

PAPER • OPEN ACCESS

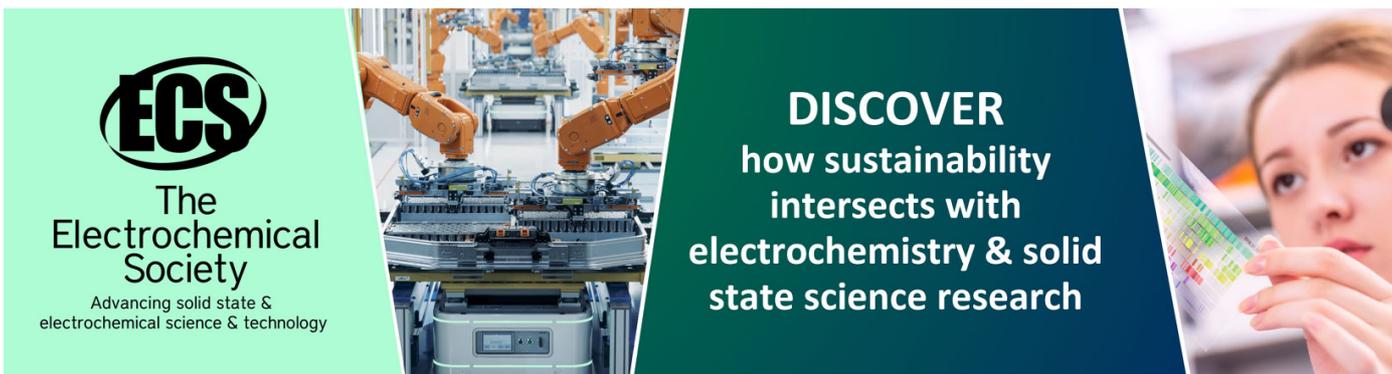
Numerical Prediction of Mixture Formation Process of an Ethanol Spray in a Rapid Compression and Expansion Machine

To cite this article: Akihiro Umeno *et al* 2019 *IOP Conf. Ser.: Mater. Sci. Eng.* **501** 012001

View the [article online](#) for updates and enhancements.

You may also like

- [Characterization of a two-dimensional temperature field within a rapid compression machine using a toluene planar laser-induced fluorescence imaging technique](#)
Camille Strozzi, Julien Sotton, Arnaud Mura *et al.*
- [Investigation of Combustion Process of Biodiesel Derived from Waste Cooking Oil, Jatropha, Palm Oil and Algae using Rapid Compression Machine](#)
Mohd Irham Anas, Amir Khalid, Norrizam Jaat *et al.*
- [Frequency domain analysis of knock images](#)
Yunliang Qi, Xin He, Zhi Wang *et al.*



ECS
The
Electrochemical
Society
Advancing solid state &
electrochemical science & technology

DISCOVER
how sustainability
intersects with
electrochemistry & solid
state science research

Numerical Prediction of Mixture Formation Process of an Ethanol Spray in a Rapid Compression and Expansion Machine

Akihiro UMENO¹, Koji UCHIDA², Norihiko WATANABE² and Hironori SAITOH^{2,*}

¹Graduate School of Mechanical Engineering, Sojo University, Ikeda 4-22-1, West Ward, Kumamoto City, 860-0082, Japan

²Department of Mechanical Engineering, Sojo University, Ikeda 4-22-1, West Ward, Kumamoto City, 860-0082, Japan

* Corresponding Author: E-mail: saitoh@mec.sojo-u.ac.jp, Telephone: +81-96-326-3729, Fax: +81-96-323-1351

Abstract. This study deals with the development of controlled-ignition technology for high performance compression ignition alcohol engines. Among the alcohol fuels, we focused on Ethanol as a promising candidate of alternative fuels replacing from petroleum. In our previous study, visualization tests of spray mixture formation process up to auto-ignition for Ethanol-Diethyl ether blend fuels had been conducted by using a constant volume electrical heating combustion chamber. Quantitative evaluation of auto-ignition quality was summarized in a form of 3D map that indicates the effects of surrounding gas pressure, temperature and Oxygen concentration on ignition delay. However, maximum surrounding gas pressure in the experiments was 2.8MPa much less than that of real engine due to the structure of the combustion chamber. As the next step, we originally designed and manufactured a RCEM (Rapid Compression and Expansion Machine with variable compression ratio) in order to investigate the mixture formation process up to auto-ignition of an Ethanol spray under surrounding gas conditions similar to real engine operating conditions with the consideration of the interaction between fluid motion of surrounding gas and fuel injection. Prior to carrying out the experiments, we numerically predicted the auto-ignition quality of an Ethanol spray in the rapid compression and expansion machine. One of the commercial CFD codes; CONVERGE was used in the computational calculation with the considerations of turbulence, atomization, evaporation and detailed chemical reaction. Effect of fluid motion and surrounding gas pressure and temperature inside the combustion chamber of the RCEM on an Ethanol spray mixture formation is mainly discussed in this paper.



