

Dual Phase High Temperature Heat Release Combustion

Gen Shibata

Central Technical Research Laboratory
Nippon Oil Corporation

Tomonori Urushihara

Nissan Research Center
Nissan Motor Co., Ltd.

Copyright © 2008 SAE International

ABSTRACT

To allow the HCCI vehicles to enter the market in the future, it is important to investigate the combustion deviations and operational range differences between the same research octane number fuels. In this paper, eighteen kinds of two hydrocarbon blended fuels, which were composed of n-heptane and another hydrocarbon, such as iso-octane, diisobutylene, 4-methyl-1-pentene, toluene or cyclopentane, were evaluated. Those fuels were blended to have the same research octane numbers of 75, 80, 85 and 90 by changing the blending volume ratio of n-heptane and counterpart hydrocarbon. Intake air was supercharged to 155 kPa abs and its temperature was kept at 58 °C. The HCCI engine was operated at 1000 rpm. Neither hot EGR, nor any other combustion stratification system was utilized in order to investigate the purely hydrocarbon effects on HCCI combustion. In-cylinder pressure data were taken at 7 different maximum pressure rise rate conditions, which were 900, 800, 700, 600, 500, 400 and 300 kPa/deg of 400 cycles averaged in-cylinder pressure traces, by changing the fuel injection quantity. The test results showed that the engine operational range of n-heptane and iso-octane blended fuels (**PRF**) were the same as those of n-heptane and diisobutylene blended fuels (**NDB**), and n-heptane and 4-methyl-1-pentene blended fuels (**NMP**). The operational ranges of n-heptane and toluene blended fuels (**NTL**) were at high IMEP conditions, but those of n-heptane and cyclopentane blended fuels (**NCP**) were only at low IMEP conditions, compared with the cases of PRF series fuels, NDB series fuels and NMP series fuels. To investigate those operational range differences, heat release data were analyzed at the same HTHR CA50 (the crank angle of 50 % burn of high temperature heat release) and IMEP conditions. As NTL fuels show the largest low temperature heat release (LTHR), high temperature heat release (HTHR) starts earlier than the other fuels. Furthermore, the HTHR combustion period of the NTL fuels was longer than the other fuels since the NTL fuels displayed dual phase high temperature heat release (DP-HTHR) combustion. The first part of the HTHR is caused by n-heptane, and second is caused by benzyl radicals and aromatics produced from

toluene. Therefore the maximum pressure rise rate can be reduced, and NTL fuel is effective in achieving low combustion noise and high IMEP engine operation.

INTRODUCTION

Though the HCCI engine has the potential for low NO_x emission, combined with diesel-like engine efficiency, the operational engine speed-torque ranges change depending on fuel composition. Octane and cetane numbers are not a sufficient fuel index for HCCI engine control. This is one of the technical barriers that block HCCI engine development in car companies. Many studies have been performed to investigate the fuel-HCCI engine interactions from simulations and engine tests [1-20].

Kalghatgi experimentally developed an "octane index", as shown in equation (1) [21-25], and showed that the combustion characteristics of fuels changed depending on the engines and HCCI operational conditions.

$$OI = (1-K) RON + K MON \quad (1)$$

OI: Octane index
 K: Factor, varies by engine and operating conditions
 RON: Research octane number
 MON: Motor octane number

We have also investigated the combustion characteristics of hydrocarbons with 23 kinds of surrogate fuels composed from 11 pure hydrocarbons, from the fuel standpoint. HCCI combustion typically occurs in two stages [26]. A low temperature heat release (**LTHR**) occurs first, followed by a high temperature heat release (**HTHR**). These combustion phases do not occur independently. For instance, **HTHR CA50** (the crank angle at 50 % burn of HTHR) can be described as a function of LTHR CA50 and LTHR heating value [27]. The oxidation and chain-branching reactions, mainly caused by n-paraffins and iso-paraffins, occur at 750-850 K. H₂O₂ is produced from two sets of HO₂ and accumulates in the range of 850-900 K [28-32]. This group of reactions can be observed as LTHR by heat release

analysis of HCCI engines. H_2O_2 decomposition into OH radicals occurs above 900 K and this is the start of HTHR [33]. HCCI engine operation is affected by the LTHR characteristics. The n-paraffins cause larger LTHR heating values and earlier LTHR CA50 timing than other fuel chemical species, while some naphthenes and olefins have a mechanism that reduces the LTHR of their mixture counterparts. This so-called **LTHR inhibitor effect** can be explained from the standpoint of hydrocarbon breakdown reactions at the first stage of the LTHR, which are strongly dependent on hydrocarbon molecular structure [27].

