

## Numerical and Experimental Study of Reduction of NO<sub>x</sub> on Diesel Combustion by Using Water Injection Systems

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### Abstract

Introduction of water into the combustion chamber has been recognized as an effective measure reducing NO<sub>x</sub> emissions from medium-speed marine diesels. There are two practical methods of water injection into the cylinder, FWE (Fuel Water Emulsion) and DWI (Direct Water Injection). However, optimization of these water injection systems has not been established yet. In this study, to observe spray propagation and combustion process of fuel-water emulsion and DWI system, experiments were carried out using a Rapid Compression and Expansion Machine (RCEM) with an electronic controlled double-needle type injector. Simulation of spray propagation and combustion processes were also carried out using three-dimensional CFD code: KIVA3V in order to evaluate the effect of water vapour distribution on cylinder temperature and NO<sub>x</sub> formation. In the DWI system, numerous and immiscible droplet collisions should happen inside the merging sprays from closely-located injection holes for water and fuel. Authors had developed the new collision models for simulating the complicated colliding behaviour of these immiscible droplets and implemented into KIVA3V code. Concentric water-in-oil type droplet had to be newly introduced as an outcome of oil and water droplet coalescence. And different treatments in calculating its breakup and evaporation processes were considered. Concentric water-in-oil type droplets were injected as an emulsion fuel in case of emulsion system. It has been concluded that when the water was injected appropriately, the temperature of flame became lower than in conventional diesel combustion. NO<sub>x</sub> emissions were reduced up to 40% with water addition of 25% of fuel mass in both the water injection technologies. The computational results were in agreement with experimental measurements and provided detailed information on the mixing process.

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### 1. Introduction

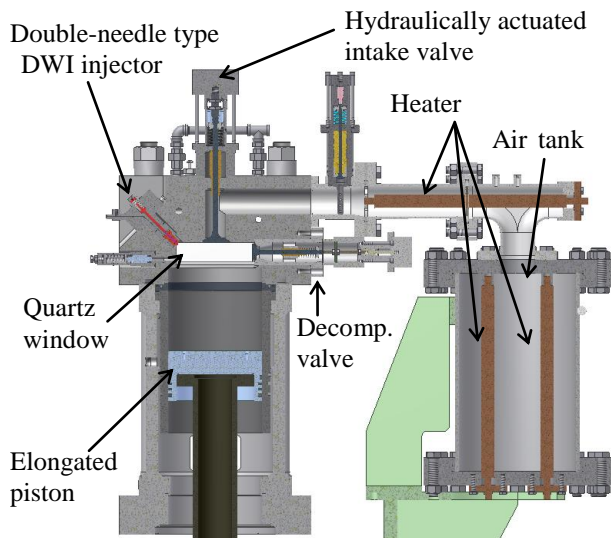
Large two stroke diesel engines have a high efficiency and it relates that shipping has low fuel oil consumption and low emission of greenhouse gasses compared to other transportation. However, they have demanded dramatically to reduce harmful regulated pollutants, which are Particulate Matter (PM) and Nitrogen Oxide. In particular, NO<sub>x</sub> regulations for marine engines will require NO<sub>x</sub> reduction as much as 80% from the level in the first Tier. Many engine designing companies and research organizations in maritime field are investigating the technologies realizing such the low-emission level. Emissions can be controlled either external reduction methods or internal methods. Various technologies such as Exhaust Gas Recirculation (EGR) [1] with a scrubber tank, Exhaust Gas Separation (EGS)[2] from MES Co., LTD and Selective Catalytic Reduction (SCR) [3] have been proposed as external reduction methods for marine diesel engines. Meanwhile, internal reduction methods focus on the combustion process and emission formation controlled by optimization of injection condition including injection pressure, timing and duration as well as technologies such as Water injection and charging gas condition of EGR. From above investigations, it is observed that mixing air with incombustible gases is effective to reduce NO<sub>x</sub> emission in the combustion process in the engine. The methods of mixing technology are proposed as water injection, EGR, Nitrogen Enrichment Humidification (NHM). However, mixing large amount of incombustible gases leads misfiring and SFOC penalty. And it is important to inject the water or incombustible gases into fuel-air mixture formation effectively for low NO<sub>x</sub> emission and fuel consumption. Some of authors have applied water injection into optical marine test engine [4],[5]. And it was reported that temperature of flame was decreased by optimized water injection timing and duration. FWE and DWI are practical methods of water injection into the cylinder; the former method is to replace the diesel fuel with diesel/water emulsions as an alternative fuel, and the latter is to inject the water directly into the combustion chamber separately from the fuel with two injectors or a single injector. However, optimization of these water injection systems has not been established yet and comparison between these two injection methods has also not been conducted.

The main objective of this paper is to observe the combustion of FWE and DWI using Rapid Compression Expansion Machine (RCEM) for optimization of these water injection methods and to reveal the difference of each case. Simulations of FWE and DWI combustion were also carried out using three-dimensional CFD code:KIVA3V modified for collision model.

