Spray Collision Modelling of Immiscible Droplets in Direct Water Injection

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Abstract

Droplet collision in a diesel spray has been studied through the observations of a binary collision system with two equivalent droplets of the same liquid. Moreover, conventional CFD (Computational Fluid Dynamics) codes only consider the coalescence and the stretching separation of two identical liquid droplets. DWI (Direct Water Injection) system recently introduced to reduce NOx emission from marine diesels, however, could have considerable collisions between the droplets of the different liquid, that is, between water droplets and fuel droplets since it has near co-axial nozzle layout and water is usually injected under much lower pressure than fuel. In this study, the criteria of the collision outcomes between immiscible droplets were newly derived theoretically and implemented into KIVA3 code. These criteria divided bounce, coalescence and reflexive or stretching separation regimes. The effective entrainment of water into fuel spray was numerically captured in the DWI system of the two-needle injector by introducing concentric fuel (inner) and water (outer) sphere after coalescence or reflexive separation. The predictions were partially confirmed through observation of the actual DWI spray in a constant volume bomb.

Introduction

Droplet collision in a diesel spray is an important phenomenon affecting spray propagation and droplet evaporation. Many researchers have been conducting numerous visual investigations on the dynamics of binary droplet collision and classifying the collision outcomes on a Weber number and an alignment index of the impact. In the spray modelling in CFD fields, probability of collision event is a main issue in the Arbitrary Lagrangian Eulerian coordinate system, which mediates between the finite volume cells fixed in a calculation domain and the droplets penetrating through them. Collision modelling for diesel spray has been dealing with "inner-spray" collision between the droplets of the same kind, and the collision event has been a sidebar issue as far as diesel sprays is concerned.

A few attempts, however, are introduced utilizing "inter-spray" collision to promote the drop breakup or to promote the entrainment of droplets of the different liquid from diesel fuel. DWI system introduced to reduce NOx emission from medium-speed marine diesels could have the considerable collisions between two separately injected sprays of water and fuel. Especially, a DWI system of two-needle type injectors is surely the case since it has near co-axial nozzle hole layout and it usually injects water under much lower pressure than its fuel injection pressure.

R. -H. Chen and C. -T. Chen [1] showed the collision between water and fuel droplets was totally different from the binary collision of identical droplets. This could explain why conventional CFD codes have not been very successful in simulating such DWI spray propagation. In view of this situation, the criteria of the collision outcomes between immiscible droplets have to be theoretically derived and objectively examined to simulate the DWI system.

Collision behavior and Outcomes of Binary Oil-Water Droplets

In general, outcomes of binary droplet collision are categorized by three non-dimensional parameters, that is, Weber number: We, impact parameter: χ, and drop size ratio: Δ. The impact parameter is defined as a dimensionless distance between the relative velocity vectors placed on the centres of two droplets. The average diameter of the two droplets is used for its normalization. Collision mode can be expressed from frontal collision at χ=0 to just grazing one at χ=1. In the case of immiscible droplet collision, We and Δ should be redefined as shown in Nomenclature.

The outcomes of droplet collision are categorized as bounce, coalescence, stretching separation, and reflexive separation as Qian et al [2] showed in Fig. 1 (a). According to Chen et al. [1], these categories are still valid in the outcomes of droplet collision between fuel and water droplets, but the criteria dividing these outcomes changes greatly such as I, II or III in Fig. 1 (b). For example, the criterion between coalescence and reflexive separation emerges at larger We and the coalescence region does not exist over We≈65 and so on. Most striking feature in the

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oil-water collision system is that merged droplets were observed to have concentric structure as a result of the coalescence and the reflexive separation. In these cases, diesel fuel spreads over the surface of water droplet and covers it completely and the consequent droplet will consist of water core and fuel shell. The reflexive separation, however, produces two smaller such concentric droplets after temporal droplet coalescence. In the stretching separation, the resulting droplets after separation are a pair of a pure fuel drop and a water drop of an extremely thin fuel layer.

