

## INVESTIGATION OF EFFECT OF NOZZLE GEOMETRY ON SPRAY WITH A 3-D EULERIAN-LAGRANGIAN SPRAY MODEL COUPLED WITH THE NOZZLE CAVITATING FLOW

by

**Genmiao GUO<sup>a</sup>, Zhixia HE<sup>b\*</sup>, Qian WANG<sup>a</sup>,  
Zhaochen JIANG<sup>a</sup>, and Liang ZHANG<sup>a</sup>**

<sup>a</sup>School of Energy and Power Engineering, Jiangsu University, China

<sup>b</sup>Institute for Energy Research, Jiangsu University, China

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*A 3-D Eulerian-Lagrangian spray model coupled with the nozzle cavitating flow was proposed to simulate the atomization and secondary break-up. The nozzle flow and near-field spray were simulated with the volume of fluid multiphase model. At a certain downstream location, where the spray is diluted, the Eulerian spray approach was switched to the conventional Lagrangian approach. This entire methodology was validated through the experimental data of liquid spray penetration under non-evaporating chamber conditions. The numerical simulations based on multi-scheme were implemented by this model to investigate the effects of nozzle geometry and configuration on the subsequent spray development.*

*Key words: Diesel engine, nozzle, X-rays, cavitating flow, primary atomization, spray model*

### Introduction

The tiny nozzle in the high-pressure common rail injection system, connected to the fuel injection upstream and downstream spray atomization, has become one of the most key components of advanced diesel injection and combustion engineering. Ranz [1] has proposed the Diesel engine nozzle spray atomization is associated with internal nozzle flow, and later numerous studies have verified the cavitation phenomenon will produce inevitably under the high injection pressure in the small orifice, which in turn influence the external spray break-up, air/fuel mixing processes, and emissions [2-4].

A number of scholars have carried out experimental and/or numerical investigations on the cavitation characteristics in the diesel orifice. Bergwerk [5] found that the discharge coefficient of the orifice is mainly dependent on the cavitation number and independent on the Reynolds number based on the experiments on simplified single-orifice acrylic nozzles. Mulemane *et al.* [6] performed experimental and numerical investigations to study the influence of operating parameters and critical injector design parameters on the dynamic performance of advanced high-pressure electronically controlled diesel injection systems. The needle lift characteristics show that the measured injection rate is a strong function of the injection pressure and the nozzle diameter. Sou *et al.* [7] studied the effects of nozzle geometries on cavitation in the orifice using 2-D nozzles with various geometries. The research

\* Corresponding author, e-mail: zxhe@ujs.edu.cn

confirmed that the thickness of the cavitation zone increases with the contraction coefficient of the cross-sectional area at upstream of the nozzle to that of the nozzle. He *et al.* [8] analyzed the effects of the needle lift, the inlet radius and the sac volume on the cavitating flow based on a testified cavitation model which was validated by the experimental data obtained from the flow visualization experiment system. Numerical results clearly reveal the distribution of the cavitation zone. Margot *et al.* [9] conducted a comprehensive study on a 3-D flow inside diesel injector-like geometries under a cavitation model implemented in a CFD code. Various numerical parameters were used to simulate cavitation under realistic Diesel engine conditions and the results show that the cavitation model was able to predict the onset of cavitation, which were verified with experiments both on the injection rate and the occurrence of choked flow.

