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Numerical Analysis on the Mixture Formation Process up to Auto-Ignition of an Ethanol Spray

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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 the promising candidate of alternative fuel. The objective of this study is to reveal the physical and chemical phenomena in the mixture formation process up to auto-ignition of an Ethanol spray. The authors has intensively investigated and reported this decade about the auto-ignition characteristics of a fuel spray for normal alcohol and Ethanol-Diethyl ether blended fuels. The quantitative evaluation of main factors that govern auto-ignition phenomenon that can be finally as the database in a form of 3D-mapping of ignition delay is now in progress. Through the series of our study, the reason of poor auto-ignition quality of alcohol sprays was theoretically and experimentally revealed. That is difficulty of simultaneous attainments of ignition-suitable concentration and temperature in a spray mixture formation. However, detailed spatial concentration and temperature distributions inside a spray and their temporal history from fuel injection are still at question. As the next step, therefore, we performed numerical analysis on the mixture formation process of an Ethanol spray in order to reveal the physical and chemical mechanisms of its auto-ignition phenomenon. One of the commercial CFD codes; CONVERGE was used in the computational calculation with the considerations of turbulence, atomization, evaporation and detailed chemical reaction. Spray mixture formation process of Ethanol and Gas oil were numerically analyzed and compared with each other. Results of numerical simulation showed that properties of Ethanol such as smaller stoichiometric air/fuel ratio and larger latent heat of evaporation induced faster lean situation and slower temperature rise in comparison with Gas oil as conventional diesel fuel. In addition, good agreement was obtained between numerical and experimental visualization results of mixture formation process up to auto-ignition.

Keywords: Ethanol Spray, Mixture Formation, Auto-Ignition, Numerical Analysis

1. Introduction

1.1 Background

Needless to say utilization of natural and renewable energy has been highlighted under the situation of global energy and environmental problems such as oil reserve depletion and climate change. Present social and industrial activities depend on the hydrocarbon combustion. As well as the automotive industry, large amount of petroleum is consumed in the various kinds of industries. Heavy duty oil is main fuel of burners that used for temperature control in green houses where many kinds of vegetables, fruits and flowers are growing and is also used for drying of agricultural and fishing products such as tea leaves and seaweed. Heat pump is better in efficiency to obtain such low level heat. Co-generation system with diesel engine and heat pump is one of the effective ways for saving energy resource. This study deals with the development of high performance diesel engines fueled by biomass-based alcohol. As well as the power unit of vehicles, diesel type high performance engines flexible for any kinds of bio-fuels including bio-Ethanol can be applied to agriculture and fishing industries as a small sized personal use electrical

power generation. That is one of the essential components for co-generation system previously introduced, and can be also applied to a large sized backup system for huge electrical power generation plants. Stable electric power supply can be also realized by the best combination with any other natural energy utilization such as solar, wind and biomass if the above proposed high performance alcohol diesel engine is developed. When renewable bio-fuel is their all power resources, sustainable community can be

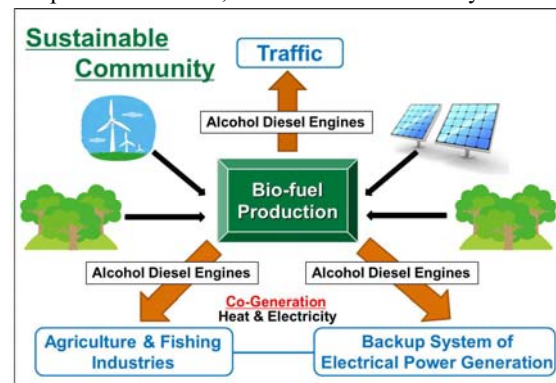


Fig.1 Conceptual figure of sustainable community with biomass energy utilization

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established as shown in Fig.1. Although electrical and thermal energy are required for bio-fuel production, such energy can be also supplied by alcohol diesels as well as solar and wind power. Therefore, success of this study induces the promotion of renewable biomass energy and a big contribution against the worldwide energy and environmental problems. Scale of the sustainable community depends on energy supply-demand relations. Therefore, the amount of feed-stock and productivity of bio-fuel have to be considered when the scale of sustainable community is decided. Although energy saving and economic growth is the trade-off relations each other, these compatibility can be possible with the development of biomass energy production and conversion technologies. This is the author's expected future image.

