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Research Article

Numerical Analysis on the Effect of Fuel Injection Timing on Auto-Ignition of an Ethanol Spray in a Rapid Compression and Expansion Machine

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Abstract:
This study deals with the development of controlled-ignition technology for high performance CI (Compression Ignition) alcohol engines. In our previous numerical analysis, it is concluded that fuel injection timing is one of the most important factors for the control of auto-ignition of an ethanol spray. We numerically investigated the effect of fuel injection timing on auto-ignition quality of an ethanol spray in a rapid compression and expansion machine (RCEM) by using the commercial CFD code "CONVERGE". Results showed that it was possible to control the auto-ignition timing of an ethanol spray in the RCEM by the adjustment of fuel injection timing. In addition, heat release patterns after auto-ignition of a fuel spray similar to the conventional DI (Direct Injection) diesel engines was numerically indicated even for ethanol direct injection by the precise control of fuel injection timing. Totally judged from the results described the above, this study showed the feasibility of diesel engine operation fueled by neat ethanol by the control of fuel injection timing.

Keywords: *Ethanol spray, Auto-ignition, Numerical analysis, Rapid compression and expansion machine*

1. Introduction

Although research trend for recent technologies of power unit has changed from internal combustion engines to battery and motors, as the enhancement of renewable/sustainable energy utilization, ignition, combustion, and emission characteristics of biofuels such as bioethanol, butanol in high performance diesel engines have been still now focused on. Recently, ignition, combustion, and emission characteristics of alcohol-diesel blended fuels have been highlighted for diesel engines [1-8]. In order to develop such diesel engines fueled by alcohol/diesel blends, correct understanding of auto-ignition of an alcohol spray is required. However, a few fundamental studies [9-14] on the physical and chemical mechanisms of auto-ignition of an alcohol spray are found in these couples of decades. Siebers and Edwards [9] pointed out the one fundamental knowledge and they showed an important direction that researchers and engineers should pay an attention in the design process. They concluded that auto-ignition in an alcohol spray is dominated by temperature of surrounding air regardless of air pressure, and they also suggested air temperature higher than 1100K at the fuel injection timing in order to obtain acceptable ignition delay. One of the authors, Saitoh, et al. [11] also reported the similar conclusions, however, they concluded that the simultaneous attainment of ignition-suitable temperature and concentration inside a spray during its mixture formation process is necessary for stable auto ignition of an alcohol spray, and mixture formation depends on the surrounding gas pressure, temperature, and oxygen concentration. Based on the above introduced recognition for stable auto ignition, required surrounding gas conditions

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were revealed in our past study [12] by using a constant volume combustion chamber (CVCC). Further investigation of numerical analysis for the RCEM with the consideration of combined effects of gas flow and temperature change in combustion chamber with crank angle was performed prior to the experiments. In this numerical analysis, fuel was injected at Top Dead Center (TDC) in order to investigate the required gas pressure and temperature at compression TDC for stable auto-ignition of an ethanol spray. In our latest report [14], it is concluded for stable auto-ignition that amount of heat supplied into a spray by the entrainment of high-temperature surrounding gas must be superior to the physical and chemical factors of temperature-increase-obstruction as follows.

1. Enhancement of ethanol evaporation due to the counter flow for fuel injection in compression stroke
2. Decrease of mean temperature of the surrounding gas in the expansion stroke
3. Endothermic reactions of H_2O_2 and HO_2 generations which occurs prior to the generations of OH radical and H atom recognized as the activated chemical species relating the chain branching reactions as auto-ignition.

Therefore, fuel injection before TDC can be one of the effective ways of improvement for the above stated temperature-increase-obstruction. The objective of this numerical study is to investigate the effect of the fuel-injection-timing (FIT) on auto-ignition quality of an ethanol spray in the RCEM.

2. Numerical Analysis

2.1 Computational Domain & Mesh Geometry

Figure 1 shows a general view of the originally designed RCEM with variable compression ratio (maximum: ε=22.5) by the variable intake and exhaust valve open/close control. The RCEM is driven by four starter motors connected with a flywheel usually used for construction vehicles. Pre-compression and heating chamber for intake gas is also equipped with the RCEM so that various surrounding gas pressure and temperature conditions before fuel injection can be examined. Figure 2 shows the computational domain of the RCEM. In the numerical analysis, results of the velocity distribution in the combustion chamber after compression stroke was used as the initial conditions for the calculation of a spray mixture formation process.