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**2. Experimental apparatus and procedure**



**Table.1** Main specifications of RCEM

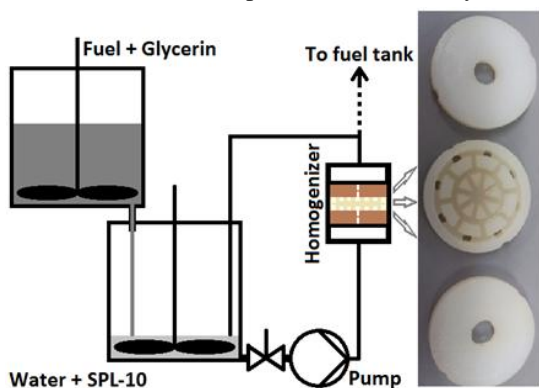
Bore × Stroke	φ240 mm × 260 mm
Clearance volume (upper, lower)	200 × 66 × 80 mm <sup>3</sup> φ240 mm × t5.4 mm
Compression ratio	9.08
Engine speed	320 rpm
Compression pressure	10MPa
Quartz window	200 × 50 × 100 mm <sup>3</sup>
Initial charging conditions	
Pressure	0.81 MPa
Temperature	353 K
Compression Pressure at TDC	10.0 MPa

**Figure 1** Schematic of RCEM

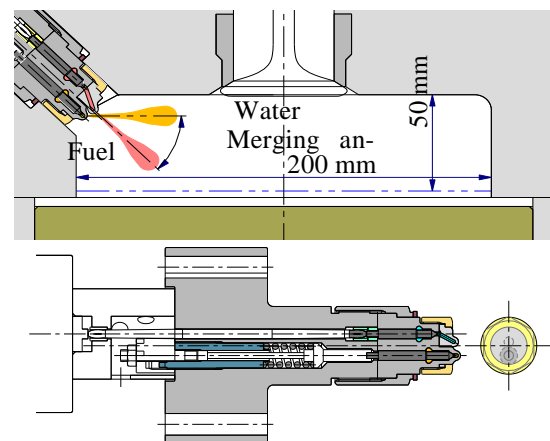
To observe the combustion process, a RCEM was used in this experiment. Table 1 shows the basic specifications of the RCEM. Figure 1 shows the schematic of RCEM. The RCEM has a bore of 240 mm and a stroke of 260 mm. Combustion chamber is cubic shaped volume consisted of 200 × 66 × 80 and it has three quartz windows on the walls for objective of visualization. Geometrical compression ratio of RCEM is 9.08. An air tank with heats is connected to the intake port of RCEM. The pressure and the temperature of the initial intake air can be controlled respectively in the air tank so that the clearance volume is large enough to observe the behavior of spray and combustion in the actual engine condition. Procedures of its one-shot firing are as follows. First it starts up motoring with its intake valve kept close, and then it actuates the valve only once synchronously with its piston motion immediately after the rating speed is reached, and finally the pre-compressed-heated charge flows into the cylinder, so as to simulate the intake and compression stroke of a real engine. After combustion, CO, CO<sub>2</sub>, O<sub>2</sub>, THC and NO<sub>x</sub> in the burned gas are measured by using exhaust gas analyzer (HORIBA:MEXA-7100). The combustion processes were taken by photographs directly using high speed camera (Photoron: Fastcam SA-4). Temperature distribution of DWI combustion was obtained from Photographs analyzed by Two Color Method (TCM). Spatial resolution of photographs is 832×224. In addition, frame rate is 20,000fps and exposure time is 5.8us.

**2.1 Injection system**

Mass of water injection was set to almost 25% of fuel injection mass cause of more water injection mass give rise to the SFOC penalty. Refined water and gas oil were used for water injection and fuel injection respectively. In FWE case, fuel is premixed with 0.1% Glycerin while the water is premixed with 0.9% RHEODOL SP-L 10; whereas percentages refer to the total emulsion volume. The chosen emulsifier guarantees reversible emulsions that can be mixed again after sedimentation of the water. As shown in Fig. 2, the fuel is slowly mixed to the water before a pump starts circulating the emulsion through a homogenizer, where the emulsion is forced with high pressure to narrow channels, leading to a sharp increase in flow velocity while the pressure declines below the saturation steam pressure, followed by an expansion.



**Figure 2** Formation of emulsion



**Figure 3** Schematic of DWI injection nozzle

Figure 3 shows illustration of DWI injector installed on the RCEM. This injector is a double needle type injector which can inject water and fuel closely to merge each other as shown in the figure. Injection rate, timing, duration can be controlled by a linear servo valve through hydraulic intensifier.

In each case, FEW and DWI case, increased amount of injection compared with fuel-only injection case was conducted by changing injection pressure or injection duration. In FEW case, water injection was conducted with two ways as shown in Fig.4; one is to inject with longer injection duration keeping same injection pressure as fuel case, and the other is to inject at higher injection pressure adjusting same injection duration as fuel case.