1.2 Objectives

The biggest challenge in the development of alcohol diesels is ignition control due to well-known its poor auto-ignition quality. Approaching way of ignition improvement is categorized by the two points of view. One is on the engine side measures as employing ignition-assist devices such as glow plug [1], spark plug [2] or heating surface [3] etc. The other is on the fuel side measures as adding of small amounts of ignition improver [4-6]. Almost all of those studies just concerned to seek the optimum configurations of ignition-assist devices and amount of additives within each examined engine and their performance. The authors [7-13] have intensively investigated and reported this decade on the effects of main factors such as fuel properties, surrounding gas pressure, temperature and Oxygen concentration on auto-ignition phenomenon of an Ethanol, Ethanol-Diethyl ether blend fuel spray, and are now in progress of drawing the map/data base that indicates how great is the influence on ignition delay for each governing parameter of auto-ignition. However, physical and chemical mechanisms of auto-ignition quality improvement is still at question. In order to develop the controlled auto-ignition technology, spray mixture formation process up to auto-ignition as physical and chemical phenomena has to be revealed. The objective of this study, therefore, is to make numerically clear Ethanol spray mixture formation process focusing on the spatial mixture concentration and temperature distributions and their temporal histories from fuel injection.

2. Theoretical Analysis

Figure 2 is a result of theoretical analysis on the spray mixture formation process for Gas oil and Ethanol [7]. This indicates the histories of mixture concentration and temperature from fuel injection, and they were evaluated, respectively, as excess air ratio of a spray tip (λ_{tip}) and mean temperature of a spray (T_{spm}). The value of (λ_{tip}) was calculated based on the spray momentum theory proposed by Wakuri et al. [14]. According to this theory reaching distance of a spray

and its excess air ratio are expressed as the function of time from fuel injection. Stable auto-ignition can be occurred if mean temperature of a spray is higher than fuels minimum ignition point ($T_{spm} > T_{ig}$) by the time when suitable mixture concentration condition ($\lambda_{tip} = 1$) is satisfied. Required heat that increases the temperature of the spray up to (T_{ig}) is expressed as follows:

$$Q = G_f [c_{fl}(T_b - T_o) + \gamma_f + c_{fg}(T_{ig} - T_b)] \quad (1)$$

First and third terms of equation (1) correspond to apparent heat in liquid and gas phase, respectively, and the second term means latent heat of evaporation. Variable (G_f) is mass of injected fuel that also is the function of time. Mean temperature (T_{spm}) was obtained from equation (2) as instantaneous heat balance assumed to be satisfied.

$$G_f [c_{fl}(T_b - T_o) + \gamma_f + c_{fg}(T_{spm} - T_b)] = G_a c_{ac}(T_c - T_{spm}) \quad (2)$$

It can be understood from Fig.2 that auto-ignition is dominated by mixture concentration for a gas oil spray because T_{spm} is higher than T_{ig} when mixture concentration is reached to $\lambda_{tip} = 1$. On the contrary for an Ethanol spray, T_{spm} does not reach to T_{ig} when $\lambda_{tip} = 1$, and leaner situation is easily expected by the time when $T_{spm} > T_{ig}$. This result of theoretical analysis allows us to make clear the reason of poor auto-ignition quality of alcohol spray. That is difficulty of simultaneous attainments of ignition-suitable concentration and temperature in a spray mixture formation. Fuel properties of alcohol fuels such as smaller stoichiometric air/fuel ratio (L_{th}) and larger latent heat of evaporation (γ) respectively induce faster lean situation and slower temperature rise in comparison with conventional diesel fuels.