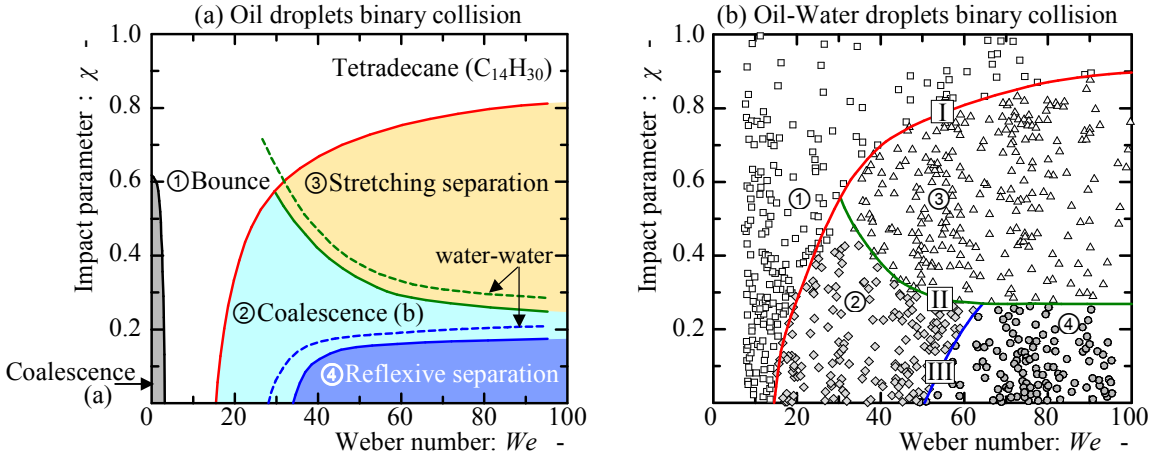

Figure 1. Criteria among collision outcomes on the experiments by Qian et al [2] (a) and Chen et al. [1] (b)

Modelling of Outcomes, Breakup and Evaporation after Oil-Water Droplet Collision

Modelling of the spray propagation in DWI system should predict the above-mentioned outcomes, momentum exchange, breakup behaviour, and evaporation process. Firstly, the former two were theoretically derived keeping the compatibility with the experimental results in Fig. 1(b), but the elicitation process has to be spared because of the limitation of space. Definitions and terminology could be referred in Nomenclature. It is worth mentioning that only criterion "II" is considered in O'Rourke collision model, which is standard in KIVA code, so that coalescence and stretching separation are the only outcomes that numerically happen, and neglect of bounce mode sometimes allows abnormal droplet growth around spray tip. Moreover, the difference between bounce and coalescence could be crucial in the case of oil-water collision since the latter generates aforementioned concentric droplets. In this study, however, further collisions between such a concentric sphere and an oil- or a water- droplet were not considered.

The criterion "I" determines the critical condition of the bounce outcome. An approach similar to TAB model was newly employed to predict the maximum deformation of an oil droplet, which was essentially given as a solution of its damped free oscillation after the impact. An oil droplet was always assumed to deform or stretch because of its smaller surface tension about one-third of water's. Critical Weber number was then obtained on the condition that the elongated axis of the oil droplet equals the semiperimeter of the paired water droplet, so that it can cover the water droplet thoroughly. The effect of a gas film between the two colliding droplets is not considered here.

$$We_{\mathrm{crit\_I}} = 2\frac{c_{\mathrm{C}}}{c_{\mathrm{F}}}\frac{1}{1-\chi^2}\left(\frac{\pi}{\Delta}-1\right)\left[1+\exp\left(\frac{c_{\mathrm{D}}\nu_{\mathrm{d}}\,\pi}{2r_{\mathrm{d}}^2\omega}\right)\right]^{-1} \quad \text{where,} \quad \omega=\sqrt{\frac{\sigma_{\mathrm{d}}}{\rho_{\mathrm{d}}\,r_{\mathrm{d}}^3}-\left(\frac{\mu_{\mathrm{d}}}{2\rho_{\mathrm{d}}\,r_{\mathrm{d}}^2}\right)^2} \qquad (1)$$

The criterion "II" determines the lower limit of the stretching separation, which happens in the range of Weber number above $We_{\mathrm{crit\_I}}(\Delta, \chi)$ and also in the range of large χ enough to make the collision more grazing rather than frontal. According to the Chen's experiments, stretching separation in DWI system should be characterised by a liquid column between two droplets, which extends from an oil droplet, bridges the water droplet temporally, and retracts into oil drop again leaving tiny satellite droplets. This criterion has been normally derived from the energy balance between initial kinetic energy of the droplets and total surface energies of the two spherical droplets and of the bridge column [3]. It is also the oil droplet that acts as an source of kinetic energy of stretching and the bridging. Assuming two-third of an oil droplet transforms to the bridging column and the interfacial surface tension between oil shell and water core can be calculated by Fowkes equation, a following equation for the critical Weber number was finally reached with interaction volume parameter ϕ_{d} and ϕ_{w} meaning how much volume of each droplet is truly effective in the relevant collision. The equation below stays within general expression although they should be con-

cretely classified into one by one according to the drop size ratio Δ and impact parameter χ. This criterion was set to be superior to the criterion III for the reflexive separation according to the aforementioned experimental results [1].