On the other hands, DWI injection settled injection pressure of water as almost a half of injection pressure of fuel as shown in Fig.5. Injection timing of water is same as it of fuel and duration is a half of fuel due to inject into a beginning of combustion for prevent a sharp rise temperature of cylinder causing formation of thermal NOx. Injection condition of each case is listed in Table 2. Injection duration of only fuel case of FWE was set shorter than case of DWI due to make a small injection amount to prevent fuel impinging on to the cylinder liner caused from expanded injection duration of FEW.

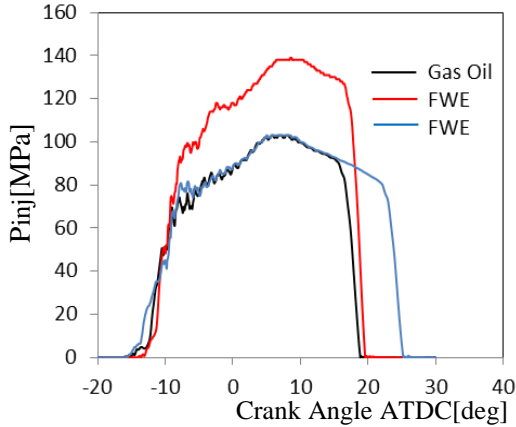


Figure 4 Injection rate in FEW case

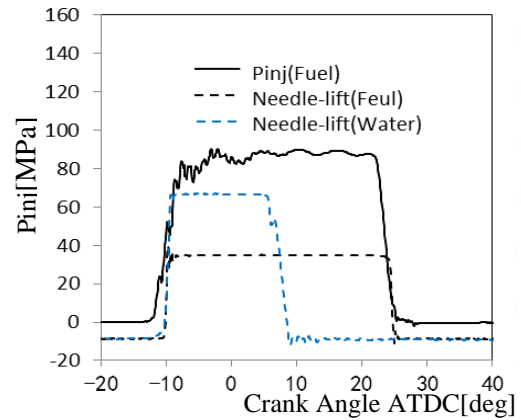


Figure 5 Injection rate and Needle-lift in DWI

Table 2 Injection condition

	FEW		DWI	
			Water	Fuel
Nozzle hole [mm]	0.23			
Injection pressure [MPa]	80	130	30	80
Merging Angle [degree]	0,5,10			
Injection timing [ATDC]	-10			
Injection duration [CA]	35	30	17.5	35
Distance between holes [mm]	7			

### 3. COMPUTAION METHOD

A combustion process in the water injection system was calculated by improving the spray sub models of the KIVA3v code. [6] The submodels used in this study are listed in Table 3.

#### Spray model

Figure 6 shows the model for water-in-fuel droplets which are treated as two layer concentric sphere; the outer layer is consisted of fuel while an inner zone is consisted of water. This model describes the droplets of FEW to be injected from nozzle hole and droplet in DWI case as an outcome of collision between fuel droplets and water droplets resulted from interaction of those spray. With this change in a treatment of droplet in each water injection system, spray model was improved as described in following part.

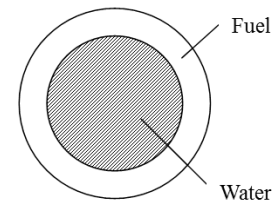


Figure 6 Model of FWE droplet

#### 3.1 breakup model

The Kelvin-Helmholtz(KH) and Rayleigh-Taylor (RT) breakup model was used to predict spray atomization. In FEW case and DWI case after collision of coalescence and reflexive separation, droplets are dealt with combined droplets between fuel and water shaped in the form of water-in-oil concentric droplet. Breakup model was also modified with a different application manner. The coalesced drop behaves as a fuel droplet in KH breakup mode because surface properties of the relevant droplet have dominant effects there, while it behaves as a water droplet because RT breakup supposedly requires large drop deformation. Consequently, droplets stripped by KH breakup were composed of only fuel.

The evaporation process of a concentric sphere starts fuel at the equilibrium temperature after the coalescence. The concentric sphere evaporates from its fuel surface assuming the water core keeps the same tempera-

ture, which means the concentric water-in-oil droplet evaporates as an oil droplet of an expanded surface area. After the fuel layer is completely vaporized, the droplet continues to evaporate as a pure water droplet. And in this paper phenomena like micro-explosion of the concentric droplet were not considered for the conclusion of the paper which explained micro-explosion would not have a drastic effect on sprays in an engine. [10]

### 3.2 Collision model

In DWI system, the collision model was modified to predict the collision outcome between fuel and water. In this simulation, O'Rourke model was used to predict the probability of collision. Collision outcome between fuel and water is categorized as four phenomena which are bounce, coalescence, stretching separation, reflexive separation. Those criteria are summarized by three non-dimensional parameters, those are, Weber number, impact parameter, droplet diameter ratio. Detail of equation dividing the outcome was suggested in the paper. [7]

### 3.3 Injection method of FWE

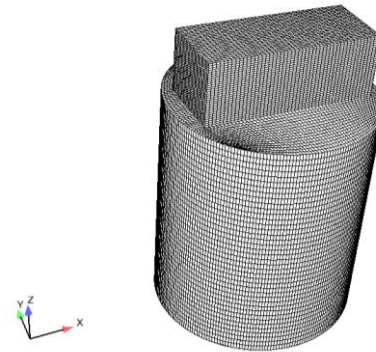
At the injection of FWE, droplets of FWE which formed two layers of fuel and water are injected, however, fuel droplets which do not contain water are also injected alternate with FEW droplets to represent the real condition of FEW fuel that not all droplets forms fuel-water merged condition.