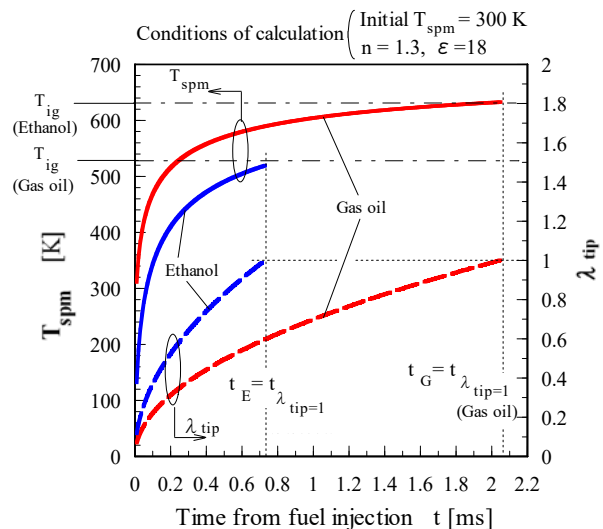


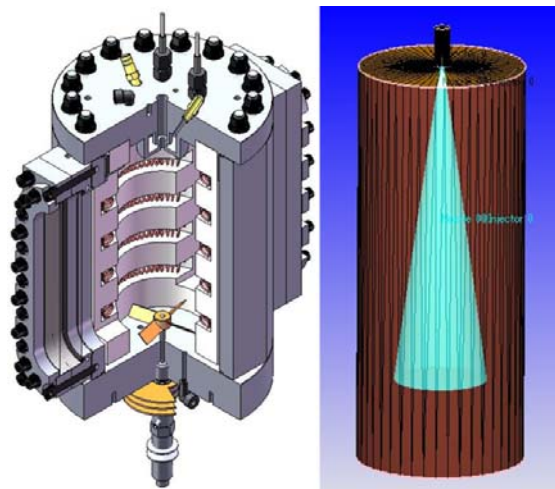
Fig.2 Estimations of λ_{tip} and T_{spm} histories for Ethanol and gas oil from fuel injection

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3. Numerical Analysis

3.1 Computational Domain and Mesh Geometry

Constant volume electrical heating chamber as shown in Fig. 3(a) was employed for the high-speed visualization of spray mixture formation up to auto-ignition in our previous research. Computational domain as shown in Fig. 3(b) is smaller than the volume of the combustion chamber to save simulation time. However, the size of computational domain was decided to be large enough to simulate the physical and chemical phenomena without the collision of a spray to the chamber wall. Table 1 represents the comparison of specifications between combustion chamber and computational domain. In order to compare with the results between experiment and numerical analysis, conditions of fuel injection were the same as those in the experiment. Table 2 shows the mesh geometry employed in the numerical analysis. Base grid size is 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 Fig.2 (light blue region) 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.



(a) Constant volume combustion chamber (b) Simple constant volume chamber model

Fig.3 Comparison between constant volume combustion chamber and computational domain

Table.1 Comparison of specification between combustion chamber and computational domain

	Constant volume chamber	Simple constant volume chamber model
Chamber Size ($\phi \times H$)	150 mm \times 420 mm	82.6 mm \times 200 mm
Volume	7250 cc	1072 cc
Injection Pressure	50 MPa	
Injection Duration	4.6 ms	
Nozzle Type ($\phi \times N$)	Hole Type (0.14 mm \times 1)	

Table.2 Specification of mesh

Base grid	x	4 mm	
	y	4 mm	
	z	4 mm	
FE (Fixed Embedding Fine Mesh)	Entity type	Cone: "INJECTOR"	
	Scale : Base grid $\times 2^{(-scale)}$	3: 4mm $\times 2^{-3}$ =0.5mm	
	Radius1	1 mm	
	Radius2	23 mm	
AMR (Adaptive Mesh Refinement)	Velocity	Max embedding Scale	6: 4mm $\times 2^{-6}$ =0.0625mm
		Sub-grid criterion	1.0 m/sec
	Temperature	Max embedding Scale	6: 4mm $\times 2^{-6}$ =0.0625mm
Sub-grid criterion		2.5 K	
Species	Max embedding Scale	5: 4mm $\times 2^{-5}$ =0.125mm	
	Sub-grid criterion	0.0001 mole fraction	

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.

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. Adiabatic condition was also applied as thermal boundary condition. Initial gas condition corresponded to the surrounding gas conditions of a fuel spray.