Nomenclature

T	: temperature [K]
t	: time [ms]
λ	: excess air ratio [-]
ε	: compression ratio

Subscripts

ig	: ignition
s_{pm}	: Mean of a spray penetration mean
tip	: spray tip

Abbreviation

AMR	: <u>A</u> daptive <u>M</u> esh <u>R</u> efinement
ATDC	: <u>A</u> fter <u>T</u> op <u>D</u> ead <u>C</u> enter
BDC	: <u>B</u> ottom <u>D</u> ead <u>C</u> enter
BRICS	: <u>B</u> razil, <u>R</u> ussia, <u>I</u> ndia, <u>C</u> hina, <u>S</u> outh Africa
BTDC	: <u>B</u> efore <u>T</u> op <u>D</u> ead <u>C</u> enter
FE	: <u>F</u> ixed <u>E</u> Embedded
IPCC	: <u>I</u> ntergovernmental <u>P</u> anel on <u>C</u> limate <u>C</u> hange
KH	: <u>K</u> elvin- <u>H</u> elmholtz
LES	: <u>L</u> arge <u>E</u> ddy <u>S</u> imulation
RCEM	: <u>R</u> apid <u>C</u> ompression and <u>E</u> xpansion <u>M</u> achine
RT	: <u>R</u> ayleigh- <u>T</u> aylor
TDC	: <u>T</u> op <u>D</u> ead <u>C</u> enter
WMO	: <u>W</u> orld <u>M</u> eteorological <u>O</u> rganization

1. Introduction

At present civil life and industrial activities are supported by mass consumption of fossil resources. Nowadays, energy consumption is increasing year by year with population growth and industrial development especially in BRICS. We have been faced the problems such as oil reserve depletion and global warming. Amount of recognized oil reserves is approximately 1071.1 billion barrels, and if we continue to consume oil at the present rate, available years is expected as 52.5 years [1]. Under the above introduced international movements with population, economic growth and industrial development depending on fossil fuel, global warming has been obviously appeared. IPCC(Intergovernmental Panel on Climate Change) founded by united nations and WMO(World Meteorological Organization) presented that carbon dioxide accounts for 60% of the total greenhouse gas emissions, and 80% of them are being emitted by consumption of fossil fuels by power plants and automobiles. Therefore, it is necessary for modern societies to pay an attention of decreasing the fossil fuel dependence and it is urgent to construct a recycling-oriented society. As one of the solutions, we focus on the development of high efficient energy conversion technology by using biomass-based alcohol fuel as an alternative fuel that is environmentally friendly and renewable.

2. Previous study and Objective

2.1. Previous study

The goal of our research is the establishment of controlled-ignition technology for high performance compression ignition alcohol engines. Among alcohol fuels, we focused on Ethanol as a promising candidate of alternative fuels replacing from petroleum. In our previous study, we conducted a theoretical calculation of mixture formation process based on the momentum theory of spray penetration proposed by Wakuri et.al [2]. In this theoretical approach, we employed two fundamental factors of mixture on auto-ignition in a spray. One was concentration factor; mixture have to be in its mixing ratio enough to advance chemical reactions. The other was temperature factor; temperature of mixture have to exceed a certain value that chemical reactions are promoted up to combustion. Focusing on this recognition, we defined concentration and temperature factors respectively as $\lambda_{tip} = 1$ and $T_{spm} \geq T_{ig}$. λ_{tip} is excess air ratio of a spray tip, T_{spm} and T_{ig} are mean temperature of a spray and minimum ignition point of fuel, respectively. In our recognition, stable auto-ignition would be obtained by fuel injection if temperature factor is cleared when concentration factor is attained. Based on this fundamental mechanism of auto-ignition, prediction of mixture formation process of an Ethanol spray and a Gas oil spray was theoretically performed. Temporal histories of (λ_{tip}) and (T_{spm}) from fuel injection for Gas oil and Ethanol is shown in figure 1.

It can be understood from figure 1 that Gas oil seems to have stable auto-ignition because T_{spm} is much higher than T_{ig} when λ_{tip} is reached its concentration factor ($\lambda_{tip} = 1$). On the other hand, in the case of Ethanol, at the timing of $\lambda_{tip} = 1$, T_{spm} does not reach to its temperature factor (T_{ig}). In addition, leaner situation is easily expected when temperature factor is satisfied. These results allowed us to draw one conclusion on the reason of poor auto-ignition quality of Ethanol spray. That is the difficulty of simultaneous attainment of auto-ignition suit concentration and temperature during mixture formation process due to smaller stoichiometric air/fuel ratio and much larger latent heat of evaporation of Ethanol comparing to Gas oil. In other words, improvement of auto-ignition quality of Ethanol seems to be possible by retardation of leaner situation and faster temperature rising. Surrounding gas conditions such as pressure, temperature and Oxygen concentration, which corresponds to the entrained gas density, temperature and amount of heat supply into a spray, also influence the λ_{tip} and T_{spm} histories from fuel injection. Higher temperature of surrounding gas result faster T_{spm} rising and higher Oxygen concentration induce faster lean situation of mixture. Higher pressure of surrounding gas has the both effects of faster lean situation and temperature rising due to higher density of entrained gas into a spray.