$$We_{\text{crit\_II}} = \frac{\frac{16}{3}\frac{\phi_{\text{d}} d_{\text{b}}}{h_{\text{b}}} + 3\left(\frac{h_{\text{b}}}{d_{\text{b}}}\right)^2 \frac{\left[\sigma_{\text{w}} - \left(\sigma_{\text{wd}} + \sigma_{\text{d}}\cos\theta\right)\right]}{\sigma_{\text{d}}}}{\rho_{\text{d}}\rho_{\text{w}}\left(\rho_{\text{w}} + \rho_{\text{d}}\Delta^3\right)^{-2}\left[\left(\Delta^3 + \frac{\rho_{\text{w}}}{\rho_{\text{d}}}\right) - \left(1-\chi^2\right)\left(\Delta^3\phi_{\text{w}} + \frac{\rho_w}{\rho_d}\phi_{\text{d}}\right)\right]} \tag{2}$$

The criterion "III" defines the minimum kinetic energy to develop the droplet coalescence into reflexive separation. This criterion has been most difficult one to formulate because of uncertainness in estimating the energy losses during deformation process that should result in re-breakup of the temporally coalesced drop. Ideas of Qian and Law [2] to identify such loses were basically continued to be used in this study. Unlike the above two criteria, however, it is a water droplet that decides whether the deformation reaches critical point or not since its water core is harder to breakup than its thin oil shell. After proper transformations setting water properties as major ones, the following equation was acquired. According to the experimental observation of Chen et al. [1] in the case of the head on collision of the fuel and water droplets, 0.275 and 0.465 was taken to be appropriate for $c_{\text{III\_1}}$ and $c_{\text{III\_2}}$ respectively.

$$We_{\text{crit\_III}} = \frac{\sqrt{\frac{\mu_{\text{w}}{}^2\sigma_{\text{w}}}{d_{\text{w}}\rho_{\text{w}}}}\left\{\frac{\alpha We_{\text{w}}{}^{5/2}}{4}\sqrt{\left(\frac{2}{\alpha We_{\text{w}}}+1\right)} + \frac{1}{6c_{\text{III\_1}}{}^{3/2}}\left(\frac{1}{c_{\text{III\_1}}{}^3}+4\right)\right\} + 4\sigma_w\left(4c_{\text{III\_1}}{}^2 + \frac{1}{c_{\text{III\_1}}} - 3\right)}{\frac{\sigma_{\text{d}}}{\Delta}\frac{\rho_{\text{w}}}{\rho_{\text{d}}}\left(\frac{\rho_{\text{d}}\Delta^3}{\rho_{\text{d}}\Delta^3+\rho_{\text{w}}}\right)\left(1-\chi^2\right)\left(1-3c_{\text{III\_2}}{}^2\right)} \tag{3}$$

where, $\alpha = \frac{1}{2We_{\text{w}}}\left\{4 - \pi \pm \sqrt{\pi^2 + \frac{1}{6}\left(We_{\text{w}}{}^3 - 64\right)}\right\}$

Fig. 2 shows the new three criteria on χ-*We* diagram. Their validity was examined in Fig. 2 (a) by comparison with the experimental results of Chen et al. Although some disagreement could be pointed out in the range of large impact parameter, where collisions seldom happen in the near coaxial DWI layout, the equations for the critical Weber numbers gave exact values on head-on collision case (χ=0) and kept proper prediction against χ as shown in the figure. Fig. 2(b) shows the effects of droplet size ratio Δ on the critical Weber numbers. The original definition of $\Delta = d_{\text{d}} / d_{\text{w}}$ is usable only in oil-water collision system. The effects were remarkable to say the least and different on each criterion. An oil droplet larger than a water droplet, for example, makes coalescence easier to happen and makes stretching separation harder, which is well within the expectation in oil-water collision system. It should be noted that the O'Rourke model does include Δ in its critical Weber number expression, but it does not show heavy