However, due to the complex interaction of vortices, cavitation and turbulence, the CFD modeling remains one of the best techniques to explore and understanding the multi-phase flow. The precise nozzle geometrical parameters provide a reliable basis for the numerical simulation, but it is rather difficult to obtain the internal accurate geometric structure by non-destructive traditional methods, which can be solved effectively by the use of synchrotron radiation technology. Lebas *et al.* [10] studied the dense spray region by implemented a 3-D model for atomization based on an Eulerian single-phase approach in a professional CFD code via AVL FIRE, which has been proved that can improve the description of the primary break-up. Hoyas *et al.* [11] captured many of the most important characteristics of the spray, such as the penetration and the axial velocity, using 2-D simulations based on the Eulerian-Lagrangian spray atomization model via STAR-CD. As can be seen in many commercial software and open source codes, the most efficient and widely-applied approach is the Lagrangian-drop-let-Eulerian-fluid (LDEF) method. Instead of solving the liquid phase as a partial-differential-equation based continuum, such as in the LDEF method treats the liquid as discrete particles. These particles are assumed to be negligible in volume and are superimposed on the continuous gas phase as material points. At the nozzle exit, liquid fuel is injected as discrete *blobs*, and a linear stability based phenomenological model is applied to account for the primary breakup [12]. In spite of its efficiency, the accuracy in the near-nozzle region is low, due to the fact that the liquid fuel is actually a continuum as observed in both experiments and direct numerical simulation (DNS). As a result, the model's connection to the nozzle flow is inherently weak, despite some efforts to model the unresolved near-nozzle physics and to consider the effects of in-nozzle cavitation and turbulence on the primary breakup [13,14].

In this paper, the accurate 3-D geometric structure of the real nozzle was measured as a basis for numerical simulations. The volume of fluid (VOF) method was used to simulate the internal nozzle flow and the primary break-up near the outlet of the nozzle orifice, and then the traditional LDEF method was set in the dilute spray region of the nozzle downstream. And then, in order to validate this simulation model, experimental data compared to were performed. Finally, the effects of different injector geometries on the spray angle, penetration, and particle size distribution under different injection pressures were investigated.

### **Synchrotron radiation measurement of nozzle structure**

The synchrotron radiation facility (SRF) applied in this paper can provide a variety of synchrotron radiations from infrared light to hard X-ray. During the measurements, 55 keV electrons penetrated the front of injector and exposure to scintillation crystal, and then the X-ray absorption image can be captured by the charge coupled device (CCD) camera in the front of injector. In the orifice measurement process, the injector seated on the sample rotation stage revolved

180° at the speed of 1.8° per second. In this process, an X-ray absorption image were captured every 0.2° with 10 seconds exposure time and 9 mm spatial resolution by the CCD camera. Much detailed information about the measurement was shown in tab. 1. The photon flux density of the SRF is  $1 \cdot 10^{10}$  phs  $s^{-1}$   $mm^{-2}$  at 20 keV and the maximal beam size can arrive 48 mm (horizontal)  $\times$  5 mm (vertical) at 20 keV, where the distance between the light and the sample is 30 m.

Figure 1(a) shows the measurement results of eight orifices of the tested nozzle, and the tab. 2 gives more detailed information about the eight different orifices. In order to simplify the calculation, we just choose one orifice (e. g. the 4<sup>th</sup> orifice) of the eight different ones to study. Figure 1(b) shows the slice of the 4<sup>th</sup> orifice of the eight different orifices which are the basis of the consequent nozzle flow and spray simulation. The left part of the axis is the mirror image of the 4<sup>th</sup> orifice which is at the right part of the axis. It is can be seen that both the inlet diameter ( $D_{in}$ ) and the outlet diameter ( $D_{out}$ ) of the 4<sup>th</sup> orifice are about 183  $\mu m$ , and the orifice length ( $L$ ) is about 598  $\mu m$ , while the orifice inlet top curvature radius ( $R_a$ ) and the orifice inlet bottom curvature radius ( $R_b$ ) are about 65  $\mu m$  and 33  $\mu m$ , respectively. The spray angle ( $\theta$ ) between orifice axis and injector axis is 62.9°.