Based on the above stated recognition, we conducted a spray visualization tests by using a constant volume electrical heating chamber under various kind of surrounding gas conditions. Ethanol-Diethyl ether blend fuel(changing blend ratio) was employed as test fuel in order to make clear the effect of fuel properties on their ignition delay. Value of fuel properties of Diethyl ether is close to Gas oil. As expected before experiments, shorter ignition delay was obtained with increasing of surrounding gas pressure, temperature and Oxygen concentration for Diethyl ether rich blend fuel. However, auto-ignition was not observed in case of Ethanol rich blend fuel even with retardation of leaner situation and faster temperature rising by surrounding gas conditions of low Oxygen concentration of 15% and 800 K in temperature, 2.8MPa in pressure. This result seemed to be attributed to insufficient surrounding gas density and temperature.

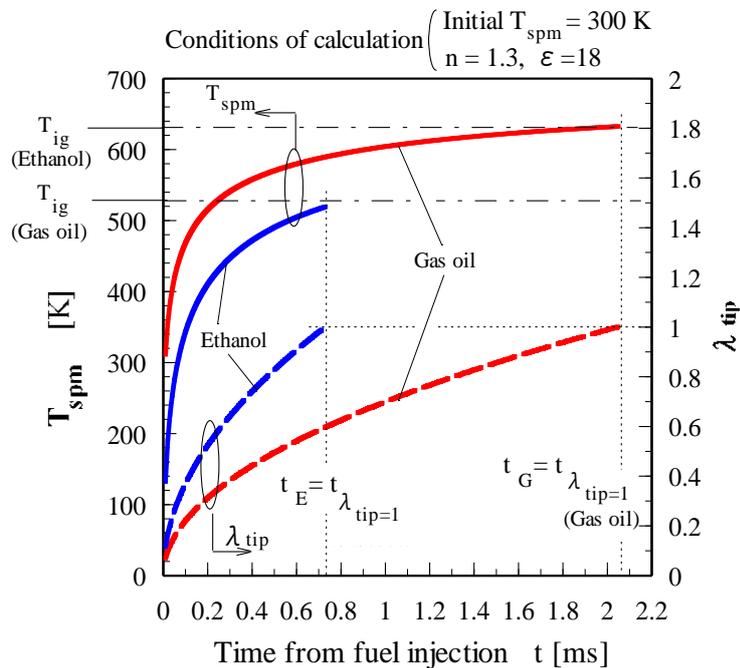


Figure 1. Theoretical evaluation of λ_{tip} and T_{spm} histories from fuel injection for Ethanol and Gas oil spray.

2.2. Objective

As the next step we originally designed and manufactured a RCEM (Rapid Compression and Expansion Machine with variable compression ratio) aiming to the observation of auto-ignition for an Ethanol spray. Figures 2(a) and (b) show the overall view of the RCEM and the cross section view of the device. RCEM consists of five parts. These are drive system, lubricating oil system, air intake/exhaust system, fuel injection system and compression parts by means of a long stroke crank-piston structure with cross-head mechanism. Compression ratio is adjustable with electronic control variable valve operating system. Maximum compression ratio is 22. Table 1 represents the principal particulars of the RCEM. Target values of compression pressure and temperature are 6.5MPa and 1000K, respectively for auto-ignition of an Ethanol spray. Prior to the experiments, in order to realize such surrounding gas conditions of high pressure and temperature we have to understand the RCEM operating conditions such as operating speed[rpm], initial intake gas condition, valve close/open timing and fuel injection timing synchronizing with crank angle. Then we performed numerical analysis of mixture formation process of an Ethanol spray with the consideration of flow behavior in combustion chamber in compression and expansion stroke. The objective of this study is to predict the spray mixture formation process of an Ethanol spray in the RCEM and to have a feasibility check for the attainment of surrounding gas conditions sufficient to occur auto-ignition.