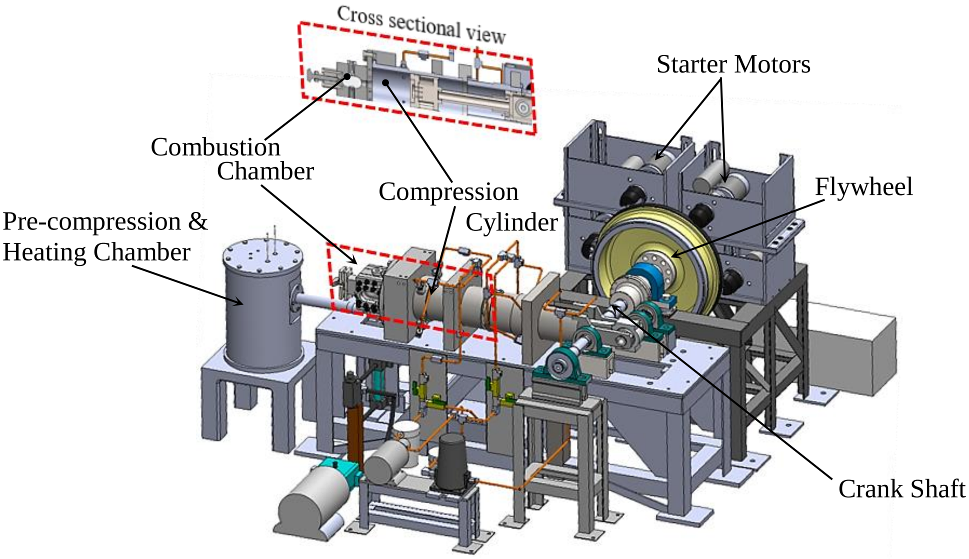

Fig. 1. Rapid Compression and Expansion Machine.

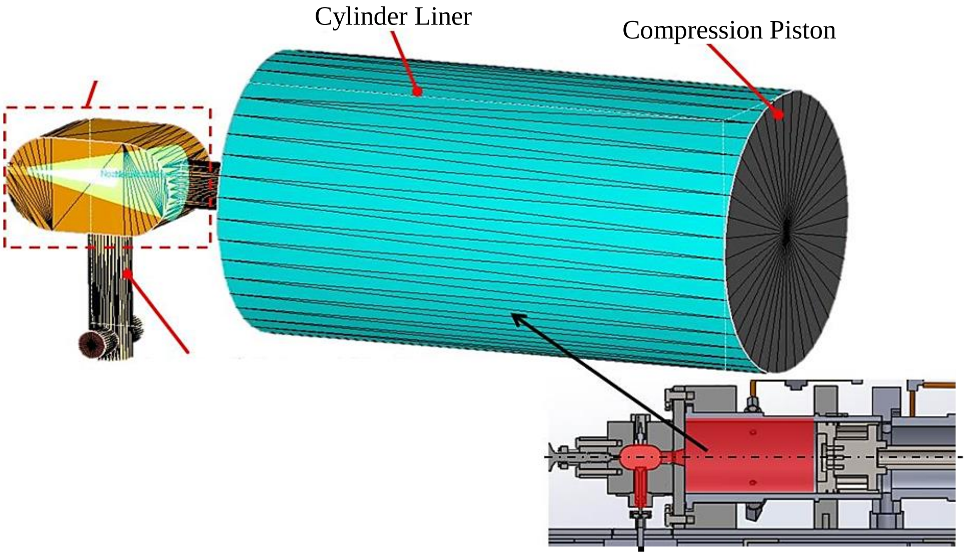

Fig. 2. Computational domain of the RCEM.

Table 1 represents the specifications of the RCEM and fuel injection conditions. Single-hole nozzle with its diameter of 0.14 mm was employed and injection duration was maintained as 6.5 degree in crank angle regardless of FIT. For the numerical analysis, a commercial CFD code; CONVERGE was used as solver. Table 2 stands for the mesh geometry and the method of mesh size control used in the numerical analysis. Although base grid size was set as 8 mm for each coordinate direction in the computational domain, fine mesh of 2 mm was set for the area where mixture formation is expected to occur. Entity of the fine mesh is cone-shape as shown in Fig. 2 (See the light green region illustrated in the combustion chamber in Fig. 2) and its geometry is expressed as “Fixed Embedding Fine Mesh” in Table 2. In addition, an automatic mesh refinement function named “AMR”: Adaptive Mesh Refinement, included in CONVERGE, was activated when finer mesh was required. AMR was applied for velocity, temperature, and chemical species as listed in Table 2, and its activation was judged at each grid point by the “sub-grid criterion”, comparing the calculated results of velocity, temperature, and chemical species with their previous-time-step-results.

