for knocking, HCCI combustion and semi-HCCI combustion (with spark assist) for different quantities of supplied fuel ($Q_{in}$). Without internal EGR, a small amount of heat release from a cool flame can be detected when n-heptane (0 RON) was used (region K in Fig. 37). In contrast, when internal EGR was applied, no sign of the passage of a cool flame can be detected in the HRR waveforms. The reason for that can be understood as follows. The application of internal EGR raises the temperature at the onset of compression, with the result that the combustion reactions pass through the temperature regime for the passage of a cool flame at an early stage and a combustion state close to ATAC exists. It is thought that this ATAC-like combustion state offers the possibility for expanding the HCCI operation region in a four-stroke engine.
CONCLUSIONS

In this study, a two-stroke engine was used to compare the characteristics of Active Thermo-Atmosphere Combustion (ATAC) under partial load and Homogeneous Charge Compression Ignition (HCCI) combustion under a WOT condition that simulated HCCI combustion in a four-stroke engine. The results obtained have made the following points clear.

Comparison Between ATAC and HCCI Combustion Processes

(1) The main differences between ATAC and HCCI combustion lie in their different low-temperature oxidation reaction characteristics, including the passage of a cool flame. The different characteristics are ascribable to differences in the state of the high-temperature residual gas, i.e., its temperature, quantity and constituents.

(2) Low-temperature oxidation reactions (i.e., cool flame) are less likely to occur in ATAC compared with HCCI combustion. In other words, autoignition in the ATAC process is governed by the higher temperature at the onset of compression due to the residual gas and by the higher temperature produced by compression resulting from piston motion. In contrast, ignition in the HCCI process is governed by the higher temperature due to compression resulting from piston motion and by the heat release from a cool flame, depending on the fuel used.

(3) Low-temperature oxidation reactions (i.e., cool flame) are less likely to occur in ATAC even when a fuel with a low octane number is used. Accordingly, varying the octane number of the fuel does not change the ignition timing appreciably. That makes it difficult to control the ignition timing arbitrarily on the basis of changing the octane number. On the other hand, combustion of the fuel is possible over a wide range of octane numbers.

(4) The HCCI combustion process is more conducive to low-temperature oxidation reactions (i.e., cool flame) compared with ATAC, and the quantity of heat released by a cool flame increases as the octane number of the fuel is reduced. As a result, the ignition timing changes. This makes it possible to vary the ignition timing by changing the octane number of the fuel. On the other hand, because the ignition timing varies depending on the octane number, the range of usable octane numbers is narrower in relation to the compression ratio on account of misfiring or premature ignition.

(5) In HCCI combustion with n-heptane (0 RON), faint light emission and degeneracy behavior were observed for HCHO at the time of heat release from a cool flame.

Influence of scavenging temperature on HCCI process

(6) Both the experimental and calculated results for HCCI combustion indicated that a higher scavenging
temperature advanced the time for the passage of a cool flame and reduced the magnitude of the cool flame. However, the interval \( \tau \) from the cool flame peak to the development of the hot flame was lengthened.

**Influence of internal EGR on HCCI process**

(7) Under HCCI combustion, both the experimental and calculated results showed a lengthening of the interval \( \tau \) from the cool flame peak to the occurrence of the hot flame when the internal EGR rate was increased. Additionally, as the internal EGR rate was increased, the ignition timing was advanced initially and then tended to be delayed.

(8) Both the experimental and calculated results for HCCI combustion showed that the passage of a cool flame occurred at an earlier crank angle as the internal EGR rate was increased and the magnitude of the cool flame also decreased.

(9) The experimental results for HCCI combustion indicated that the combustion interval \( \theta_{comb} \) was lengthened at internal EGR rates above 54%.

(10) Under HCCI with internal EGR condition, the ignition timing differed substantially in relation to the different octane numbers of the fuel under a condition of a small internal EGR rate. However, as the internal EGR rate was increased, the ignition timings of the test fuels converged.

(11) Under HCCI combustion, the application of internal EGR expanded the stable operation region of the test engine on the lean mixture side and the high speed side, resulting in a combustion state resembling ATAC.

(12) The use of negative valve overlap to apply internal EGR in the HCCI process seems to result in combustion characteristics that approach those of ATAC as described above. Therefore, when using internal EGR or a multifuel blend in an effort to expand the operation region of HCCI engines, the relationship between the octane number and ignition timing may vary greatly depending on the engine operating conditions.

**REFERENCE**


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DEFINITIONS, ACRONYMS, ABBREVIATIONS