### 3.4 Computational grid and calculation condition

Figure 7 shows a computational grid shaped in the form of RCEM and used in this study. The computational mesh is composed of approximately 260000 at BDC. The calculation is performed from -124 deg.ATDC to 50 deg.ATDC. Injection timing and duration and pressure are the same as experimental results.

**Table 3** Submodels adopted in KIVA3V

Phenomenon	Sub model
Primary breakup	Blob model
Secondary breakup	Modified KH-RT model
Collision and Coalescence	Model of O'Rourke (water, fuel) Immiscible drop model (water-fuel)
Evaporation	Model of Amsden (water, fuel) + Two-step evap of coaxial drops of water(inner) and fuel (outer)
Turbulence	RNG k- $\epsilon$ model
Ignition	Shell model
Combustion	CTC model



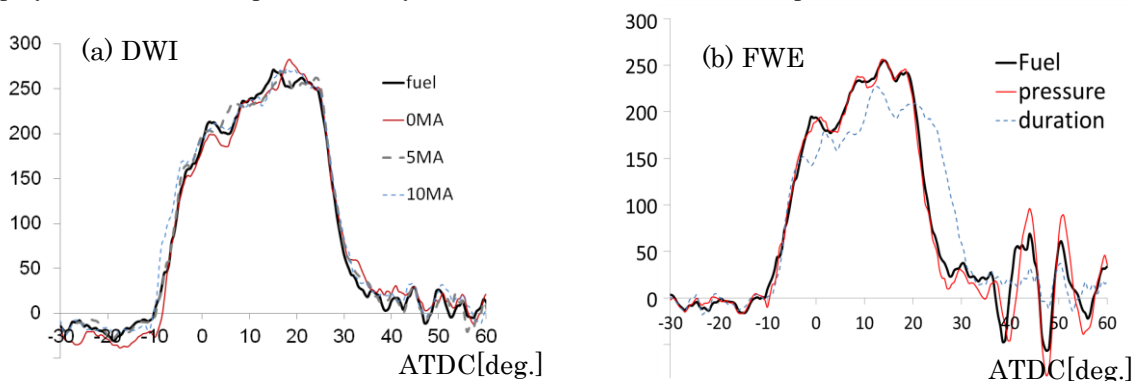
**Figure 7** Computational grid at BDC

## 4. Result and discussion

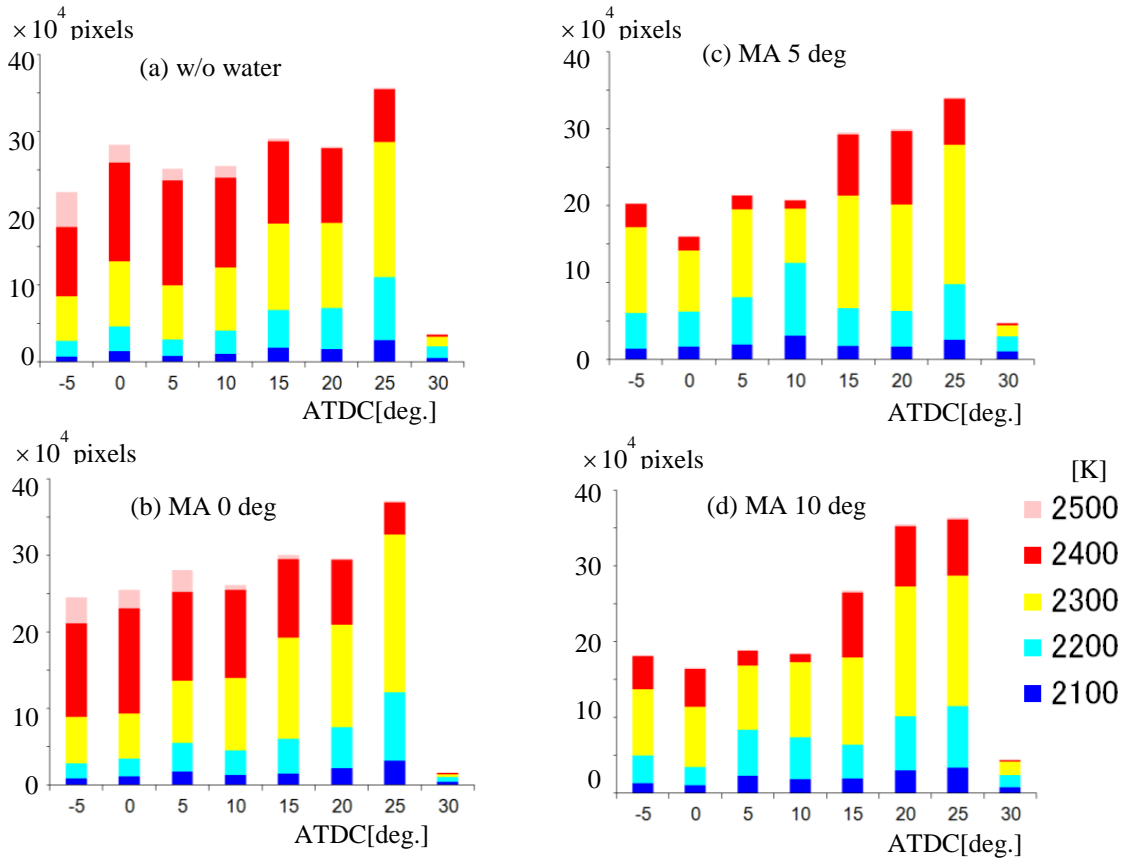
### 4.1 Experimental result

Figure 8 shows the comparison of apparent heat release rate of DWI case and FWE case. Changes of merging angle in DWI case and changes of injection pressure and duration in FWE are shown in each graph and "fuel" represents only fuel injection without water injection. As can be seen in the graph of DWI case, there is little difference among heat release rate of each case although water was injected. This result is the same trend as high pressure injection of FWE case. This means that 25% water injection mass could not lead to SFOC penalty in any case of this experiment. There is also little difference with ignition delay.

Figure 9 and 10 shows the histograms and images of flame temperature distribution of DWI obtained by two-color method at different water injection angle and without water injection in the same timing. As can be seen in these figures, high temperature distribution area was decrease clearly by injection of water. Especially, temperature dropped at lower portion of flame cause of the water spray exists there. In the water injection cases, the area of high temperature were reduced as MA was increased. However, flame area was spread Penetration of DWI spray was become longer and spread, because momentum of DWI spray was increased due to merge each spray. As a result, the vapor was widely distributed and area of flame was spread.