Table 1: Specification of the RCEM & fuel injection conditions.

Bore × Stroke	150 mm × 280 mm
Rotation Speed	244 rpm
Compression Ratio	Variable max. 22.5
Fuel Injection Pressure	50 MPa
Fuel Injection Duration	6.5 deg. in crank angle
Injector Nozzle diameter × number	ϕ 0.14 mm × 1

Table 2: Specification of the mesh.

Maximum number of cells			700,000
Base grid		X	8 mm
		Y	8 mm
		z	8 mm
FE (Fixed Embedding Fine Mesh)		Entity type	Cone: ‘Injector’
		Scale: Base grid × 2^(-scale)	$3{:}8\times2^{-3} = 1$ mm
		Radius 1	2 mm
		Radius 2	20 mm
		Length	80 mm
AMR (Adaptive Mesh Refinement)	Velocity	Max. embedding scale	$6{:}8\times2^{-6} = 0.125$ mm
		Sub-grid criterion	12.0 m/s
	Temperature	Max. embedding scale	$6{:}8\times2^{-6} = 0.125$ mm
		Sub-grid criterion	6.0 K
	Chemical Species	Max. embedding scale	$6{:}8\times2^{-5} = 0.25$ mm
		Sub-grid criterion	0.0001 mole fraction

2.2 Governing Equations & Boundary Conditions

Conservation law of mass, momentum, and energy were expressed by the finite volume method. Three-dimensional equations of continuity, Navier-Stokes equation, and energy equation with the consideration of fluid compressibility were employed in the calculation of flow and temperature fields in intake, compression and expansion strokes. Transport equation of chemical species was also applied for the calculation of spray mixture formation process by fuel injection. Law of wall was applied for velocity and thermal boundary conditions. Therefore, the velocity and temperature profiles in their boundary layer were defined and calculated by the wall function. Boundary condition for chemical reactions at cylinder surface was not considered because no collision of spray to the combustion chamber wall occurred.

2.3 Physical & Chemical Models

Large eddy simulation (LES) was used as turbulence model. Kelvin-Helmholtz and Rayleigh-Taylor models were employed for atomization and evaporation of fuel droplets. Detailed chemical reaction model was also used in the calculation. We referenced chemical kinetic mechanism of Ethanol proposed by Marinov [15].

3. Results and Discussions

Four cases of FIT in Before Top Dead Center (BTDC) 2.5 deg., 5.0 deg, 7.5 deg, and 10 deg., respectively, indexed as “CASE 1, CASE 2, CASE 3, and CASE 4” in Table 3 were examined under the surrounding gas conditions of P=5.5MPa and T=1100K at compression TDC. Therefore, both the in-cylinder gas pressure and temperature were lower than 5.5MPa and 1100K when fuel was injected in CASE 1 – CASE 4. CASE 0, fuel injection timing of TDC, was the reference which was obtained in our previous study. Table 3 also shows the results indicating whether auto-ignition occurred or not. Although auto-ignition was not obtained in CASE 0, it was indicated that auto-ignition occurred in CASE 1, CASE 3, and CASE 4. In CASE 2, auto-ignition was not clearly observed. However, it was confirmed/predicted numerically that auto-ignition of an ethanol spray can be obtained by change of FIT before compression TDC.

Table 3: Examined fuel injection timing with each auto-ignition quality.

Index	CASE 0	CASE 1	CASE 2	CASE 3	CASE 4
Injection timing	TDC	BTDC 2.5 deg.	BTDC 5.0 deg.	BTDC 7.5 deg.	BTDC 10 deg.
Auto-Ignition	×	O	Δ	O	O