3.3 Physical and Chemical Models

Large eddy simulation (LES) was used as turbulence model. Kelvin-Helmholtz and Rayleigh-Taylor models represented as KH-LT model was employed for atomization and evaporation of fuel droplets. SAGE detailed chemical reaction model was also used in the case with the consideration of combustion after spray mixture formation.

3.4 Analysis Conditions

Table 3 shows the analysis conditions. Five kinds of simulations were performed for Gas oil and Ethanol sprays as listed in Table 3. Simulations that are indexed as No.1 – No.4 were compared with the experiment under the same surrounding gas pressure, temperature and Oxygen concentration conditions of 2.5 MPa, 800 K and 21 vol. % respectively. Ethanol spray mixture formation process was also calculated under the surrounding gas pressure and temperature

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conditions of 6.5 MPa and 1000 K which are the conditions that auto-ignition seems to be obtained. Fuel properties substituted in the calculation are listed in Table 4.

Table.3 Analysis Conditions

Index of calculation	No.1	No.2	No.3	No.4	No.5
Fuel	Gas Oil	Ethanol	Gas Oil	Ethanol	Ethanol
Surrounding Gas Temperature	800 K				1000 K
Surrounding Gas Pressure	2.5 MPa				6.5 MPa
Surrounding Gas O ₂ concentration	21% (vol.)				
Turbulence Model	LES Model				
Spray Model	KH-RT Model				
SAGE Detailed Chemical Reaction Model	off	off	on	on	on

KH: Kelvin-Helmholtz, RT: Rayleigh-Taylor

4. Results and Discussion

Figure 4 shows the comparison of mixture formation process between Gas oil and Ethanol sprays. Upper and lower parts of Fig.4 are results of calculation without chemical reaction indexed as No.1 and No.2 in Table 3. Spatial distributions of excess air ratio (λ) and temperature are indicated with time from fuel injection. Both results of Gas oil and Ethanol consist of 12 temporal frames. Faster leaner situation of Ethanol in comparison with Gas oil is confirmed

Table.4 Fuel Properties

Properties	Fuel notation	Ethanol	Gas oil
	Stoichiometric a/f ratio: L_{th}	[kg/kg]	9.01
Density: ρ_f	[kg/m ³]	785	825
Specific heat (liquid): c_{fl}	[kJ/(kg·K)]	2.723	2.372
Specific heat (gas): c_{fg}	[kJ/(kg·K)]	2.329	1.915
Boiling point: T_b	[K]	351.7	443~663
Heat of evaporation: γ_f	[kJ/kg]	854.8	187.2
Minimum ignition temp.: T_{ig}	[K]	636	530
Lower heating value: Hu	[MJ/kg]	26.8	44.4

※ Under Atmospheric Pressure Condition

from λ distribution results, and slower temperature rise of Ethanol is also observed in temperature distribution results. These seem to be attributed to smaller stoichiometric air-fuel ratio (L_{th}) and larger latent heat of evaporation (γ) of Ethanol represented in Table 4. In addition mixture formation region of Ethanol is larger than that of Gas oil due to the easier evaporation characteristic of Ethanol. This can promote to prevent from heat-up an Ethanol spray. At the numerical result for Gas oil as shown in the 7th frame from the left, mean temperature of a spray (T_{spm}) was higher than 700K that is much higher than Gas oil minimum ignition temperature (T_{ig}) represented in Table 4, and