### Spray simulation coupled with nozzle flow

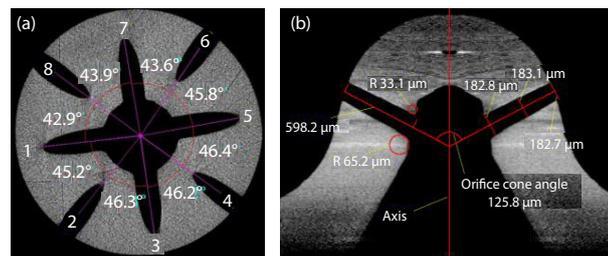
#### Models of hydrodynamic cavitation

In this paper, VOF multiphase model was employed to deal with the internal cavitating flow and the near-field dense spray. VOF model is mainly based on transportation of the volume fraction, that is, a source term representing phase transition which is governed by the difference between the local pressure and the vapor pressure. According to the vapor fraction transport equation, cavitation is assumed to occur due to the bubble nuclei or micro bubbles in the liquid, which can grow or collapse with the changing of the surrounding conditions. Moreover, the growth and collapse of the bubbles are taken into account according to the Rayleigh's simplified bubble dynamics equation [15].

The bubble distribution can be described by a single scalar field which is the vapor volume fraction  $\alpha_v$ , because it is assumed that all vapor bubbles in the control volume have

**Table 1. Main parameters of the experiment**

Energy range	8~72.5 keV
Energy resolution	$\leq 3 \cdot 10^{-3}$
Photon flux density	$1 \cdot 10^{10}$ phs $s^{-1}$ $mm^{-2}$
Maximal beam size	48 mm (H) 5 mm (V)



**Figure 1. The slice of injector in different directions; (a) the measurement results of eight orifices of the tested nozzle, and (b) the slice of the 4<sup>th</sup> orifice of the eight different orifices**

**Table 2. Measurement results of eight different orifices**

$D_{in}$ [ $\mu m$ ]	$D_{out}$ [ $\mu m$ ]	$L$ [ $\mu m$ ]	$R_a$ [ $\mu m$ ]	$R_b$ [ $\mu m$ ]	$\theta$ [ $^\circ$ ]
184	183	589	70	35	62.8
181	184	602	62	30	62.3
180	182	595	58	28	62.5
183	183	598	65	33	62.9
185	184	588	61	32	63.1
182	185	595	62	31	62.6
181	183	598	68	34	62.8
185	182	603	70	33	62.7

the same radius and a homogenous distribution. Also, assuming that only exists a single liquid phase, and the bubbles will occupy the corresponding control volume when the cavitation take place. Equation (1) is a description for the relationship between the vapor volume fraction  $\alpha_v$  and the average vapor bubble radius  $R$ :

$$\alpha_v = \frac{V_v}{V_{tot}} = \frac{N_{bub} \frac{4}{3} \pi R^3}{V_l + V_v} = \frac{n_0 V_l \frac{4}{3} \pi R^3}{V_l + n_0 V_l \frac{4}{3} \pi R^3} = \frac{n_0 \frac{4}{3} \pi R^3}{1 + n_0 \frac{4}{3} \pi R^3} \quad (1)$$

where  $V_v$  and  $V_l$  are the volume occupied by the vapor phase and liquid phase, respectively, and  $V_{tot}$  – the total cells volume,  $N_{bub}$  – the number of vapor bubbles in the control volume, and  $n_0$  – the number density of bubbles per volume of liquid.

The vapor volume fraction  $\alpha_v$  in the control volume will change with the convective transport and bubbles' growth or collapse. The eq. (2) describing the transport of  $\alpha_v$  based on the assumption that the vapor density is much smaller than that of the liquid density:

$$\frac{d}{dt} \int_V \alpha_v dV + \int_S \alpha_v (v - v_s) d\alpha = \int_V \frac{n_0 \frac{4}{3} \pi R^3}{1 + n_0 \frac{4}{3} \pi R^3} \frac{d}{dt} \left( \frac{4}{3} \pi R^3 \right) dV \quad (2)$$