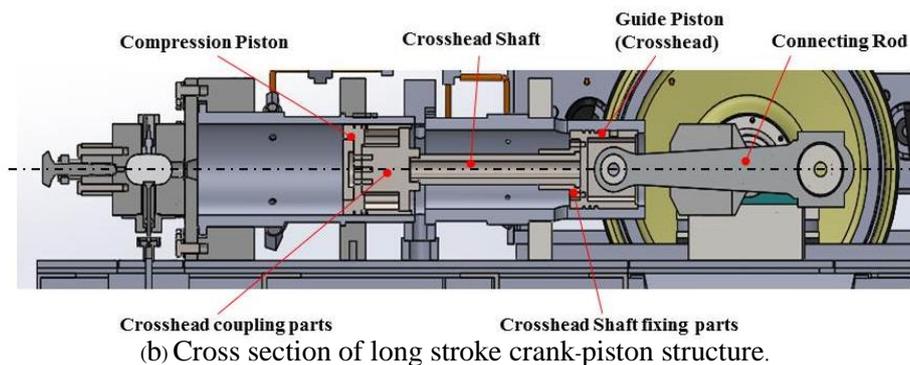
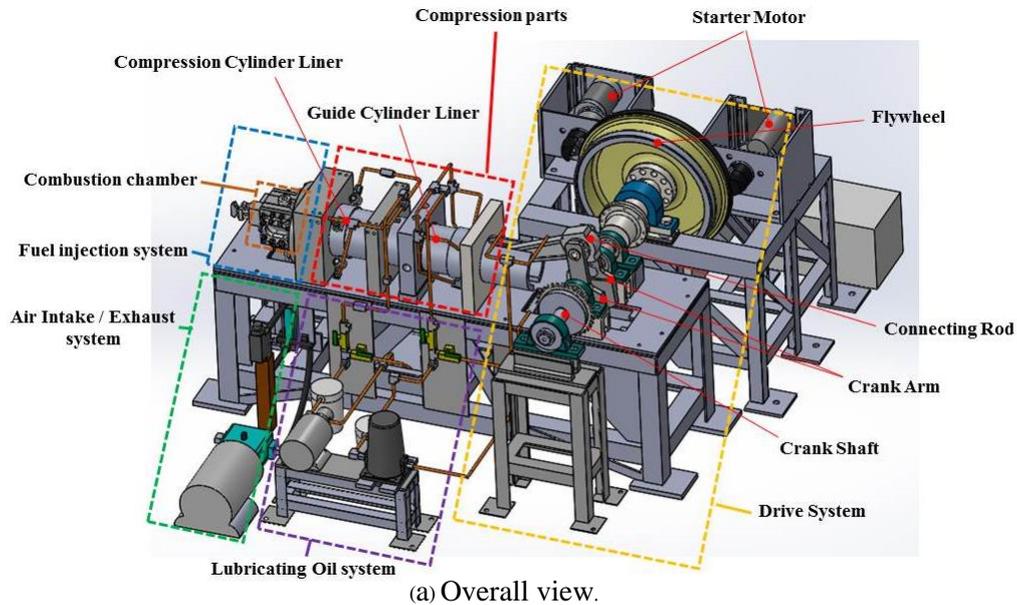


Figure 2. General view of the RCEM.

Table 1. Specification of the rapid compression and expansion machine with variable compression ratio.

Cylinder Bore [mm]	150
Stroke [mm]	280
Maximum Volume[mm ³]	5.18×10 ⁶
Target Compression Temperature [K]	1000 (1200K pre-heating)
Target Compression Pressure [MPa]	6.5
Maximum Compression Ratio	22
Fuel Injection Pressure [MPa]	50
Fuel Injection Duration [ms]	4.5
Injector Nozzle (type, diameter:φ[mm]×number)	Hole type, 0.14×1

3. Numerical Analysis

3.1. Computational Domain and Mesh Geometry

Computational domain as shown in figure 3 consists of intake/exhaust port, combustion chamber and cylinder with changing its size by piston movement. Table 2 shows the mesh geometry employed in the numerical analysis. Base grid size was 4mm. Fine mesh of 0.5mm was set in the expected area where mixture formation is occurred. Entity of the fine mesh is cone shape as shown in figure 3 (light green region in the combustion chamber) and its geometry is presented as “Fixed Embedding Fine Mesh” in table 2. Commercial CFD code; CONVERGE used in the numerical analysis has an automatic mesh refinement function named “AMR”: Adaptive Mesh Refinement. We applied AMR for velocity, temperature and chemical species as listed in table 2. For each grid point, AMR activation is judged by the “sub-grid criterion” comparing to the calculated results of velocity, temperature and chemical species to their previous time step results at the same grid. Minimum mesh size of 0.0625mm was applied by AMR in the numerical analysis for correct calculation. Table 3 shows the analysis conditions. RCEM operating speed was set as 244 rpm calculated from the rotational speed of starter motor and gear ratio between starter motor and flywheel, intake air was set as suction from atmosphere with 0.1MPa in pressure, 300K in temperature and 21 volume % in Oxygen concentration. Large eddy simulation (LES) was used as turbulence model. Kelvin-Helmholtz and Rayleigh-Taylor models represented as KH-RT model was employed for atomization and evaporation of fuel droplets. SAGE detailed chemical elementary reaction model was also used in the case with the consideration of combustion after spray mixture formation.