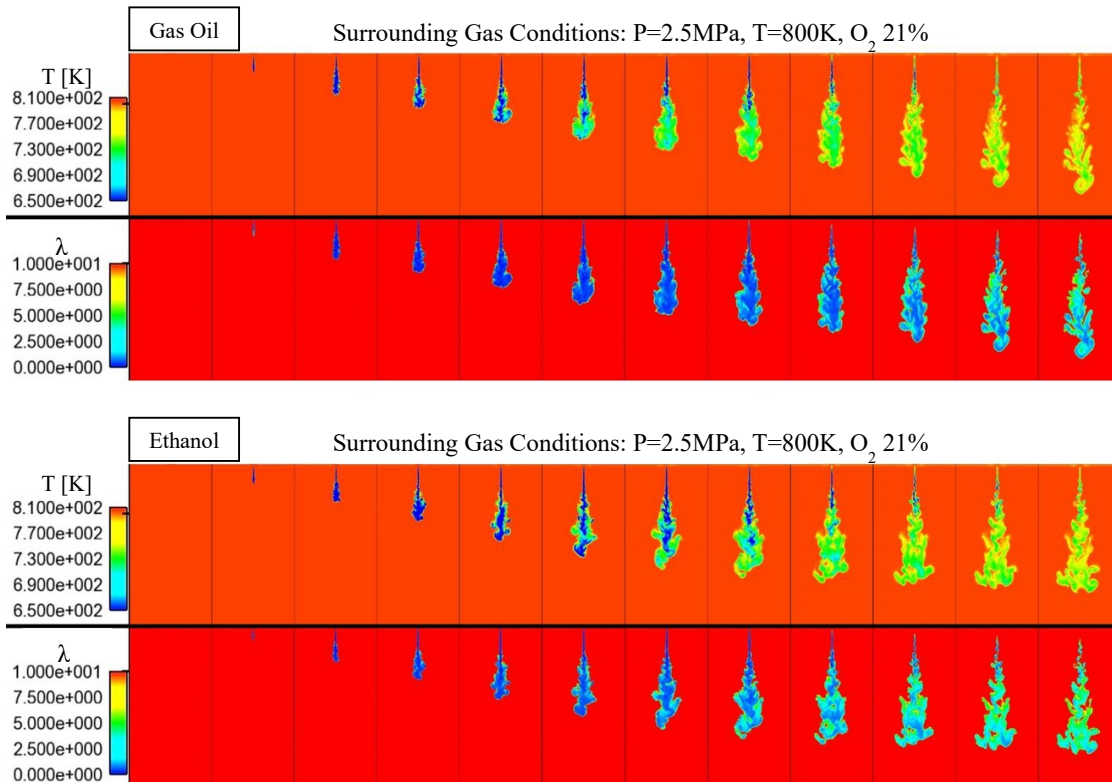


Fig.4 Comparison of mixture formation process between Gas oil and Ethanol sprays

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at the same timing, excess air ratio (λ) was smaller than 1, which corresponds to fuel rich mixture. Contrary for an Ethanol spray, mean temperature of a spray (T_{spm}) was lower than that of Gas oil at the same timing of 7th frame from the left and excess air ratio (λ) was clearly greater than that of Gas oil. Computational calculation resulted spatial and temporal mismatch of auto-ignition suit concentration and temperature in Ethanol spray mixture formation. This shows the same tendency obtained from theoretical analysis previously introduced in chapter 2.

Figure 5 presents the comparison of Gas oil spray mixture formation process between theoretical analysis

and numerical analysis. Temporal excess air ratio (λ) and temperature distributions of cross section (y-z plane) perpendicular to spray axis are also drawn in Fig.5. Numerically analyzed excess air ratio (λ) and temperature (T[K]) histories represented as “<CFD> λ /T[k]” were calculated as the area-averaged λ and T of maximum y-z cross section area in a spray. Numerical data of λ showed good agreement with theoretical analysis after 1ms from fuel injection. However, before 1ms from fuel injection, big difference of λ between <CFD> and <theory> was indicated. The value of <CFD> λ was much higher than that of <theory>. In the numerical analysis, liquid