The right side of eq. (2) is the cavitation bubble growth rate of the model, which can be obtained by the observation on the Lagrangian of a cloud of bubbles and the conventional bubble dynamic observation of a single bubble in an infinite stagnant liquid, respectively. This analysis results is the extended Rayleigh-Plesset equation:

$$R \frac{d^2 R}{dt^2} + \frac{3}{2} \left( \frac{dR}{dt} \right)^2 = \frac{P_{sat} - P_\infty}{\rho_l} - \frac{2\sigma}{\rho_l R} - 4 \frac{\mu_l}{\rho_l R} \frac{dR}{dt} \quad (3)$$

where,  $P_{sat}$  is the saturation pressure corresponding to the temperature at the bubble surface,  $P_\infty$  – the pressure of the surrounding liquid,  $\rho_l$  and  $\mu_l$  are the liquid density and viscosity, respectively, and  $\sigma$  – the surface tension coefficient.

The precise geometry structure of the 4<sup>th</sup> orifice of the nozzle obtained by synchrotron

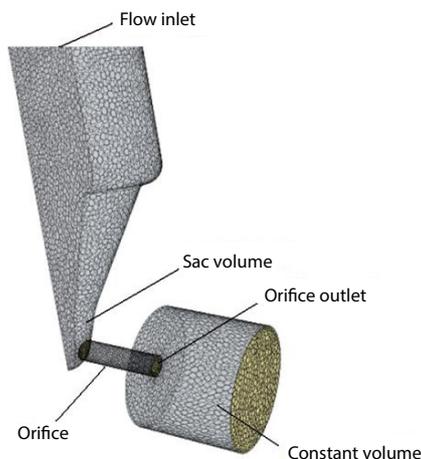


Figure 2. The mesh of injector used (the 4<sup>th</sup> orifice) for nozzle flow simulation

radiation measurement was used to simulate the nozzle flow. Figure 2 was the structure and the mesh used for nozzle flow simulation, and the total grid number chosen was 102529 based on the grid independence tests. All simulations were made with the standard  $k-\epsilon$  turbulence model with standard wall functions. The solver applied was based on the pressure correction and the algorithm applied was SIMPLEC. What the discretization of the  $k-\epsilon$  turbulence model equations used was the upwind differencing scheme and the cavitation model used was based on the Rayleigh equation and associated with the rate of change of the bubble radius depended on the local pressure, where the density of liquid and vapor were constant and there is no slip between the bubbles and the liquid.

### Eulerian-Lagrangian spray model

The near-field dense spray is simulated with the VOF multiphase model the same as the flow in the orifice. The atomization of diesel sprays is modeled as a turbulent mixing process of the liquid fuel with the ambient gas. At a certain downstream location, where the spray is diluted, this Eulerian spray approach was switched to conventional Lagrangian approach which thought the droplet parcels as the control liquid volumes in the computational domain of spray and could depicted the mutual effects between droplets and gas, evaporation and break-up and so on. Figure 3 is the diagram for the Eulerian-Lagrangian coupled spray model, which gives the thought of this spray model clearly.

The conventional Lagrangian spray was simulated by STAR-CD. Theoretical studies provided a criterion for the onset of break-up and an estimate of the stable droplet diameter ( $D_{d, stable}$ ) and the characteristic time scale  $\tau_b$  of the break-up process, simultaneously. The break-up rate of the spray can be calculated by eq. (4):

$$\frac{dD_d}{dt} = -\frac{D_d - D_{d,stable}}{\tau_b} \quad (4)$$

where  $D_d$  is the instantaneous droplet diameter.

Instability of the spray is determined by a critical value of the Weber number ( $We$ ) and the droplet Reynolds number ( $Re$ ), eqs. (5) and (6):

$$We_d = \frac{\rho |u - u_d|^2 D_d}{2\sigma_d} \quad (5)$$

$$Re = \frac{\rho |\mu - \mu_d| D_d}{\mu} \quad (6)$$

The criterion for the onset of this Stripping break-up regime:

$$\frac{We_d}{\sqrt{Re_d}} \geq C_{s1} \quad (7)$$

The characteristic time scale for this Stripping break-up regime:

$$\tau_b = \frac{C_{s2}}{2} \sqrt{\frac{\rho_d}{\rho}} \frac{D_d}{|u - u_d|} \quad (8)$$

Here, the empirical coefficient  $C_{s1}$  is 0.5 and,  $C_{s2}$  is in the range from 2-20.