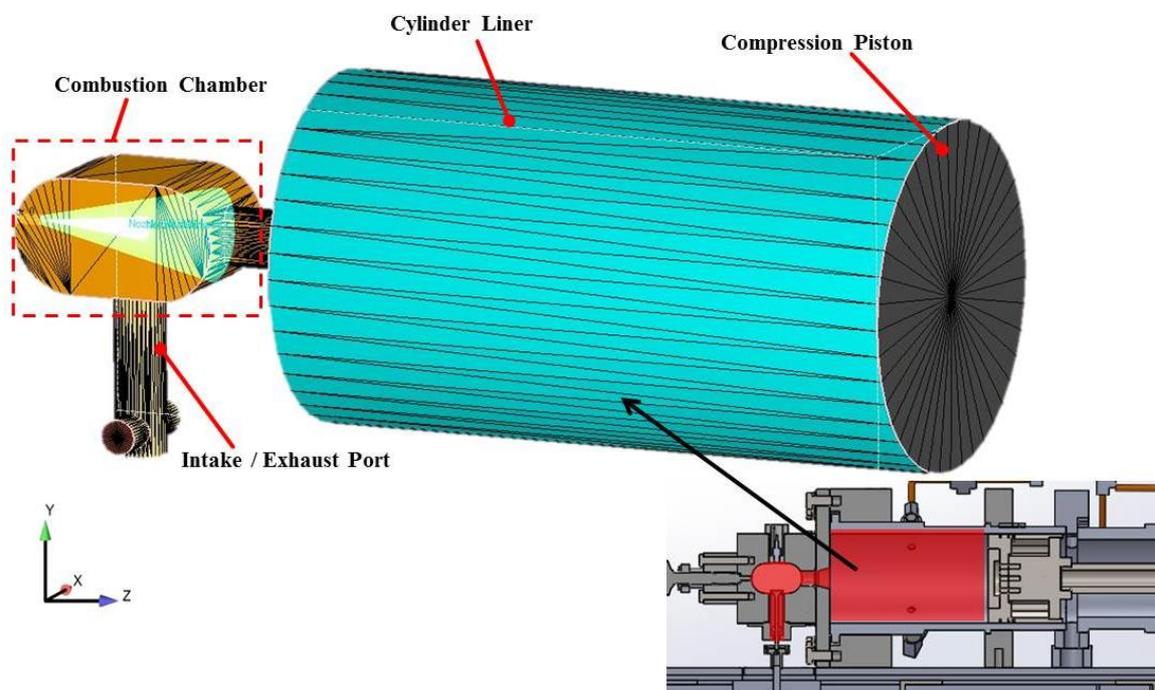


Figure 3. Computational domain.

Table 2. Mesh geometry in the numerical analysis.

Base grid	x	4 mm	
	y	4 mm	
	z	4 mm	
FE (Fixed Embedded)	Entity type	Cone: INJECTOR	
	Scale: Base grid $\times 2^{(-scale)}$	3: $4\text{mm} \times 2^{-3} = 0.5\text{ mm}$	
	Radius 1	2 mm	
	Radius 2	20 m	
	Length	80 mm	
AMR (Adaptive Mesh Refinement)	Velocity	Max embedded Scale	6: $4\text{mm} \times 2^{-6} = 0.0625\text{ mm}$
		Sub-grid criterion	1.0 m/sec
	Temperature	Max embedded Scale	6: $4\text{mm} \times 2^{-6} = 0.0625\text{ mm}$
		Sub-grid criterion	2.5 K
	Species	Max embedded Scale	5: $4\text{ mm} \times 2^{-5} = 0.125\text{ mm}$
		Sub-grid criterion	0.001 mole fraction

Table 3. Analysis conditions.

RCEM Operating Speed [rpm]	244
Fuel	Ethanol
Intake Gas Temperature [K]	300
Intake Gas Pressure [MPa]	0.1
Intake Gas Oxygen Concentration	21% (vol.)
Fuel Injection Pressure [MPa]	50
Fuel Injection Duration [ms]	4.5
Turbulence Model	LES
Spray Model	KH-RT Model
Chemical reaction Model	SAGE Detailed elementary reaction model

KH : Kelvin-Helmholtz, RT : Rayleigh-Taylor

3.2. Governing Equations and Boundary Conditions

Flow and temperature fields were solved under the conservation law of mass, momentum and energy. Three dimensional equation of continuity, Navier-Stokes equation and energy equation were employed with the consideration of fluid compressibility. Transport equation of chemical species was also applied for the calculation of combustion. Flow and temperature fields were numerically solved by finite volume method for the above introduced governing equations.

Non-slip condition was applied for flow field at the boundary of computational domain. Law of wall condition was also applied as thermal boundary condition.

4. Results and Discussion

Figure 4 shows the calculation result of flow field during intake and compression stroke. Although complicated flow with large-scale vortices was observed with valve motion during intake stroke, such complicated flow was disappeared and uniform velocity was formed in the combustion chamber at the crank angle around BTDC 40 degree in compression stroke. However, at TDC the end of compression stroke, asymmetric velocity distribution was observed again. In the region near the valve, higher velocity was obtained. In addition, temporal velocity fluctuation (acceleration and deceleration) was almost followed the piston speed.