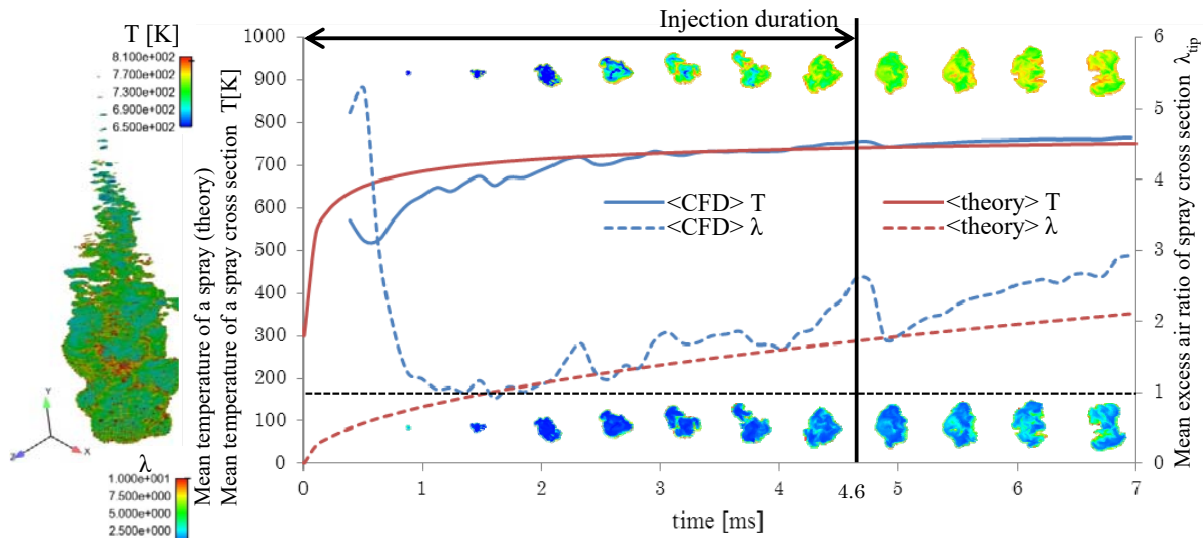


Fig.5 Verification of numerical analysis for a gas oil spray by comparison with theoretical prediction obtained from spray momentum theory (conditions of surrounding gas : $P=2.5\text{MPa}$, $T=800\text{K}$, O_2 21 %)

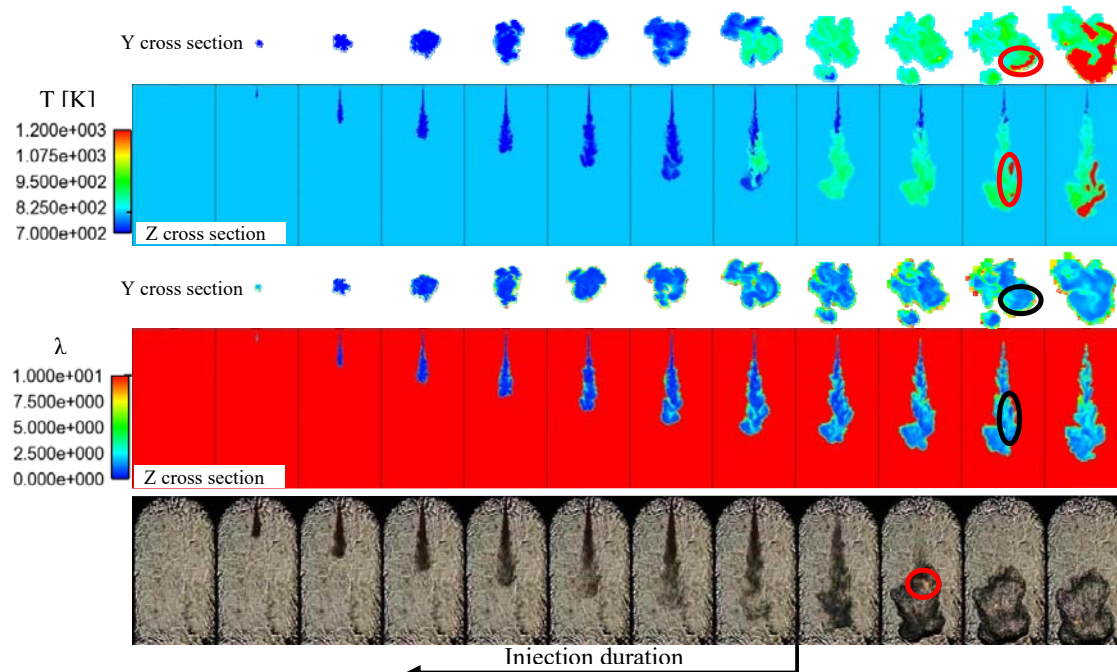


Fig.6 Verification of numerical analysis for a gas oil spray by comparison with experimental result (conditions of surrounding gas: $P=2.5\text{MPa}$, $T=800\text{K}$, O_2 21 %)