Surround Gas Conditions: P = 5.5 MPa, T = 1100 K at compression TDC

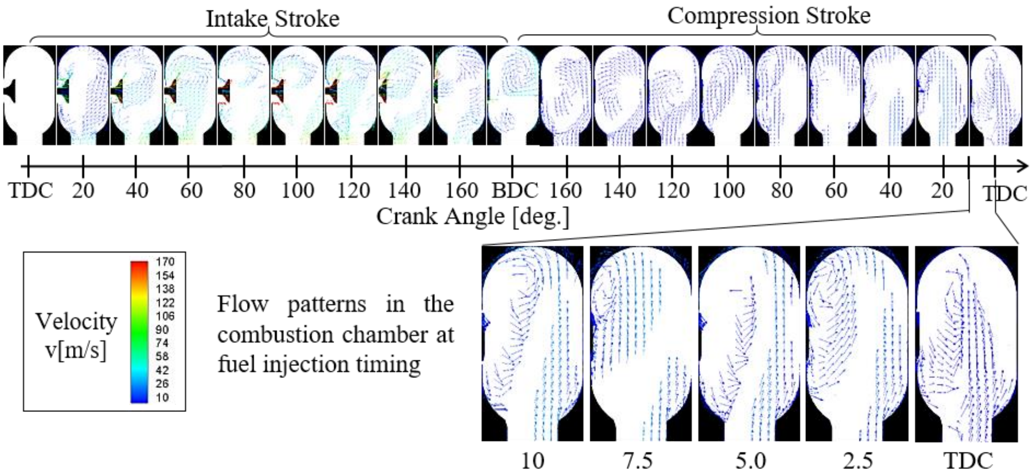

Fig. 3. Results of flow analysis during intake and compression strokes.

Visualization results of flow field in the combustion chamber are shown in Fig. 3. Upper figure shows the flow patterns in the intake and the compression strokes. The lower five figures indicate the velocity distributions formed in the combustion chamber before fuel injection of each examined case. Although velocity distribution at FIT showed different patterns among five cases, flow in the opposite direction for fuel injection was observed for all the cases. It was confirmed that the counter flow against fuel injection caused the enhancement of atomization and evaporation compared with the results obtained in a CVCC in our past study [12].

Figure 4 shows the histories of mean temperature of a spray for each FIT case. Temperature rapidly decreased when fuel was injected due to the enhancement of atomization and evaporation of ethanol droplets, and after that temperature increased with its gradient change twice. This tendency was observed for all the FIT case except for CASE 2 and this was also obtained for CASE 0 in our previous study [14]. The mechanism of this temperature history from fuel injection was discussed and concluded that second temperature gradient with drastic temperature rising can be caused by auto-ignition, on the other hand, obstruction of temperature rising after the first temperature gradient change can be attributed to the start of endothermic reactions of H_2O_2 and HO_2 generations. According to these recognitions, auto-ignition seemed to occur before TDC in CASE 3 (BTDC 7.5 deg.) and CASE 4 (BTDC 10 deg.). Contrary, auto-ignition seemed to occur after TDC in CASE 1 (BTDC 2.5 deg.) Auto-ignition is ideally obtained close to TDC for higher thermal efficiency, therefore, optimum FIT seems to exist between CASE 1 and CASE 3. However, drastic temperature rising as auto-ignition was not indicated in CASE 2. Earlier FIT means lower surrounding gas temperature and stronger counter flow when fuel injection is started and getting higher in surrounding gas temperature until TDC. The former and the latter corresponds to negative and positive factors, respectively, for temperature rising of a spray, therefore, auto-ignition seems to depend on which factor is superior to the other. In CASE 2, negative factors can be superior to positive one. Optimum FIT seems to exist between BTDC 2.5 deg. and 5.0 deg., or between BTDC 5.0 deg. and 7.5 deg.