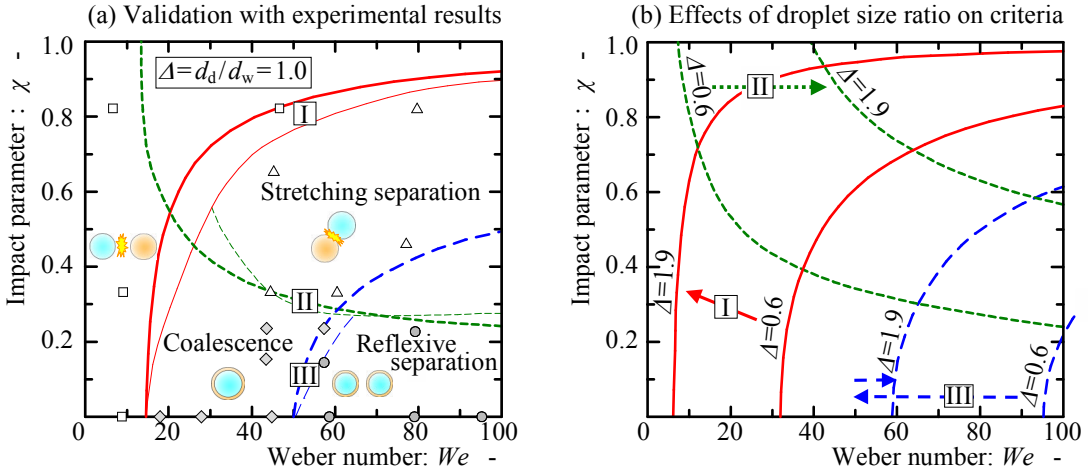

Figure 2. Theoretical criteria dividing outcomes of immiscible binary droplet collision in DWI system

dependency on Δ. All in all, the elicitation of critical Weber numbers in this study was successfully done and its implementation into CFD codes could have great influence over the simulation of the DWI spray propagation.

Next, the momentum (and the temperature) of the resulting droplets after the immiscible droplet collision should be identified in order to continue tracing their behaviour, which is essential to spray simulation.

In bounce mode there is no substantial difference from O'Rourke model considering two colliding droplets of the same liquid in calculating the after-collision momentum. Momentum values of both droplets are as follows.

$$\boldsymbol{u}_{\mathrm{col\_w}} = \frac{\left[m_{\mathrm{d}}\boldsymbol{u}_{\mathrm{d}} + m_{\mathrm{w}}\boldsymbol{u}_{\mathrm{w}} - m_{\mathrm{d}}\left(\boldsymbol{u}_{\mathrm{d}} - \boldsymbol{u}_{\mathrm{w}}\right)\right]\left(\chi - \chi_{\mathrm{crit}}\right)}{\left(m_{\mathrm{d}} + m_{\mathrm{w}}\right)\left(1 - \chi_{\mathrm{crit}}\right)}, \quad \boldsymbol{u}_{\mathrm{col\_d}} = \frac{\left[m_{\mathrm{d}}\boldsymbol{u}_{\mathrm{d}} + m_{\mathrm{w}}\boldsymbol{u}_{\mathrm{w}} + m_{\mathrm{w}}\left(\boldsymbol{u}_{\mathrm{d}} - \boldsymbol{u}_{\mathrm{w}}\right)\right]\left(\chi - \chi_{\mathrm{crit}}\right)}{\left(m_{\mathrm{d}} + m_{\mathrm{w}}\right)\left(1 - \chi_{\mathrm{crit}}\right)} \tag{4}$$

In stretching separation both momentum of oil and water droplets would remain unchanged considering that the growth and the break of the oil-bridge acts only internally in the colliding system and the rotation of the temporally bridged droplets induced by grazing contact could be negligible in the case of the DWI spray configuration.

In coalescence mode the properties of a coalesced droplet could be simply calculated thorough weighed mean.

$$\boldsymbol{u}_{\mathrm{col}} = \frac{m_{\mathrm{d}}\boldsymbol{u}_{\mathrm{d}} + m_{\mathrm{w}}\boldsymbol{u}_{\mathrm{w}}}{m_{\mathrm{d}} + m_{\mathrm{w}}}, \quad T_{\mathrm{col}} = \frac{m_{\mathrm{d}}C_{\mathrm{d}}T_{\mathrm{d}} + m_{\mathrm{w}}C_{\mathrm{w}}T_{\mathrm{w}}}{m_{\mathrm{d}}C_{\mathrm{d}} + m_{\mathrm{w}}C_{\mathrm{w}}} \tag{5}$$