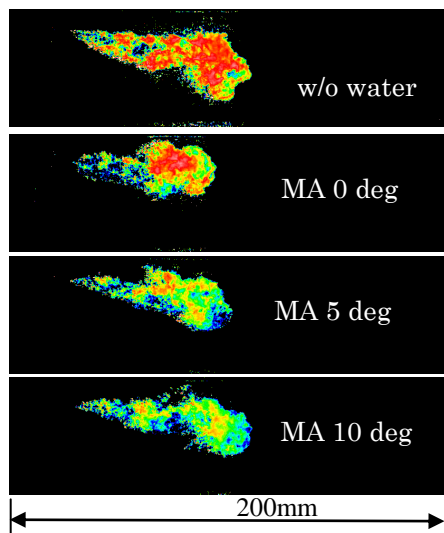


**Figure 8** Time history of Apparent Heat Release Rate(AHRR)



**Figure 9** Temperature distribution of the flame at each crank angle

Thermal NO<sub>x</sub> formation is highly temperature dependent and the formation rate is increased exponentially when the temperature is higher. Decrease of a portion of high temperature is more important than reduction of flame area. As can be seen from these figures, a portion of highest temperature in the case “w/o water injection” was largest of all at CA-5deg. However, after CA 15 deg. referring to termination of water injection, each temperature distributions of other cases were almost same although water vapor remains in the combustion chamber. This means water spray cooled the mixture formation by latent heat of evaporation and the lower temperature of mixture formation lead to lower temperature combustion. In cases of water injection, high temperature distribution was dramatically reduced between MA 0deg. and MA 5deg. This shows that the merging of spray is important in DWI spray. Because, MA 0deg denotes that water was injected parallel to fuel injection direction and MA 5deg denotes that water was injected into fuel spray with a slight angle. Therefore Interaction of spray was caused in DWI spray and influences behavior of the spray and combustion.



**Table 4** Rate of NO reduction at 3 merging angles in DWI

Setting	NO (with water) /NO (w/o water) %
MA 0 deg.	58.4
MA 5 deg.	57.9
MA10 deg.	51.8

**Table 5** Rate of NO reduction at 2 injection in FWE

Setting	NO /NO %
High Pres.	59.3
Long duration	57.4

**Figure 10** The Images of flame temperature obtained by TCM at -5 deg. ATDC in various merging angle

Table 4 shows NO reduction ratio calculated measured data of burned gas in the closed combustion chamber after one-shot firing. Reduction ratio was calculated from NO of water injection case divided by NO of only fuel case. To prevent the error of cycle by cycle, NO of only fuel case was measured after NO of water injection case each time. Assuming that MA 10 is effective of all cases from the temperature distribution in the Fig.10, MA 10 resulted in lowest NO reduction ratio calculated from measured data.