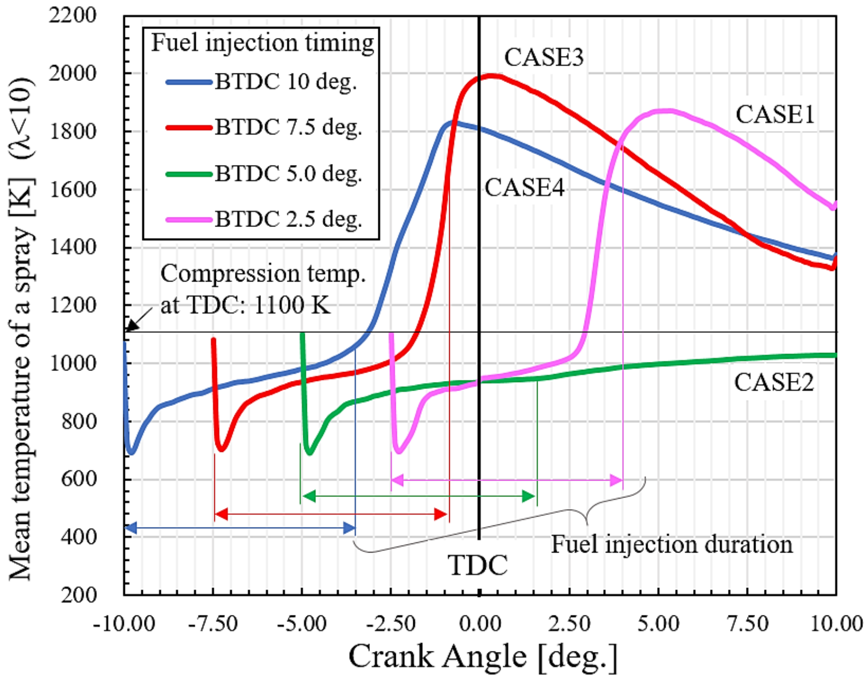

Fig. 4. History of mean temperature of a spray for each examined fuel injection timing.

Figure 5 shows the temporal visualization results on temperature and excess air ratio of an ethanol spray from fuel injection of CASE 1 with comparison in temperature of CASE 0. In CASE 1, auto-ignition occurred close to the end of fuel injection duration. On the other hand, auto-ignition was not observed in CASE 0. It is understood from Fig. 5 that auto-ignition depends on the mixture formation before TDC, though the duration of mixture formation is only 2.5 deg. in crank angle.

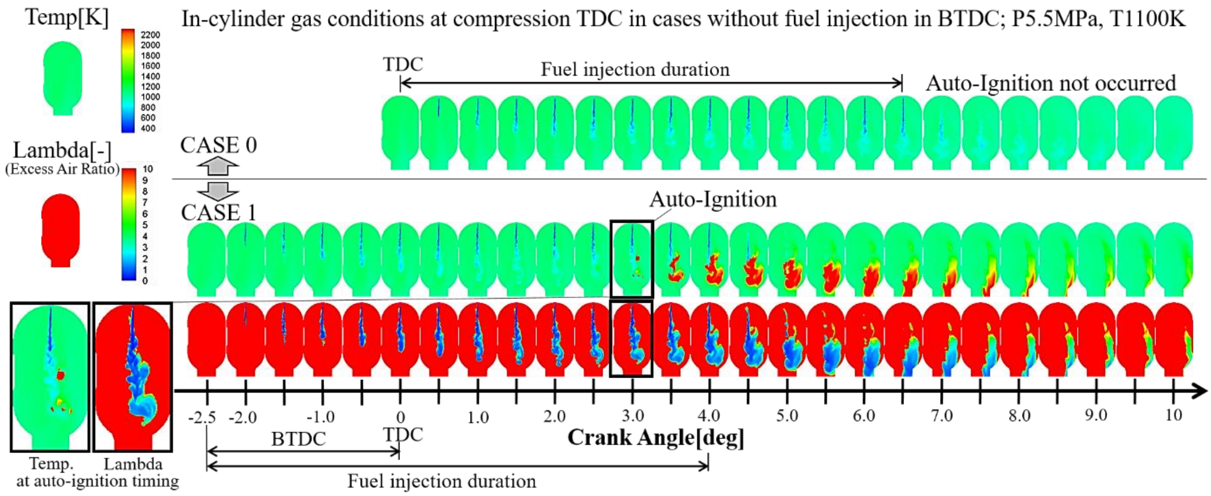

Fig. 5. Temporal visualization results on temperature and excess air ratio of an ethanol spray from fuel injection of the CASE 1 with comparison in temperature of the CASE 0.