In reflexive separation the energy dissipation should be considered in course of re-breakup of a temporally coalesced drop. It may be noteworthy that two identical concentric droplets generate in the present collision model, but they acquire different velocities to each other to reflect the initial momentum difference of oil and water droplets. Dissipation factor φ was set to 0.5 according to the theoretical analysis of Jiang et al [4]. The results are as follows.

$$\boldsymbol{u}_{\mathrm{temp}} = \frac{m_{\mathrm{d}}\left(\boldsymbol{u}_{\mathrm{d0}} - \boldsymbol{u}_{\mathrm{d}}\right) + m_{\mathrm{w}}\left(\boldsymbol{u}_{\mathrm{w0}} - \boldsymbol{u}_{\mathrm{w}}\right)}{m_{\mathrm{d}} + m_{\mathrm{w}}}, \quad \boldsymbol{u}_{\mathrm{col\_1}} = \boldsymbol{u}_{\mathrm{temp}} + \varphi\,\boldsymbol{u}_{\mathrm{d}}, \quad \boldsymbol{u}_{\mathrm{col\_2}} = \boldsymbol{u}_{\mathrm{temp}} + \varphi\,\boldsymbol{u}_{\mathrm{w}} \tag{6}$$

Finally, the breakup and the evaporation process in DWI system can be discussed. Naturally it is the coalesced water-in-oil concentric droplet again that matters in these processes. As for breakup, a hybrid model of KT (Kelvin-Helmholtz) breakup model and RT (Rayleigh-Taylor) break up model, which is a popular secondary breakup model in marine diesel simulations, was continuously adopted to the coalesced droplet with different application manner. The coalesced drop behaves as an oil 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 deformation of the drop. The effects of droplet size ratio were disregarded in breakup calculation.

The evaporation process of the concentric spheres starts at the equilibrium temperature (5) immediately reached after coalescence. A concentric sphere evaporates from its fuel surface assuming the water core keeps the same temperature, which means the concentric water–in-oil droplet evaporates as an oil droplet of an expanded surface area and phenomena like micro-explosion of the coalesced droplet was not considered in this study. After the fuel layer is completely vaporized, the droplet continues to evaporate (and also to breakup) as a pure water droplet.

Results and Discussion

The sub-models used in the computation by KIVA3V code are summarized in Table 1. The inner-spray phenomena such as collision, breakup and evaporation of each liquid coexisted with the oil-water spray interaction, and were handled in a conventional way. The model constants are defined individually for fuel and water so as to fit the spray tip penetrations of a single spray of fuel and water observed in a VCC (visual combustion chamber). For comparison, the simulation of fuel-water interacting spray was conducted with and without the present collision model. In case of the conventional collision, the outcome from the collision between fuel and water droplets was assumed to result in the bounce mode. In the DWI, spray formation is thought to be asymmetric because two inclined sprays are interacting. Therefore, a rectangular solid having 200 mm in height, 50 mm in width and in depth was chosen for a computational domain. In order to reduce the grid dependency in the region where two sprays interact, refinement

Table 1. Sub-models used in computation

Phenomenon	Sub-model	Phenomenon	Sub-model
Primary breakup	Blob method	Turbulence	standard k-ε model
Secondary breakup	KH-RT model	Ignition	Shell model
Collision	model of O'Rourke (water, fuel)	Combustion	LaTCT model (Magnussen model)
	theoretical collision criteria (water-fuel)	NO generation	Extended Zeldovich mechanism
Evaporation	model of Amsden (water, fuel), two-step evaporation for concentric drops		

was provided in the centre region where the injectors were located and also in the upper 65 mm region of the domain, resulting in some 110,000 cells. Up to 15,000 of parcels was provided to express both fuel and water sprays.