Figure 11 shows the histogram of flame temperature distribution in FEW case obtained by two-color method at different injection pressure and injection duration and without water injection case as comparison. As can be seen in these figures, high temperature distribution area was decrease clearly by injection of water like DWI case, and this can be seen in temperature distribution at 5 deg ATDC in Fig.12 and 13. Momentum of FWE spray should be increased due to additional water amount however penetration of FEW spray was not changed between with water and without water. The reason is that the flame formed by emit from soot was decreased due to soot decreased by emulsified fuel. And penetration cannot be detected.

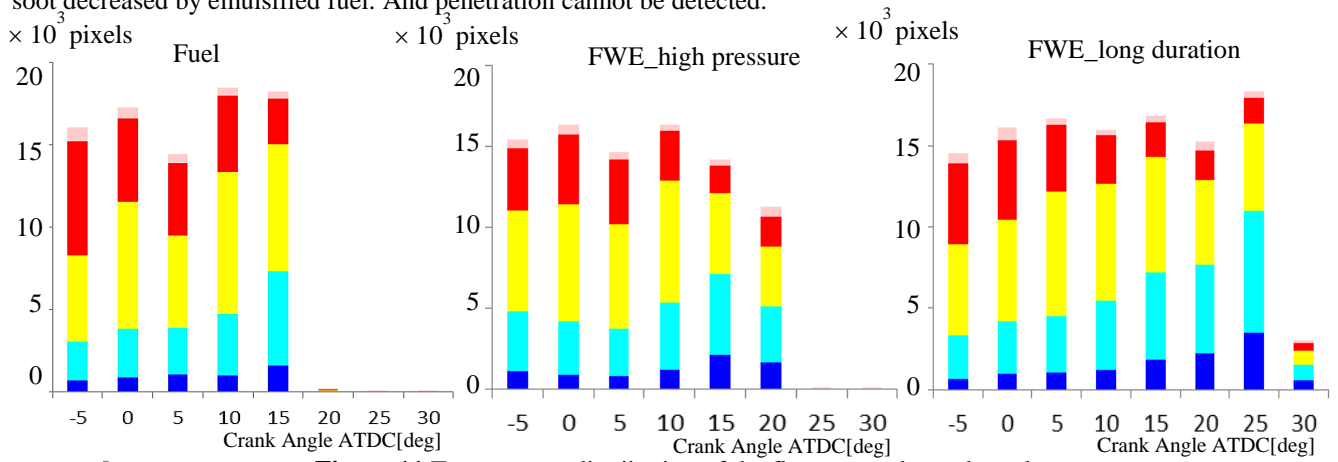


Figure 11 Temperature distribution of the flame at each crank angle

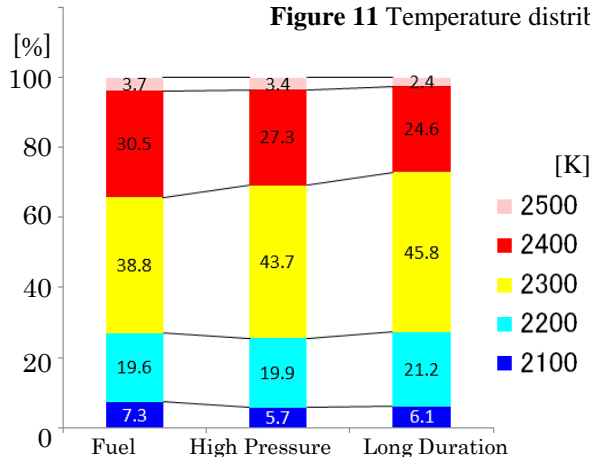


Figure 12 Temperature distribution at 5 deg ATDC

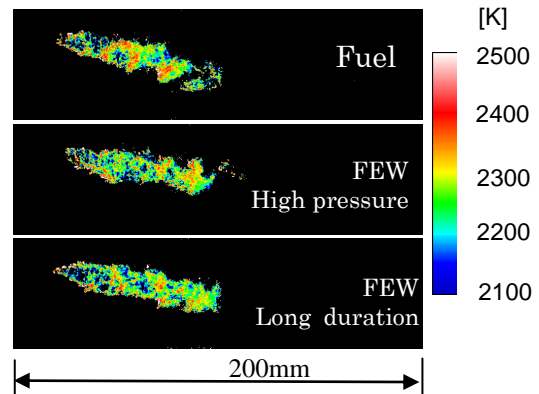


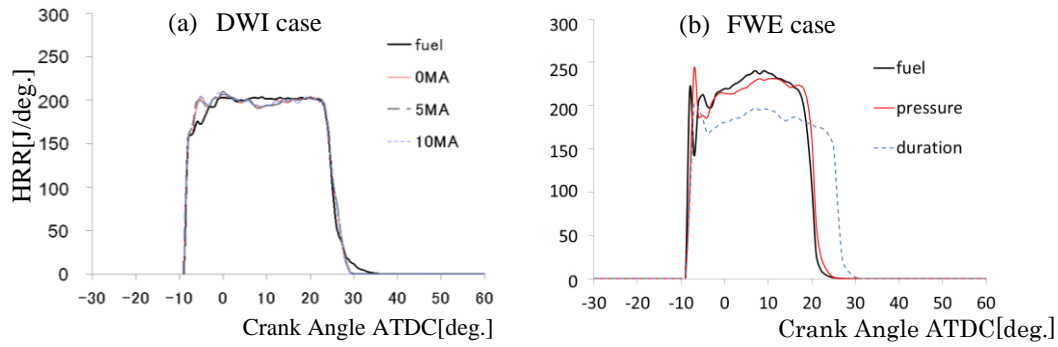
Figure 13 Temperature distribution image at 5deg ATDC

Table 5 shows NO reduction ratio calculated measured data. Assuming that case of long duration is effective of all cases from the temperature distribution in the Fig.14, but these cases were not changed in NO reduction ratio caused of longer combustion time. And in comparison between DWI and FEW, MA 10 resulted in lowest NO reduction ratio.