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phase fuel jet existed along the spray axis during 1ms from fuel injection. On the other hand, in the theoretical analysis, continuous two-phase flow was assumed with instantaneous evaporation of injected fuel. Therefore, numerical area-averaged λ seemed to indicate higher value compared with theoretical one, and drastic decrease of λ during 1ms can be attributed to the promotion of evaporation with fuel injection. Based on this recognition, spray mixture formation process seems to be correctly simulated as physical phenomena.

Results of numerical analysis for Gas oil with the consideration of chemical reaction (No.3) is presented in Fig. 6. Visualized images of Gas oil spray mixture formation up to auto-ignition are also shown in Fig. 6 in order to verify the results of numerical analysis. In “CONVERGE” the CFD software we employed is programed that calculation of chemical reaction is started when each cell temperature is higher than 600K or the mole-fraction of burnable component such as Hydro Carbon (HC) and Carbon mono-Oxide (CO) is reached to 1.0×10^{-8} . Judgement of auto-ignition depends on the operator’s definition. Mixture temperature as shown after 9th frame from the left is obviously higher than the surrounding gas temperature; therefore, we can understand that at least chemical reaction was promoted up to combustion.

Although several kinds of numerical definitions of auto-ignition has to be examined in order to precisely reveal the auto-ignition timing, we defined from Fig.6 that auto-ignition was occurred at the timing of 11th frame judged by radical local temperature increase within a spray, which is pointed by an ellipse in Fig.6. Value of excess air ratio (λ) and temperature (T[K]) at auto-ignition timing were around 1 and 1200K, respectively. On the other hand for experiment, auto-ignition was confirmed at the timing of 10th frame from the left. Although there is one frame difference corresponding to approximately 0.12ms difference of ignition timing, numerical result shows good agreement with experimental result. Based on this recognition, spray mixture formation up to auto-ignition and following combustion seem to be correctly simulated as physical and chemical phenomena.

Figure 7 shows the result of numerical analysis with the consideration of chemical reaction for an Ethanol spray under the surrounding gas pressure and temperature conditions of 6.5MPa and 1000K which corresponds to the gas conditions at the end of compression stroke of an actual diesel engine with its compression ratio of 22 and with pre-heating of intake gas up to around 70°C. History of λ showed greater increasing-gradient in comparison with Gas oil spray