Fig. 3 (a) shows the shadowgraph images of a single fuel- or water- spray and a fuel-water interacting spray under 2.5 MPa of closed ambient nitrogen at 300 K and 750 K. Both two injectors had a single nozzle hole of 0.23 mm in diameter. The distance between the two holes was set to 6 mm and the angle between the centre lines of these holes was set to 5°. Water was injected at pressure of 28 MPa whereas diesel fuel was injected at 80 MPa. Measured spray tip penetrations are shown in Fig. 3 (b) with prediction results. (Hereafter the fuel-water interacting spray is abbreviated as "DWI". Time after start of injection will be denoted as 'ASOI'.) DWI spray penetration was more straightforward than the other and also the longest of all, which implies the spray interacting hardly changes spray shape and the total spray momentum determines spray propagation, so that slower water droplets can help it. When compared with the 300 K case, spray penetrations in 750 K case clearly increased by approximately 30 % both in fuel and water spray whereas some 11 % increase in the DWI spray. Leaner ambient gas density and much enhanced droplet evaporation are surely the reason, and yet denser spray body in the DWI case weakened evaporation effect.

As can be seen in the Fig. 3 (b), the effect of the collision model was rather sidebar since the spray penetration with the oil-water collision model showed reasonable but slightly shorter penetration than the conventional model. This can be explained by the consideration of the kinetic energy consumption in the droplet deforming process, and also the conventional collision model would do at least to predict the DWI spray penetration. Just after the breakup length, however, unreasonable deceleration was observed in the present collision model. Consumption of kinetic energy may be too much in the very beginning of secondary breakup process at present calculation.

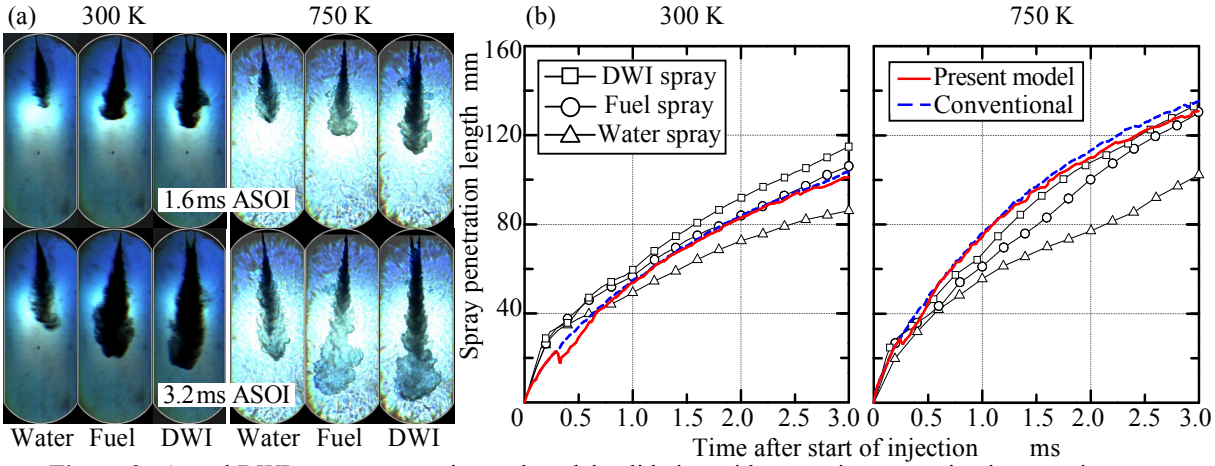

Figure 3. Actual DWI spray propagation and model validation with spray tip penetration in pure nitrogen