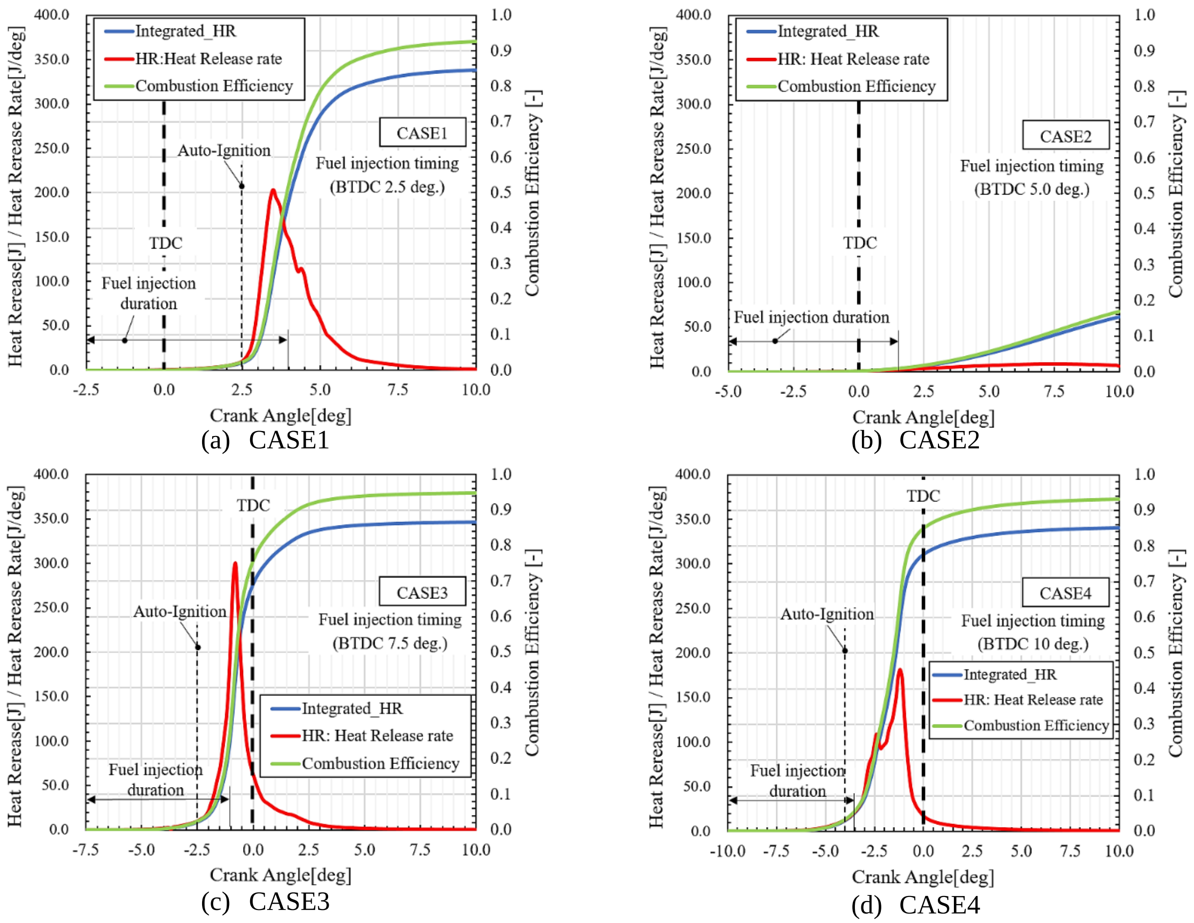

Fig. 6. Variations of heat release pattern and combustion efficiency with different FITs.

Figures 6 (a), (b), (c), and (d) show, respectively, heat release pattern and combustion efficiency in CASE 1, CASE 2, CASE 3, and CASE 4. Earlier auto-ignition timing was obtained with earlier FIT; however, also longer ignition delay was obtained with earlier FIT. As the result, pre-mixed combustion mainly occurred in CASE 1, CASE 3, and CASE 4 due to long ignition delay. Although small amount of heat release was confirmed in CASE 2, combustion could not be maintained due to insufficient heat supply by the entrainment of the surrounding gas. In addition, combustion efficiency showed less than 100% for all the FIT cases.

Four cases of FIT in BTDC 0.5 deg., 1.0 deg, 2.5 deg, and 5.0 deg were also examined under the surrounding gas conditions of P=4.5MPa and T=1200K at compression TDC. Results of the simulation are shown in Table 4. Auto-ignition occurred in BTDC region even in the FIT cases of 2.5 deg. and 5.0 deg., therefore, it is understood that shorter ignition delay was obtained in comparison with lower surrounding gas temperature cases as previously introduced. The most ideal auto-ignition timing was observed when FIT was BTDC 1.0 deg. as indexed as CASE 5 in Table 4.

Table 4: Examined fuel injection timing with each auto-ignition quality.

			CASE 5		
Injection timing	TDC	BTDC 0.5 deg.	BTDC 1.0 deg.	BTDC 2.5 deg.	BTDC 5.0 deg.
Auto-Ignition	O	O (ATDC)	O (ATDC)	O (BTDC)	O (BTDC)