Researching the auto-ignition of air-fuel mixtures has been performed in our previous works [8, 27, 33, 34]. Equation (2) is an absolute HCCI auto-ignition fuel index that we have developed [34]. This index is calculated from the LTHR heat release analysis, LTHR inhibitor effect and HTHR characteristics under no LTHR conditions. Each coefficient of parameter is characterized depending on the in-cylinder temperature range at 15bar during the compression stroke, as shown in Table 1. The difference between equations (1) and (2) is a relative and absolute HCCI auto-ignition fuel index, respectively. But basically both equations have the same meaning, as a result [34].

HCCI Index (abs) = rRON+a'(n-P)+b'(i-P)+c'(O)+d'(A)+e'(OX)+Y'

(2)

(RON: Research octane number, n-P: n-Paraffins vol%, i-P: iso-Paraffins vol%, O: Olefins vol%, A: Aromatics vol%, OX: Oxygenates vol%)

Table 1 Coefficients of parameters against temperature at 15bar (1.5MPa) in-cylinder pressure

Temp. @15bar (1.5MPa)		-670K	670-700K	700-730K	730-790K	790-820K	820K -
RON	r	0.848	0.858	0.831	0.523	0.207	0.161
n-Paraffin	a'	-0.203	-0.256	-0.320	-0.244	-0.103	-0.050
iso-Paraffin	b'	-0.198	-0.267	-0.336	-0.187	-0.012	0.014
Olefin	c'	-0.134	-0.193	-0.259	-0.176	-0.064	-0.043
Aromatic	d'	0.006	-0.087	-0.186	-0.109	-0.009	0.008
ETBE	e'	-0.032	-0.072	-0.132	-0.088	-0.003	0.018
Et-OH	e'	0.172	0.089	-0.036	-0.054	-0.026	-0.020
MTBE	e'	0.025	0.023	0.004	-0.004	0.018	0.031
y-intercept	Y'	-60.028	-56.041	-48.828	-32.109	-18.947	-19.276

For ideal high performance HCCI engine development, both the optimization of the engine and fuel developments are required. Since gasoline and diesel fuels on the market are not appropriate for full range HCCI operation, the development of combustion control has been required. For gasoline HCCI, HCCI operation is restricted to low engine speed and torque operation surrounded by knock and misfire limits [35]. As gasoline is well vaporized and mixed with air, the mixture auto ignites at the same time. This leads to heavy HCCI engine knocking. To avoid this rapid in-cylinder combustion, the stratification techniques of A/F, temperature and EGR in-cylinder have been reported [36, 37]. The aim of these techniques is lengthen the combustion period, and avoid of rapid combustion, to operate the HCCI engine at high load conditions.

From the fuel stand point, the effects of fuels on HTHR have not been sufficiently researched. It is known that the hydrocarbon fuel composition affects the LTHR characteristics, and thus changes the HTHR combustion timing. But the characteristics of HTHR itself have not

been thoroughly discussed. In our previous paper [34], we reported that there exists a HTHR case without LTHR, as shown in Figure 1. This figure shows that the individual auto-ignition characteristics are different for each hydrocarbon.

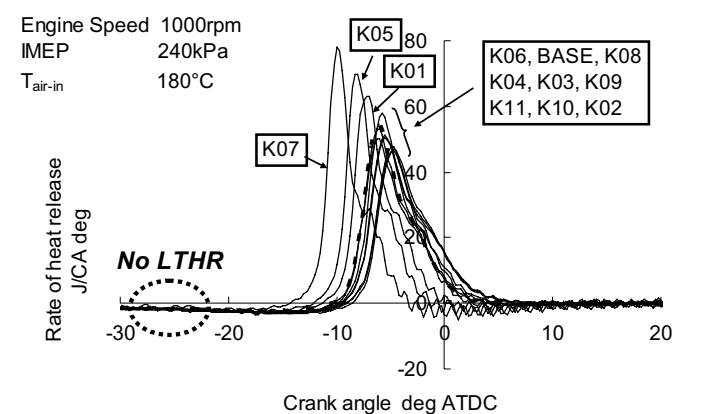


Figure 1 Difference of HTHRs without LTHR case [34]

Equation (2) shows the effects of fuel components on HTHR CA20 (or HTHR CA50), but it does not show the HTHR combustion period and phasing. The fuels, which show the same HTHR CA50 but different combustion period and phasing, can be considerable. The HTHR combustion period and phasing must also be taken into account for HCCI engine operation. To investigate this subject, several kinds of fuels with the same research octane number were prepared. All fuels were composed of two hydrocarbons; one was n-heptane and the other hydrocarbon was iso-octane, diisobutylene, 4-methyl-1-pentene, toluene or cyclopentane. The engine was operated at 1000 rpm and intake air was supercharged to 155 kPa abs pressure. Heat release data were taken at 7 different maximum pressure rise rate conditions. The operation range of each fuel was first investigated. Then HTHR characteristics were compared at the same HTHR CA50 and IMEP conditions.