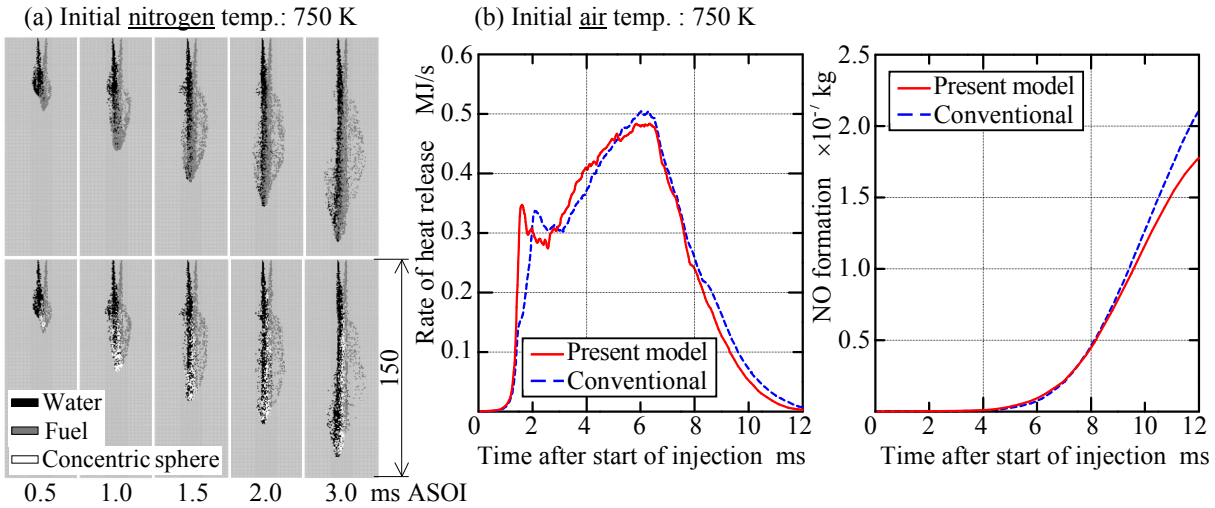

Figure 4. Predicted DWI spray propagation and collision model effects on combustion process

Fig.4 (a) shows the comparison of the simulation results of DWI liquid spray trajectory with or without the consideration of fuel-water droplet collision at ambient temperature of 750 K. In the figure, each droplet is depicted as grey dot for fuel, black dot for water, and white dot for coalesced concentric-sphere. It was proved that more than 60 % of near ten thousand collision events by 3 ms ASOI resulted in bounce mode and coalescence (14 %) and reflexive separation (7 %) were not major outcomes even in the fuel-water collision model. And yet their existence was clear right after the contact of fuel and water sprays, and penetrated down to the spray tip along the boundary face of fuel-water sprays. It can be said as remarkable that the concentric spheres of the extended fuel surface promoted fuel vaporization so that liquid water droplets became dominant around the spray head as the DWI spray propagated, which implies the concentric spheres tuned back to pure water droplets and more fuel vapour accumulated before ignition. In contrast, the conventional collision model left more fuel droplets and less water droplets.

Fig. 4 (b) shows the simulation results of the combustion process using the same conditions except for changing the in-chamber gas from nitrogen to air. The effects of fuel-water collision model on the history of in-cylinder rate of heat release (ROHR) and NO generation were distinctly displayed in the figure. As referred above, the promoted fuel evaporation by the present model gave sharper premixed combustion peak in RHOR than the conventional collision model, and at the same time it gave more controlled combustion thanks to the reserved water droplets. The latter effect helped realizing lower ROHR peak and fewer NO generation by as much as 10 % reduction. Of course, these results just mean the collision model between the immiscible droplets is something valiant to consider and do not secure the validity of the model. To improve the DWI system by CFD simulation, more experiments especially in actual engines and more refinements on the model are clearly needed.

Conclusions

Theoretical collision model for the inter-spray collision between fuel oil and water droplets was implemented in KIVA3V code to predict the spray behaviour in direct water injection (DWI) system. Conclusions were as follows.

- New collision model between immiscible oil and water droplets was introduced. Collision outcomes were divided into full four cases, and effects of drop size ratio and momentum distribution were taken into account.
- Concentric water-in-oil type droplet had to be newly introduced as an outcome of oil and water droplet coalescence. Different treatments in calculating its breakup and evaporation processes were necessary.
- The new collision model gave more enhanced fuel evaporation through the production of the concentric droplets and made more water droplets remaining around the spray tip. This would affect the subsequent ignition and combustion processes greatly, so that NO formation process in DWI system should be discussed carefully.

Nomenclature

Variables				Subscripts	
symbol	meaning	symbol	meaning	symbol	meaning
c	model constant	χ	impact parameter = $X/(r_d+r_w)$	0	initial properties
C	specific heat	Δ	drop size ratio: $r_d/r_w = d_d/d_w$	1, 2	id for reflex. separation
d	diameter	ϕ	interaction volume parameter	b	bridge in stretching separation
E	energy	φ	energy dissipation factor		
h	height	μ	kinetic viscosity	d	diesel fuel : oil
m	mass	θ	impact angle = $\cos^{-1}(1-\chi^2)^{0.5}$	w	water
r	radius	ρ	density	C	conservation force term
$\boldsymbol{u}$	velocity	σ	surface tension	F	external force term
We	Weber number in DWI = $(\rho_d d_d \boldsymbol{u}_{rel}^2)/\sigma_d$	ω	angular velocity	D	damping force term
				crit	critical property
We_w	Weber number @ water base = $(\rho_w d_w \boldsymbol{u}_w^2)/\sigma_w$			rel	relative component
				temp	temporal component
X	impact offset distance			col	collision result

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