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Units</th>
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<tbody>
<tr>
<td>$\varepsilon$</td>
<td>Effective Compression Ratio</td>
<td>[-]</td>
</tr>
<tr>
<td>$\phi$</td>
<td>Intake Equivalence Ratio</td>
<td>[-]</td>
</tr>
<tr>
<td>$\eta_s$</td>
<td>Scavenging Efficiency</td>
<td>[-]</td>
</tr>
<tr>
<td>$\kappa$</td>
<td>Specific Heat Ratio (c_p/c_v)</td>
<td>[-]</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Crank Angle</td>
<td>[deg.]</td>
</tr>
<tr>
<td>$\theta_{cool}$</td>
<td>Cool Flame Peak Timing</td>
<td>[deg.]</td>
</tr>
<tr>
<td>$\theta_{on}$</td>
<td>Ignition Timing</td>
<td>[deg.]</td>
</tr>
<tr>
<td>$\theta_{peak}$</td>
<td>Hot Flame Peak Timing</td>
<td>[deg.]</td>
</tr>
<tr>
<td>$\theta_{off}$</td>
<td>End of Combustion</td>
<td>[deg.]</td>
</tr>
<tr>
<td>$\theta_{comb}$</td>
<td>Combustion (Hot Flame) Period</td>
<td>[deg.]</td>
</tr>
<tr>
<td>$\rho_a$</td>
<td>Ambient Density</td>
<td>[kg/m$^3$]</td>
</tr>
<tr>
<td>$\tau$</td>
<td>Ignition Delay After the Cool Flame Peak</td>
<td>[deg.]</td>
</tr>
<tr>
<td>$c_p$</td>
<td>Specific Heat at Constant Pressure</td>
<td>[J/kg K]</td>
</tr>
<tr>
<td>$c_v$</td>
<td>Specific Heat at Constant Volume</td>
<td>[J/kg K]</td>
</tr>
<tr>
<td>HRR</td>
<td>Heat Release Rate</td>
<td>[J/deg.]</td>
</tr>
<tr>
<td>L</td>
<td>Corrected Delivery Ratio</td>
<td>[-]</td>
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</tbody>
</table>

\[ L = \frac{M_{as}}{M_{ref}} = \frac{M_{as}}{V_{epc} \times \rho_a} \]

Mas Mass of Delivered Air [kg]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Definition</th>
<th>Units</th>
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</thead>
<tbody>
<tr>
<td>$\text{Mepc}$</td>
<td>In-cylinder Mass at the Exhaust Port Close</td>
<td>[kg]</td>
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<tr>
<td>$\text{Mref}$</td>
<td>Reference Mass</td>
<td>[kg]</td>
</tr>
<tr>
<td>$n$</td>
<td>Polytropic Index</td>
<td>[-]</td>
</tr>
<tr>
<td>N</td>
<td>Engine Speed</td>
<td>[rpm]</td>
</tr>
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</table>

OOQOOH Hydroperoxy Alkylperoxy Radicals

P In-cylinder Pressure [MPa]

Pepo In-cylinder Pressure at the Exhaust Port Open [MPa]

Pmax Maximum In-cylinder Pressure [MPa]

Qin Quantity of Fuel Supply [mg/cycle]

OOOH Hydroperoxy Alkyl Radicals

R Alkyl Radicals

Sp Instantaneous Piston Speed [m/sec]

$T_{\text{EGR}}$ EGR Gas Temperature [K]

$T_{\text{epc}}$ In-cylinder Gas Temperature at the Exhaust Port Close [K] (In-cylinder temperature at the onset of the compression)

\[ T_{\text{epc}} = \frac{M_{sc} \cdot T_{sc} \cdot C_{p_s} + M_{\text{EGR}} \cdot T_{EGR} \cdot C_{p_{\text{EGR}}}}{M_{\text{epc}} \cdot C_{p_{\text{epc}}}} \]

\[ = \frac{M_{\text{epc}} \cdot \eta_s \cdot T_{sc} \cdot C_{p_s}}{M_{\text{epc}} \cdot C_{p_{\text{epc}}}} \cdot \frac{(1 - \eta_s) \cdot T_{\text{EGR}} \cdot C_{p_{\text{EGR}}}}{M_{\text{epc}} \cdot C_{p_{\text{epc}}}} \]

\[ \approx T_{sc} \eta_s + T_{\text{EGR}} (1 - \eta_s) \]

$T_{\text{epo}}$ In-cylinder Gas Temperature at the Exhaust Port Open [K] (Blowdown Gas Temperature)

Tex Exhaust Gas Temperature [K]

Tsc Scavenging Temperature [K]

Tsp Spark Plug Washer Temperature [K]

Tm Mean Gas Temperature [K]

Tmax Maximum In-cylinder Gas Temperature [K]

Vepc Cylinder Volume at the Exhaust Port Closing [m$^3$] (Effective Displacement Volume)

AI Auto-ignition

AR Activated Radical
APPENDIX

[a] Calculation of the EGR Gas Temperature ($T_{EGR}$)

The EGR gas temperature was estimated as follows:

$$T_{EGR} \approx \frac{T_{es} + T_{e po}}{2}$$

$$T_{e po} \approx T_{max} \left( \frac{P_{e po}}{P_{max}} \right)^{\frac{k-1}{k}}$$

[b] Scavenging efficiency in a two-stroke engine

Typical scavenging models for two-stroke engines include the “perfect displacement model” and the “perfect mixing model.” A comparison of the scavenging efficiency of each model is given in Fig. A-1. With the Schnurle scavenging method used in this study, the scavenging efficiency is higher than that assumed for perfect mixing scavenging and lower than that assumed for perfect displacement scavenging. Because the internal EGR rate used in this study assumes perfect mixing scavenging, it is likely that the internal EGR was estimated slightly larger than the actual value. However, the internal EGR rate was used here for the purpose of making a qualitative assessment of combustion characteristics due to the relative change in the quantity of internal EGR applied. For that reason, perfect mixing scavenging was assumed.

![Fig. A-1 Scavenging efficiency in a two-stroke engine.](image-url)