The effects of hydrocarbon composition on HTHR combustion period and phasing are the main issues discussed in this paper.

EXPERIMENTAL DESCRIPTION

ENGINE BENCH SETUP

The engine was operated in an environmentally controlled chamber where the temperature, relative humidity and atmospheric pressure were maintained at 20 °C, 60 % and 101 kPa abs, respectively, to ensure constant intake air conditions. A schematic of the research engine bench is shown in Figure 2.

The engine employed in the experiment was a research, supercharged, 4-cylinder engine with high compression pistons (compression ratio=15:1), 4 valves per cylinder, and centrally located spark plugs. The intake manifold was

equipped with separate electric heaters for each cylinder (200 V, total 6 kW) allowing independent control of intake air temperature up to 200 °C at 1500 rpm. The engine was equipped with a pressure transducer for each cylinder. Pressure data was transmitted to the PC at 400 cycles of crank angle resolved pressure data for each test condition. Each injector fuel quantity was independently controlled to yield the same IMEP for each cylinder.

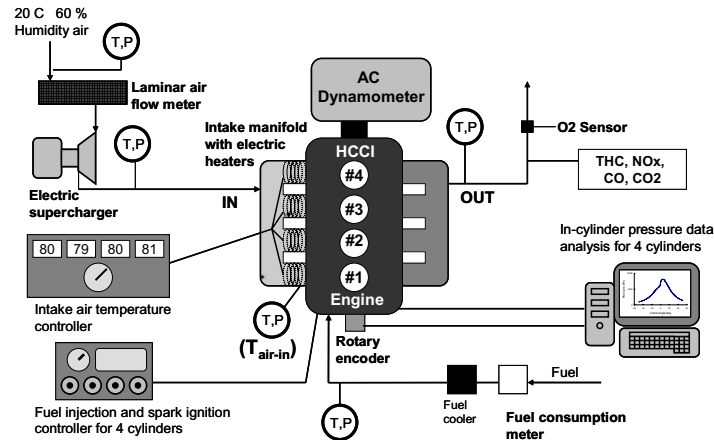


Figure 2 Experimental engine set-up schematic

The specifications of the HCCI engine are given in Table 2. For all test conditions in this paper, the water jacket temperature and engine oil temperature were maintained at 80 °C.

Table 2 HCCI engine specifications

Engine type	4 cylinder MPI
Compression ratio	15:1
Bore	86mm
Stroke	86mm
Displacement	1998cc
Exhaust valve open	53°CA BBDC
Exhaust valve close	7°CA ATDC
Intake valve open	1°CA ATDC
Intake valve close	19°CA ABDC

FUELS

The test fuels are shown in Table 3. All the test fuels were blended from two hydrocarbons. One hydrocarbon was n-heptane and the other hydrocarbon varied between the fuel types. The counterpart hydrocarbons of PRF series fuels, NDB series fuels, NMP series fuels, NTL series fuels and NCP series fuels are iso-octane, diisobutylene, 4-methyl-1-pentene, toluene and cyclopentane respectively. The LTHR characteristics of those hydrocarbons have been well researched. The molecular structures of those hydrocarbons are shown in Figure 3. Iso-octane is an iso-paraffin, and a very small LTHR can be observed. Diisobutylene is a hydrocarbon in the olefin family. The molecular structures of iso-octane and diisobutylene are quite similar, but diisobutylene has a double bond in its molecule, as shown in Figure 3. Therefore the existence of

the double bond can be examined from the combustion data of the PRF series fuels and NDB series fuels. 4-Methyl-1-pentene is also an olefin hydrocarbon, but the LTHR inhibitor effect is weaker than diisobutylene.