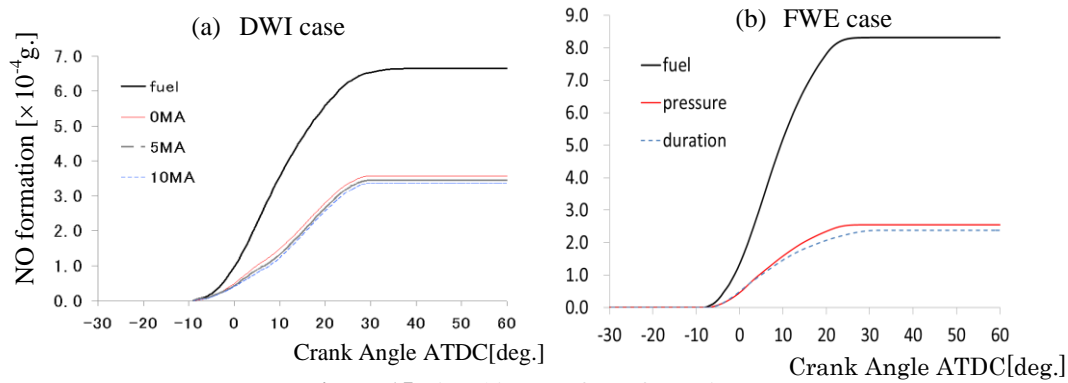
**4.2 Simulation result**

Figure 14 shows the history of Heater Release Rate obtained from simulation. As can be seen in DWI case, there is little difference among heat release rate of each case as well as experimental ones. And simulation of FWE case also has same trends as experimental results. Therefore, these simulations were reproduced well.

From comparison of them in DWI, peak of premixed combustion was a slightly higher with water injection and after-combustion was shortened. In FWE case, peak of ROHR of high pressure injection become higher than that of only fuel injection due to longer ignition delay from additional water vapor. In the case of long duration, the peak became lower than only fuel injection even longer ignition delay due to small amount of fuel vapor mass. Figure 15 shows a comparison of NO formation. In DWI case, differences of NO formation appear until CA 5 deg. among water injection cases. After that time, those differences are kept to the end. As a result, it was consider that there is a factor which gives the difference of each NO formation before CA 5deg in the DWI combustion process. In FEW case, the longer injection duration case has a low of NO formation rate during combustion process and it is resulted in a lowest NO formation even longer combustion time.