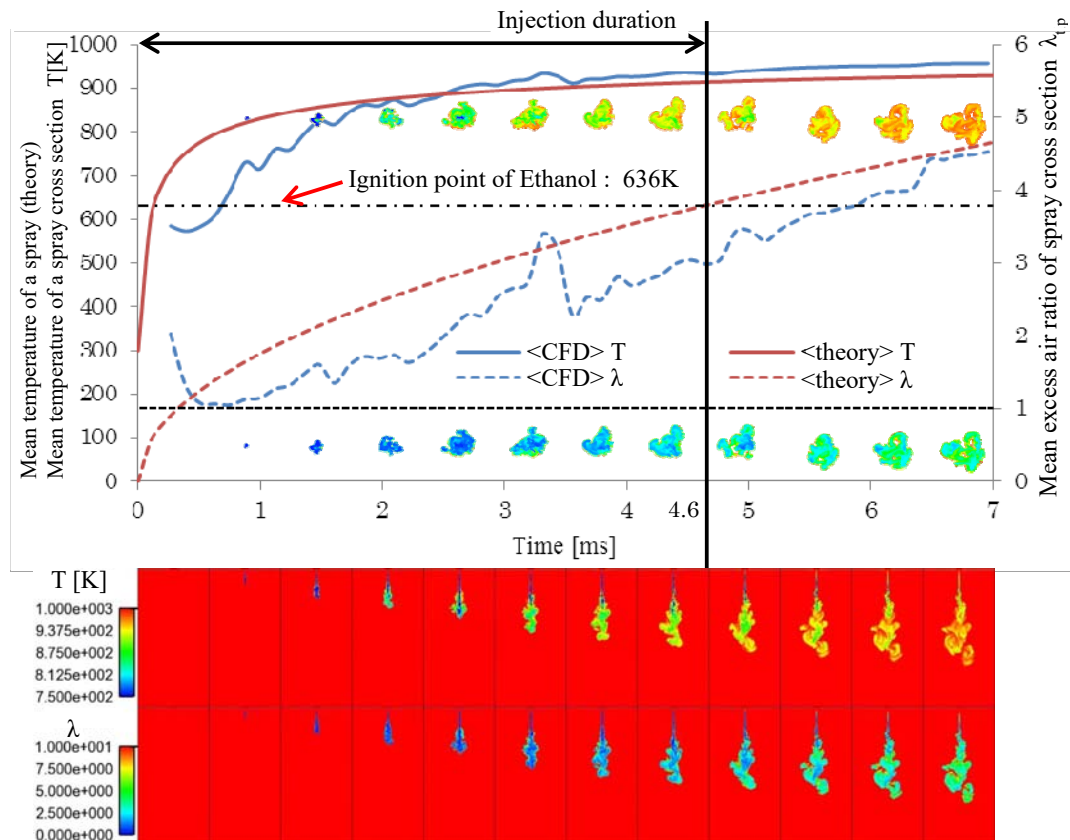


Fig.7 Verification of numerical analysis for an Ethanol spray by comparison with theoretical prediction obtained from spray momentum theory (conditions of surrounding gas: $P=6.5\text{MPa}$, $T=1000\text{K}$, O_2 21%)

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mixture formation due to higher density of entrained gas as well as smaller stoichiometric air-fuel ratio (L_{th}) of Ethanol. This stands for faster lean situation of an Ethanol spray. Focusing on the temperature history and its spatial distribution, we cannot find radical increase. Therefore, auto-ignition seems not to be occurred, although averaged cross section temperature of a spray showed higher value of the ignition point of Ethanol. Surrounding gas temperature of 1000K was insufficient for auto-ignition of an Ethanol spray. Higher surrounding gas pressure due to higher compression ratio yields higher and faster temperature rise, however, simultaneously it results faster lean situation in spray mixture formation process. In order to obtain stable auto-ignition of an Ethanol spray under feasible compression ratio, it should be paid an attention for the retardation of lean situation.

5. Conclusions

- In mixture formation process, excess air ratio and temperature distribution inside an Ethanol spray and their histories from fuel injection are completely different from those of Gas oil spray. In addition, shape of a spray is also different from each other.
- Spray can be recognized as two-phase flow after 1ms from fuel injection in sort of the prediction of averaged cross sectional excess air ratio.
- Under high pressure surrounding gas condition of 6.5MPa, 1000K is insufficient in surrounding gas temperature for stable auto-ignition of an Ethanol spray. Retardation of lean situation of mixture is effective and feasible way to develop controlled-ignition technology by fuel injection.

6. Acknowledgement

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.

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Nomenclature

c	: specific heat	[kJ/(kg·K)]
d_N	: diameter of spray nozzle	[mm]
G_a	: mass of the entrained air	[kg]
G_f	: mass of injected fuel	[kg]

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H_u	: lower heating value	[MJ/kg]
L_{th}	: stoichiometric air / fuel ratio	[kg _a /kg _f]
n	: polytropic exponent	[-]
Δp_{inj}	: effective pressure difference in fuel injection	[MPa]
Q	: required heat for auto-ignition	[kJ]
T	: temperature	[K]
t	: time from fuel injection	[msec]
V	: volume of a spray	[m ³]
X	: reaching distance of a spray tip	[m]
γ	: latent heat of evaporation	[kJ/kg]
θ	: 1/2 injection angle	[deg]
λ	: excess air ratio	[-]
ρ	: density of fuel	[kg/m ³]

Subscripts

a	: air
b	: boiling point
c	: compression
f	: fuel
fg	: fuel (gas phase)
fl	: fuel (liquid phase)
ig	: ignition
o	: initial value
tip	: spray tip