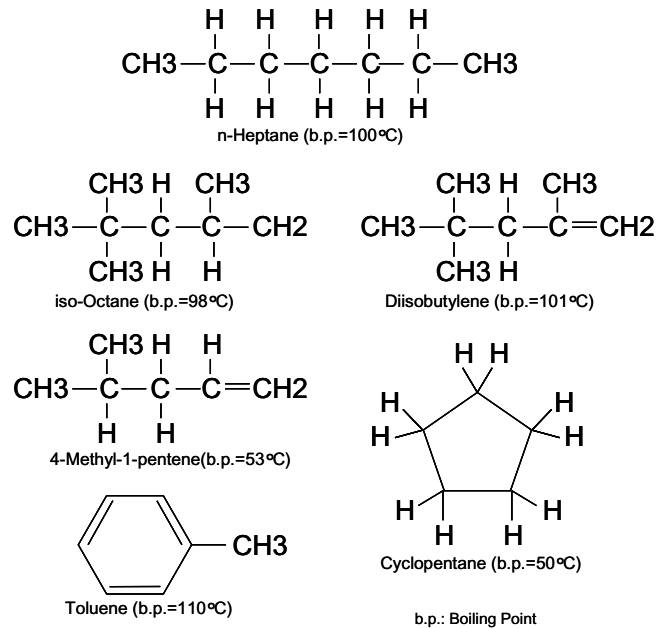


Figure 3 Structures of the hydrocarbons used in this test

Toluene is representative of the aromatic family. Toluene produces a small reaction during the LTHR period and changes to benzyl radicals and aromatics, as shown in Figure 4 [38]. Those benzyl radicals and aromatics are quite stable and do not react until the hot flame combustion starts. Cyclopentane is a naphthene. Its ring breaks during the LTHR period and changes to olefins [33]. Each hydrocarbon was blended with n-heptane to be 75, 80, 85 and 90 research octane numbers by changing the blending ratio of the two hydrocarbons. For example, NDB80 fuel was composed from n-heptane and diisobutylene, and its research octane number was 80. For NCP series fuels, the engine could not be run with NCP85 and NCP90 fuels. So those data were deleted from Table 3. For this engine, engine operational range of NTL90 fuel was small. So a NTL70 fuel was newly blended and tested in stead of NTL90 fuel, as listed in Table 3.

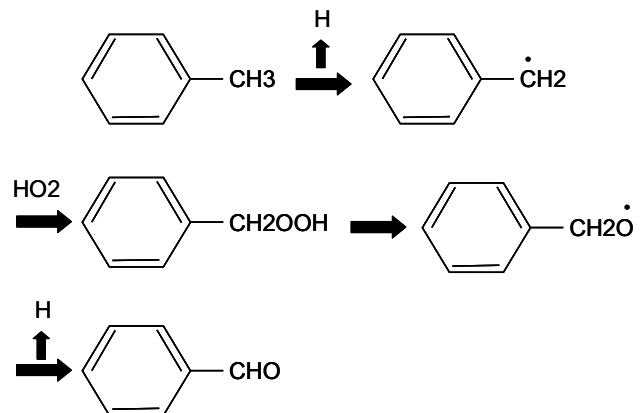


Figure 4 Toluene reaction during the LTHR period [38]

Table 3 Description of test fuel properties

		PRF75	PRF80	PRF85	PRF90	NDB75	NDB80	NDB85	NDB90	NMP75	NMP80	NMP85	NMP90	NTL70	NTL75	NTL80	NTL85	NCP75	NCP80
Density 15C	g/cm3	0.694	0.694	0.694	0.695	0.704	0.706	0.707	0.709	0.675	0.674	0.673	0.671	0.792	0.799	0.807	0.815	0.721	0.724
RON		75.0	80.0	85.0	90.0	75.0	80.0	85.0	89.3	75.3	80.0	85.0	89.0	70.0	74.5	80.0	84.8	74.5	79.8
C%	wt%	84.06	84.07	84.08	84.09	84.77	84.84	84.92	84.99	85.09	85.19	85.28	85.37	88.38	88.69	89.00	89.31	84.88	84.95
H%	wt%	15.94	15.93	15.92	15.91	15.23	15.16	15.08	15.01	14.91	14.81	14.72	14.63	11.62	11.31	11.00	10.69	15.12	15.05
H/C		2.275	2.273	2.271	2.270	2.156	2.144	2.132	2.119	2.102	2.087	2.071	2.056	1.578	1.530	1.483	1.437	2.138	2.126
Stoic A/F		15.13	15.13	15.12	15.12	14.97	14.95	14.93	14.92	14.89	14.87	14.85	14.83	14.14	14.07	14.00	13.93	14.94	14.93
Heating value	kJ/kg	44399	44388	44378	44367	44312	44291	44270	44249	44290	44270	44249	44227	42101	41928	41759	41592	44122	44090
n-Heptane	vol%	25.00	20.00	15.00	10.00	50.89	46.62	42.35	38.08	30.27	24.98	19.69	14.39	44.82	40.31	35.80	31.29	45.57	41.39
iso-Octane	vol%	75.00	80.00	85.00	90.00														
Diisobutylene	vol%					49.11	53.38	57.65	61.92										
4Methyl-1-pentene	vol%									69.73	75.02	80.31	85.61						
Toluene	vol%													55.18	59.69	64.20	68.71		
Cyclopentane	vol%																	54.43	58.61
n-Heptane	mass%	24.78	19.81	14.85	9.90	49.77	45.52	41.26	37.02	30.88	25.51	20.13	14.72	39.05	34.76	30.55	26.43	43.46	39.33
iso-Octane	mass%	75.22	80.19	85.15	90.10														
Diisobutylene	mass%					50.23	54.48	58.74	62.98										
4Methyl-1-pentene	mass%									69.12	74.49	79.87	85.28						
Toluene	mass%													60.95	65.24	69.45	73.57		
Cyclopentane	mass%																	56.54	60.67