### Switch method of the Eulerian- Lagrangian model

The calculation data of injector flow (cavitation and turbulence) delivered to downstream conventional Lagrangian spray simulation by the mean of subroutine in STAR-CD,

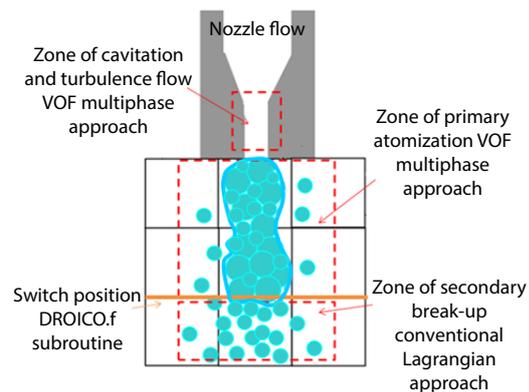


Figure 3. Zones division of coupled spray model

which contained 13 return values. Figure 4 shows the detail information of these parameters. The velocity (magnitude and direction) and density of the upstream Euler flow were made as the initial conditions of the downstream applying the conventional Lagrangian approach.

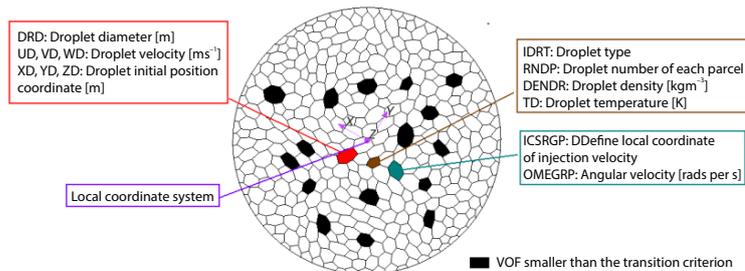


Figure 4. The detail information of return values

fuel injector cells. The positions of these cells were considered as the position of the droplet parcels injected and the velocities of these cells were considered as the initial velocities (magnitude and direction) of droplets. So this model could simulate the spray angle and it was not needed to give previously. The initial droplet size was determined by the fuel liquid volume of fraction. The diameters of fuel droplets were proportional to the volume of fraction value of fuel liquid. It was assumed that the initial size was the orifice diameter multiply by corresponding scale factor [16].

### Validation of Eulerian-Lagrangian spray model

Traditional spray model means simulating the spray directly without coupled the nozzle flow, Eulerian-Lagrangian coupled spray model on STAR-CD that is the model applied in this paper, and coupled spray model on FIRE [17] were simulated based on the 4<sup>th</sup> nozzle. From fig. 5, it can be easily found that the simulation data of coupled spray were much closer to

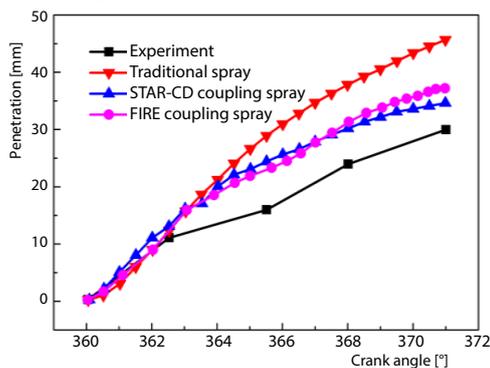


Figure 5. Tip penetrations of traditional spray, coupled spray and experiment data

the experimental data [17] than traditional spray model, which verified the accuracy of the coupled spray mode. Meanwhile, the data obtained from the coupled spray model on FIRE is consistent with that got from the Eulerian-Lagrangian coupled spray model on STAR-CD, which justifying the subprogram compiled coupled the cavitating flow to spray model was feasible in some degree, and the calculation precision of model proposed in this paper can meet the current mainstream commercial software. What obtained from the two kind of coupled spray mode further verified the accuracy of the Eulerian-Lagrangian coupled spray model.