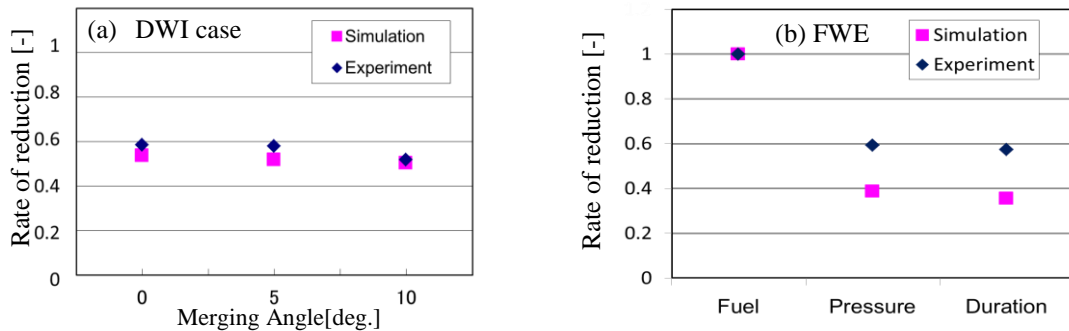


**Figure 14** Time history of Heat Release Rate(HRR)



**Figure 15** Time history of NO formation (DWI)

Figure 16 shows the comparison of a series of NO reduction ratio with water injection between experiment and simulation. Both trends of experiment and simulation are that rate of the NO reduction was decreased with increasing merging angle and NO formation was decreased with adding the water. However, the change for merging angle in the simulation was smaller than the change obtained by experiment. Because, the collision phenomenon become an important role to reproduce the interaction of DWI spray in the simulation. Model to predict collision outcome in the collision model was modified in this study, yet, model to predict the chance of droplet collision was used conventional O'Rourke model, which remains the problem of mesh dependency. The number of collision was less due to mesh dependency and the collision affected lightly behavior of spray involved propagation and combustion process. Therefore it is necessary to modify the collision model for interspray as like DWI spray. In case of FEW, Tendency of decreasing NO with water injection case can be seen in both experiment and simulation results, however, simulation over estimate the amount of NO reduction. The addition of water to the fuel as an emulsion results to high OH radical production cause that the water in emulsion remains longer in high temperature region of the flame compared with DWI case. And this may affects OH radical on NO formation reaction.[8] In this study, NO formation is calculation by Zeldovich mechanism.[9] However, this model does not take account of OH radical from water, which leads difference between experiment and simulation in FEW case.

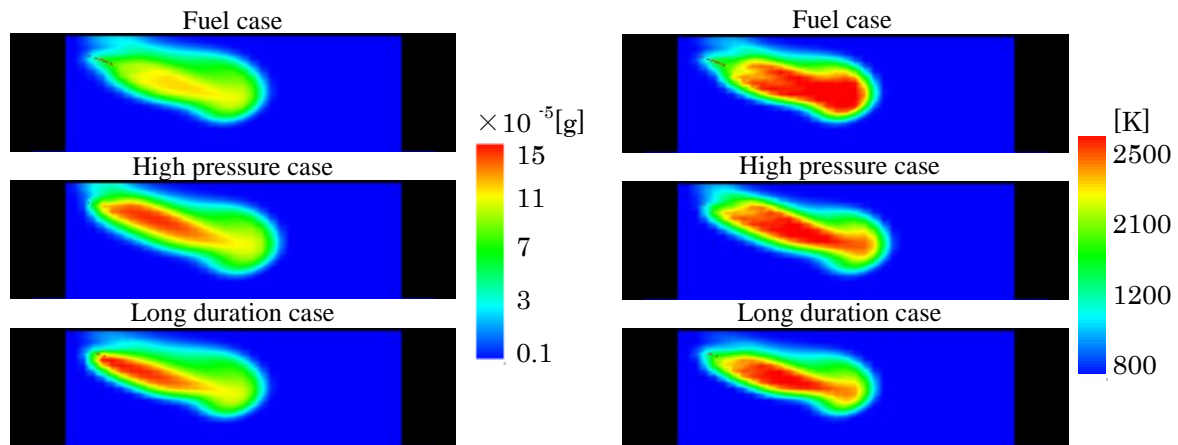


**Figure 16** Comparison of rate of NO reduction between Experiment and Simulation

Figure 17 shows simulation results of water distribution and temperature distribution in FWE case.

Increased water vapour region can be seen in both high pressure case and long duration case of FWE injection, and high pressure case shows wider spread compared with long duration case as a result of higher injection rate from high pressure. Long duration injection also has a longer penetration compared with only fuel case due to increasing density of droplets by containing water.

High temperature area in the fuel injection case cannot be seen in both FWE case especially at the spray tip.



**Figure 17** Water distribution and Temperature distribution in FWE case at 5 deg. ATDC

## 5. Conclusion

Two methods of water injection, FWE and DWI, were investigated in this study. For investigation of the effect of NO<sub>x</sub> formation by water supplying strategies, spray propagation and combustion process of FEW and DWI system with a double-needle type injector were observed in detail using a RCEM. In this experiment, injection direction of water spray was changed with three patterns in DWI and injection pressure and duration was changed in FWE. Simultaneously Simulation was carried out by using KIVA3V code. Conclusions of this study are follows

- Apparent heat release rate of each case has only little difference with same injection amount of fuel during same injection duration although water was injected
- From observing flame analyzed by the Two Color Method, high temperature distribution area was decrease clearly by injection of water in both FWE and DWI. Moreover, high temperature of flame in DWI case was reduced as Merging Angle was increased. In the cases of MA10, NO formation was most reduced of all cases.
- Numerical analysis can be reproduced trend of the DWI and FWE combustion processes by using the modified KIVA3V code about breakup and collision and evaporation processes. However, it could not reproduce the NO formation in FWE cause of the NO<sub>x</sub> model which does not take account of OH radical from water.
- High temperature area of flame was decreased especially at the spray tip by using FWE method.

## 6. REFERENCES

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## NOMENCLATURE

MA	: Marging Angle [degree]
CA	: Crank Angle [degree]
TDC	: Top Dead Center [degree]
ATDC	: After TDC[degree]
ROHR	: Rate of Heat Release