Surrounding Gas Conditions: P = 4.5 MPa, T = 1200 K at compression TDC

Figure 7 shows the temperature history with the spatial temperature distribution of CASE 5. Typical temperature history when auto-ignition occurs as introduced in Fig. 4 was indicated in Fig 7. That is; ① rapid temperature decrease at the beginning of fuel injection due to enhancement of atomization and evaporation of fuel droplets, ② rapid temperature increase by the amount of heat supplied into a spray by the high temperature surrounding gas entrainment, ③ first temperature-gradient-change after temperature rising, ④ obstruction of temperature increase due to the endothermic reactions of H_2O_2 and HO_2 generations, ⑤ drastic temperature rising caused by auto-ignition. Compared this graph with Fig. 4, shorter region of ④ is indicated. In addition, after auto-ignition, mean temperature of a spray was maintained during fuel injection indexed as ⑥ in Fig. 7. This can be caused by continuous heat generation as diffusion combustion under surrounding gas temperature decrease situation in expansion stroke. Spatial temperature distributions illustrated in Fig. 7 endorse the above introduced understanding of this phenomena. In Figure 4, this tendency was not observed due to almost pre-mixed combustion induced by long ignition delay due to insufficient surrounding gas temperature. Ignition delay was 1.8 deg. in crank angle that approximately corresponds to 1.23ms in time. This is an acceptable ignition delay for actual engines.

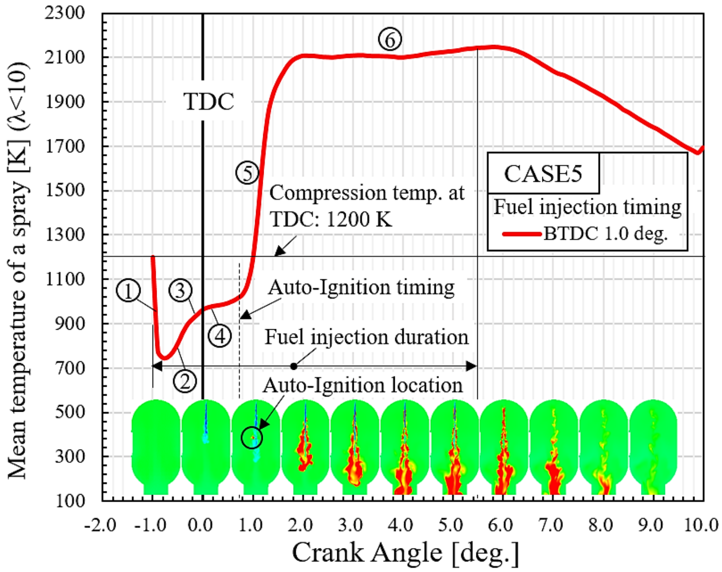

Fig. 7. Temperature history of an ethanol spray in the case when acceptable ignition delay was obtained.

Heat release pattern in CASE 5 is shown in Fig. 8. First peak of heat release corresponds to pre-mixed combustion of mixture formed during ignition delay. Continuous diffusion combustion after pre-mixed combustion is also indicated in Fig. 8. This indicates the similar one as typical diffusion combustion in a conventional diesel engine fueled by gas-oil or heavy duty oil. In addition, combustion efficiency reached 100% at 2.5 deg. after fuel injection was finished. It is clearly understood from Figs. 7 and 8 that auto-ignition and diffusion combustion can be realized even for an ethanol spray by the control of fuel injection timing under sufficient surrounding gas pressure and temperature.

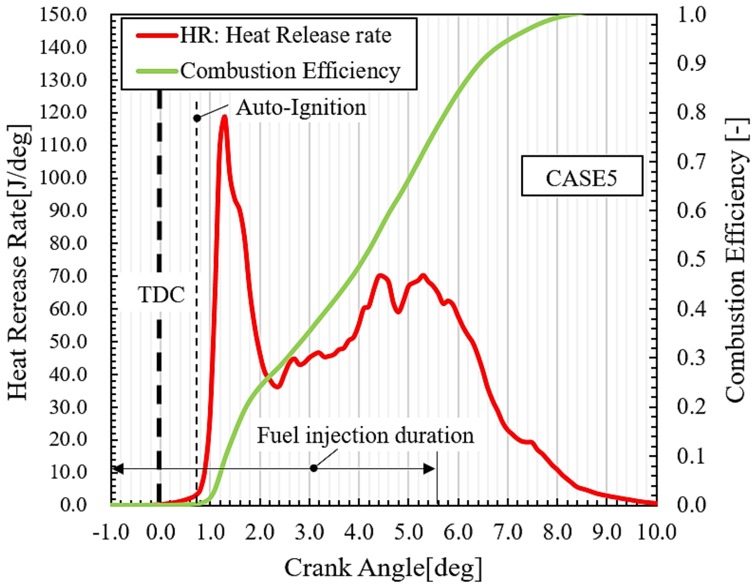

Fig. 8. Heat release pattern and combustion efficiency in the case when acceptable ignition delay was obtained.