Though the predicted results of the coupled spray mode were higher than the experimental, results obtained from spray simulations which coupled with internal cavitating flow were superior to that traditional spray model which did not consider the influence of internal cavitating flow. For the slight unavoidable differences between predicted and experimental results, the errors in the measurement of spray penetration distance and simplification of the boundary conditions in spray simulation were regarded as the dominant causes.

It was assumed that the spray zones, where the distance to orifice outlet is longer than 2 mm, were dilute spray zone. The simulation cells of switch location cross-section, whose liquid volume of fraction was bigger than 0.5, were chosen as the

the experimental data [17] than traditional spray model, which verified the accuracy of the coupled spray mode. Meanwhile, the data obtained from the coupled spray model on FIRE is consistent with that got from the Eulerian-Lagrangian coupled spray model on STAR-CD, which justifying the subprogram compiled coupled the cavitating flow to spray model was feasible in some degree, and the calculation precision of model proposed in this paper can meet the current mainstream commercial software. What obtained from the two kind of coupled spray mode further verified the accuracy of the Eulerian-Lagrangian coupled spray model.

Based on the verification above, numerical simulation was conducted with the Eulerian-Lagrangian coupled spray model on STAR-CD. The conditions were same as the experiment by Verhoeven *et al.* [18], that is, the injection pressure is 50 MPa, and the back pressure is 2 MPa. As shown in fig. 6 is the distribution of the spray droplet diameter obtained by different methods, though the Eulerian-Lagrangian coupled spray model on STAR-CD simulations result was less than the traditional spray model, the spray penetration was much closer to the experiment, especially the spray near the outlet of the orifice because of considering the flow inside the nozzle.

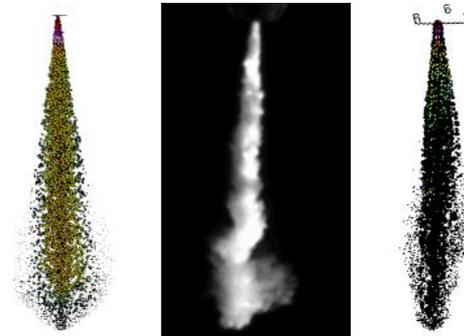


Figure 6. The distribution of the spray droplet diameter obtained by traditional spray, experiment and coupled spray; (a) traditional spray (b) experiment, and (c) STAR-CD coupled spray

### Effects of different injector geometries on the spray characteristics

According to the study [8], the injector geometries have important effects on the spray. In this paper, using the above verified coupled spray model, the multi-scheme numerical simulations were carried out for the different nozzle geometry parameters, such as the ratio of nozzle orifice length to diameter ( $L/D$ ), orifice entrance curvature radius ( $R$ ) and the different nozzle configurations like the standard (STD) type, valve covered orifice (VCO) type, and the improved (IMPROVED) type, to analyze the effects of the nozzle geometries on the subsequent spray.

#### Effects of the $L/D$ and $r$ on the spray characteristics

The nozzle configuration was the STD type, and the pressure at the inlet was 50 MPa and the back pressure was 0.5 MPa.

When studying the effect of the different ( $L/D$ ) on the spray characteristics, the orifice entrance curvature radius ( $R$ ) is 0, and the orifice diameter ( $D_d$ ) is 0.228 mm. The simulation results for different ratios of nozzle orifice length to diameter ( $L/D = 2, 3, \text{ and } 4$ ) were shown in fig. 7. The spray tip penetration is increased with the ratio of length to diameter increased, and the sauter mean diameter (SMD) would increase.