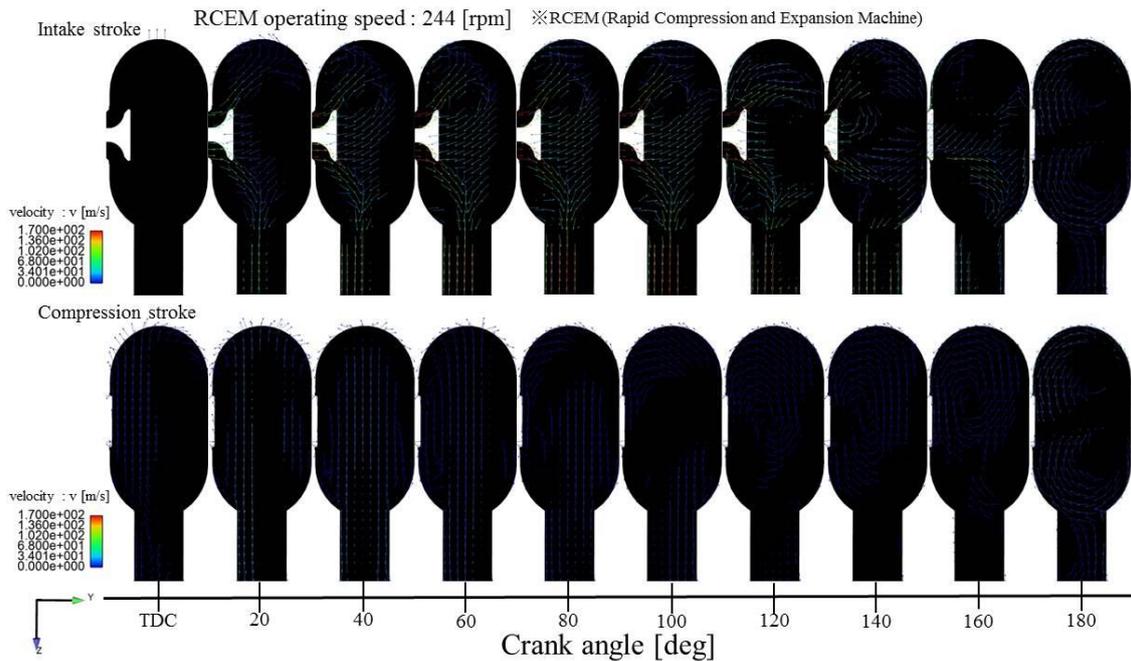


Figure 4. Numerical result of flow field in the combustion chamber during intake and compression stroke under the RCEM operating speed of 244rpm.

Figure 5 presents the temporal in-chamber gas pressure and temperature change during intake and compression stroke. Approximately 24% pumping loss was indicated in intake stroke. At the beginning of compression stroke at BDC, gas pressure and temperature was respectively indicated as 0.076MPa and 290K. Due to such pumping loss resulted compression pressure and temperature as 4.3MPa and 772K less than each target value. Therefore, decrease of pumping loss up to zero or device of supercharge is required to obtain the target compression pressure and temperature (6.5MPa and 1000K).

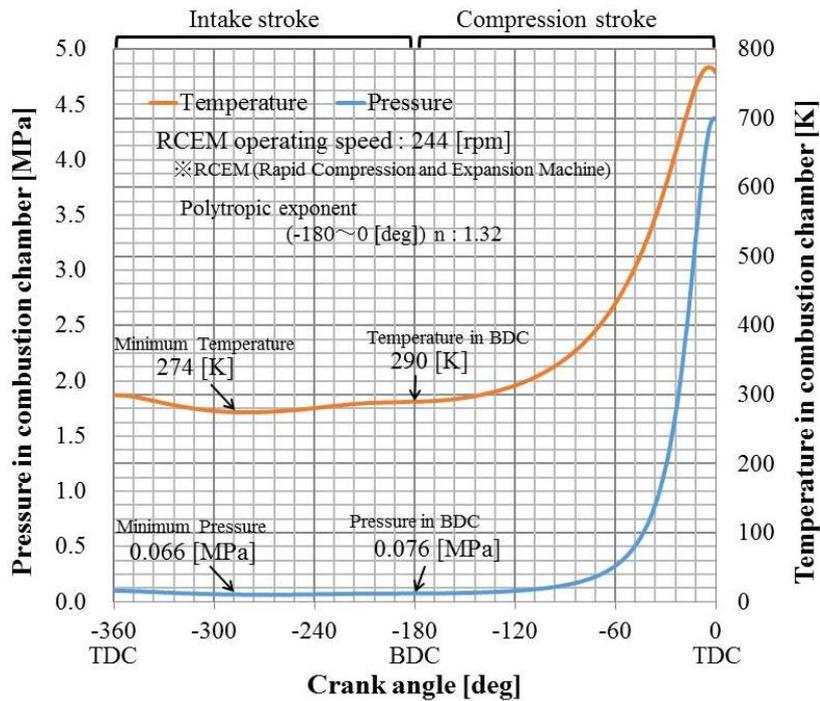


Figure 5. Pressure and temperature of in-chamber gas during intake and compression stroke.