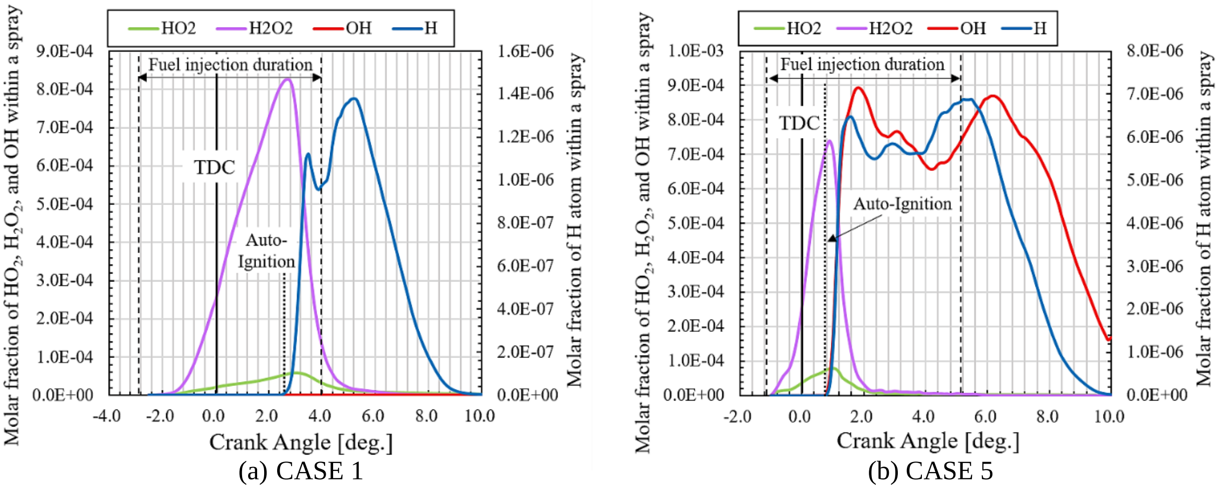

Fig. 9. Comparison of activated-chemical-species generation between CASE 1 and CASE. 5

Figure 9 shows the comparison of four kinds of activated-chemical-species generation between CASE 1 and CASE 5. Auto-ignition timing coincided with the generations of OH and H for both cases. However, OH generation was negligibly small in CASE 1, therefore, auto-ignition was chemically dominated by the H generation in CASE 1 where pre-mixed combustion mainly occurred. Although auto-ignition was observed in CASE 1, peak value of molar fraction of H atom was less than half of that in CASE 5. In addition, duration of H atom generation was shorter than that in CASE 5. Therefore, combustion/chain branching reaction seemed not be maintained. Lower combustion efficiency in CASE 1 can be attributed to this chemical reason. Contrary, auto-ignition seemed to be dominated by OH generation in CASE 5 where diffusion combustion mainly occurred. Duration of OH radical and H atom generations were continued until the end of fuel injection. This knowledge is fundamental understanding of chemical reaction not special for ethanol spray. In sort of chemical aspect, it seems that auto-ignition depends on the continuous OH radical and H atom generation with heat generation in chain branching reactions regardless of fuel.

4. Conclusions

Results of numerical analysis introduced in the previous chapter allow us to draw the following conclusions.

1. It is possible to control the auto-ignition of an ethanol spray in the RCEM by the adjustment of fuel injection timing.
2. Precise control of injection timing associated with the surrounding gas temperature is required to realize the acceptable ignition delay time short enough for actual diesel engine operations fuelled by neat ethanol.

5. Future Work

The RCEM is not under operation yet, it is now under the final check of its drive-system for safe experimentation, and data acquisition system with the signal synchronization between crank angle signal and fuel injection trigger one has to be checked/adjusted before carrying out the experiments. Validation between the numerical results introduced in this paper and the experimental data obtained in the future study is required for further discussion.

Nomenclature

P	pressure, MPa
T	temperature, K
v	velocity, m/s
λ	excess air ratio= actual air fuel ratio / stoichiometric air fuel ratio

Abbreviations

AMR	Adaptive Mesh Refinement
BTDC	Before Top Dead Center
CI	Compression Ignition
DI	Direct Injection
FIT	Fuel Injection Timing
LES	Large Eddy Simulation
RCEM	Rapid Compression and Expansion Machine
TDC	Top Dead Center

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