The boiling point temperatures of n-heptane, iso-octane and diisobutylene are almost 100 °C. That of toluene is 110 °C. Therefore, the differences in vaporization characteristics of PRF series fuels, NDB series fuels, and NTL series fuels can be neglected. The boiling point of 4-methyl-1-pentene is 53 °C and the affect of fuel homogeneity on this engine can be estimated.

Fuel is injected by a port fuel injection system. Neither hot EGR, nor any other combustion stratification system was utilized in order to investigate the purely hydrocarbon effects on HCCI combustion.

ENGINE TEST CONDITIONS

The HCCI engine was operated at 1000 rpm. Intake air was supercharged to 155 kPa abs and its temperature was kept at 58 °C. Engine test data were recorded for 7 different maximum pressure rise rates. Rates of 900, 800, 700, 600, 500, 400 and 300 kPa/deg were achieved by changing the fuel injection quantity and were processed from the 400 cycles averaged in-cylinder pressure data, as shown in Figure 5.

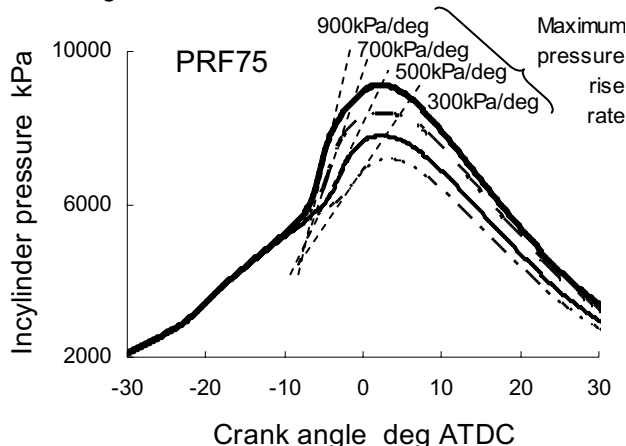


Figure 5 Relation between measured in-cylinder pressure and maximum pressure rise rate (PRF75)

DEFINITION OF HEAT RELEASE DATA

Figure 6 shows the definitions used in the analysis of heat release in this paper. All the heat release data and in-cylinder temperatures in this paper were calculated from the pressure data taken by the #1 cylinder pressure sensor. After the averaged 400 cycles of pressure data were converted to heat release data, the start and end points of the HTHR were chosen as the x-axis intercepts. The dashed area in Figure 6 is the integrated heating value of HTHR. HTHR CA50 is the crank angle timing at 50 % completion of HTHR combustion. The crank angle resolution had 0.25 CA degrees. Maximum pressure rise rate was calculated from each maximum pressure rise rate over 400 cycles.

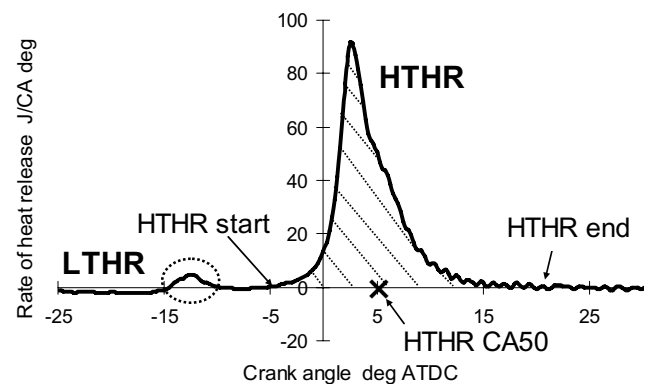


Figure 6 Definition of heat release data

RESULTS AND DISCUSSION

EFFECT OF OCTANE NUMBERS AND MAXIMUM PRESSURE RISE RATES ON ENGINE OPERATION

Figure 7 shows the IMEP-HTHR CA50 operational range of PRF series fuels. As research octane number increases, HTHR CA50 retards and the IMEP increases.