Mixture formation of an Ethanol spray was simulated in expansion stroke from TDC to ATDC 7 degree in crank angle that corresponded to 4.78ms in time from fuel injection. Previously introduced flow (velocity distribution), pressure and temperature fields in the combustion chamber at the end of compression stroke was used as the initial gas condition at TDC before fuel injection. Result of calculation is shown in figure 6. Upper part of this figure indicates the history of spatial excess air ratio (λ) distribution along the axis of fuel injection (z direction), and lower part corresponds to those of temperature distribution. Although spray developed straight downward, both the excess air ratio and temperature inside a spray showed asymmetric distributions. Leaner and higher temperature mixture was observed in valve-side region. This can be resulted by promotion of evaporation due to stronger entrained gas flow, and this phenomenon can be caused by the asymmetric velocity distribution in the combustion chamber at TDC as represented in figure 4. In addition, auto-ignition was not confirmed under this surrounding gas conditions. Surrounding gas temperature was decreased at every crank angle due to increase of volume in expansion stroke. Figure 7 presents the excess air ratio (λ) and temperature (T) histories from fuel injection. They were calculated as the area-averaged λ and T of maximum x - y cross section in a spray. Both of the λ and T slightly increased with crank angle. This tendency is different from that previously introduced in figure 1 as theoretical analysis. This can be attributed to the decrease of entrained gas pressure and temperature at every crank angle in expansion stroke. Although temperature (T) exceeded the minimum ignition point of Ethanol around 0.5 degree in crank angle, at that timing excess air ratio (λ) showed the value greater than 1 defined as concentration factor for auto-ignition in figure 1.

In order to make clear the reason why auto-ignition was not occurred, we focused on instantaneous spatial λ and T distribution inside a spray from the viewpoint of temporal and spatial matching of auto-ignition suit mixture concentration and temperature.

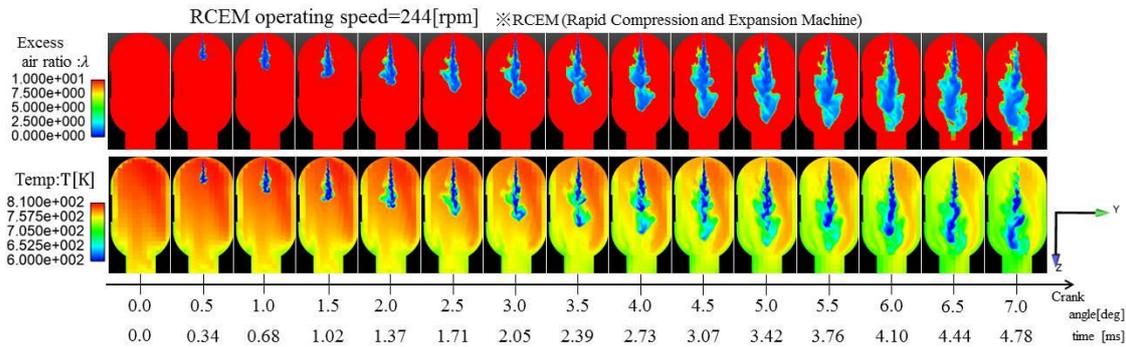


Figure 6. Prediction of the mixture formation process of an Ethanol spray in expansion stroke from TDC to ATDC 7.0 degree.

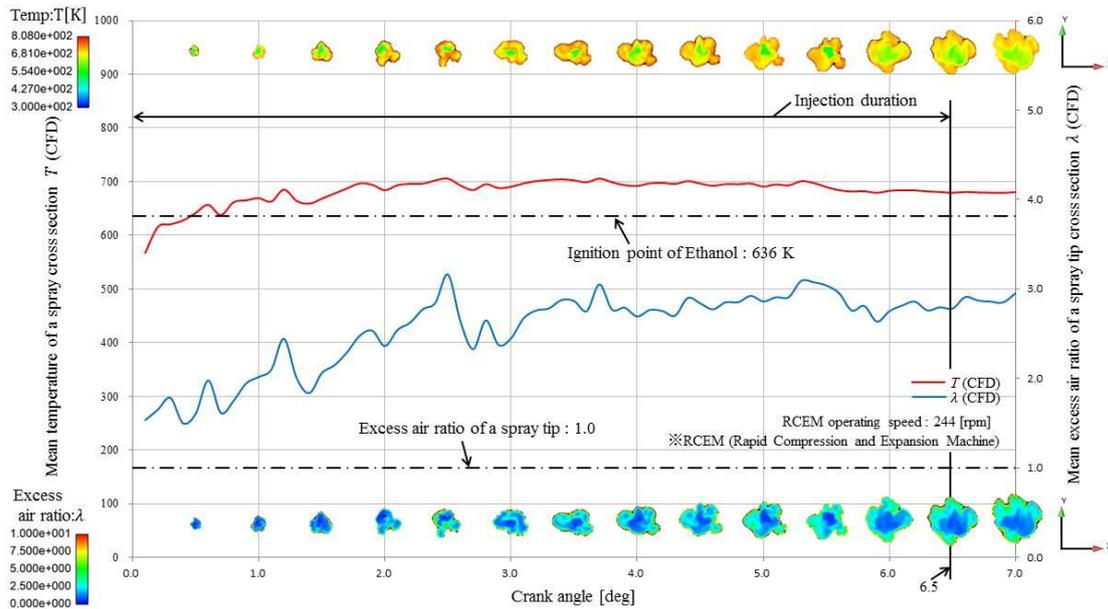


Figure 7. Numerically analyzed histories of mean excess air ration and temperature of an Ethanol spray cross section.

Figure 8 shows the local area of concentration and temperature factor attainment ($\lambda_{tip} = 1, T_{spm} \cong T_{ig}$) and their change with crank angle. Upper part of this figure indicates λ distribution of y-z and x-y cross sections. Local area of concentration factor attainment for auto-ignition is coloured blue. Lower part corresponds to T distribution and local area of temperature factor attainment is coloured orange. Lowest part is the overlapped image of λ and T distributions at each crank angle. It is clearly confirmed from this figure that no overlapped area of two colours is found. Therefore, auto-ignition seemed not to be obtained.

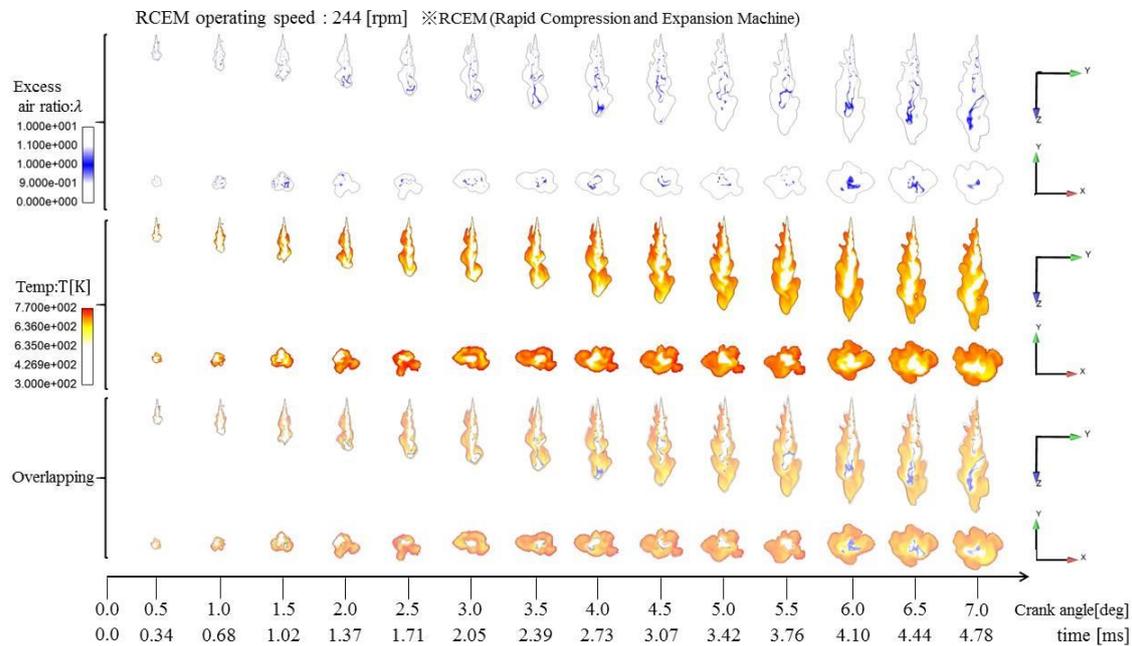


Figure 8. Temporal and spatial mismatch of auto-ignition suit concentration and temperature during the mixture formation process of an Ethanol spray.

5. Conclusions

1. Velocity distribution in combustion chamber at the end of compression stroke influences spray mixture formation process. Flow in the combustion chamber before fuel injection promote atomization and evaporation.
2. RCEM (Rapid Compression and Expansion Machine) has to be modified with negligible small pumping loss or supercharging device to realize target compression pressure and temperature (6.5MPa and 1000K).
3. As well as a spatial averaged discussion, in sort of local distributions of excess air ratio and temperature inside a spray, it is revealed that difficulty of simultaneous attainment of auto-ignition suit concentration and temperature during mixture formation process is the reason of poor auto-ignition quality of an Ethanol spray.
4. Decreasing of surrounding gas pressure and temperature with crank angle in expansion stroke prevents faster lean situation and faster temperature rising of an Ethanol spray, and based on this fact, we have to come up with new ideas to establish a new technology with stable auto-ignition in order to develop high performance alcohol engines.

Acknowledgments

The authors would like to express a special appreciation to the Japanese ministry of education, culture, sports, science and technology and Japan society for the promotion of science for their money support as grant-in-aid for scientific research.

References

- [1] Narita T 2016 Resource Energy Yearbook Editorial Committee 2016 *Resource energy yearbook*, ed Resource energy yearbook editorial committee (Japan: Tsusan data publication association Ltd.) pp 215-218
- [2] Wakuri Y, Fujii M, Amitani T and Tsuneya R 1960 Studies on the Phenomena of Fuel Spray of Diesel Engine. *Transactions of the JSME*. **25** 820-826
- [3] Saitoh H and Uchida K 2015 Surrounding Gas Pressure and Temperature Dependence of the Spray Auto-ignition Phenomenon for Ethanol-Diethyl Ether Blended Fuels. *Transaction of the TSME 2016*. **4** 79-86
- [4] Saitoh H, Tohjo Y and Uchida K 2016 Numerical Analysis on the Mixture Formation Process up to Auto-Ignition of an Ethanol Spray (AEC0025). *The 7th TSME Int. Conf. on Mechanical Engineering 13-16 Dec. 2016*