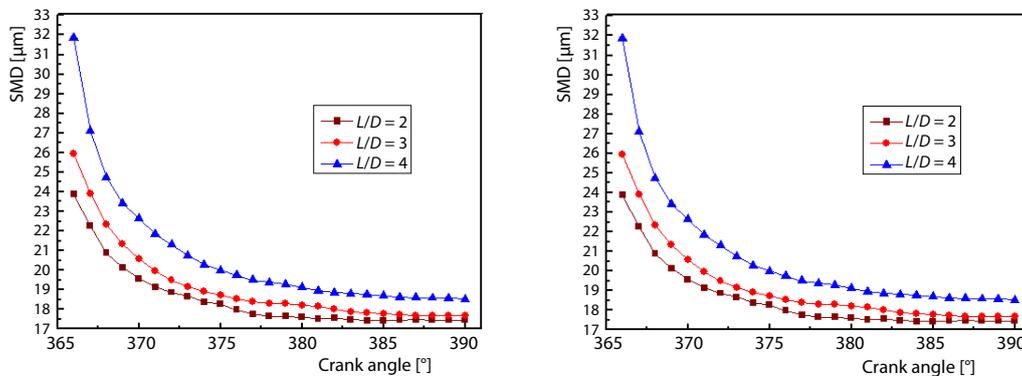


Figure 7. Spray tip penetration and SMD for  $L/D = 2, 3, \text{ and } 4$

As for investigating the effect of the orifice entrance curvature radius ( $R$ ) on the spray characteristics, the ratio of orifice length to diameter ( $L/D$ ) was 4. Figure 8 showed the simulation results for the three different kinds of orifice entrance curvature radius, that is  $R = 0$ ,  $R = 0.0228$  mm, and  $R = 0.0456$  mm. It presented that if the entrance curvature radius decreased, the spray tip penetration and the SMD were decreased rapidly. It could find that both at  $R = 0.0228$  and  $R = 0.0456$  mm the spray tip penetration and the SMD were nearly similar, but had a large distinction compared to the condition of  $R = 0$ . It could be supposed that the existence of entrance curvature radius may reduce the cavitation inside the orifice.

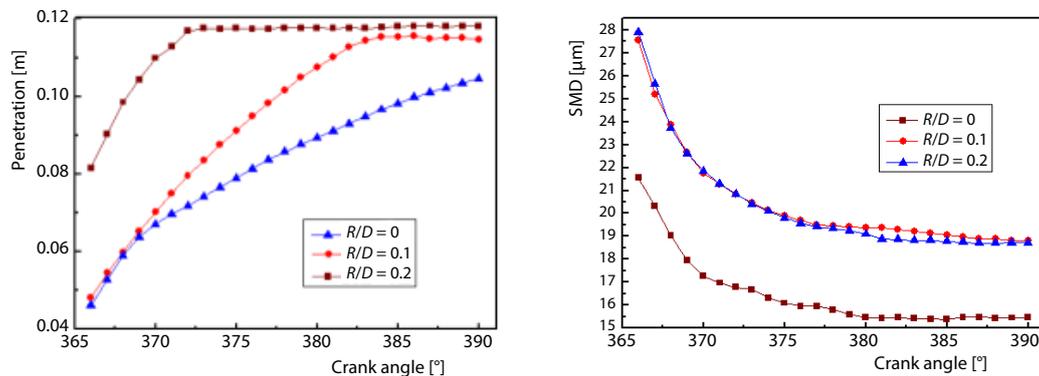


Figure 8. Spray tip penetration and SMD for  $R = 0, 0.0228, \text{ and } 0.0456$  mm

#### Effect of the types of sac volume on the spray characteristics

The main difference of the STD, VCO, and IMPROVED type nozzle is the relative location of the orifice and the needle valve seat, so there are different sac volume, as shown in fig. 9.

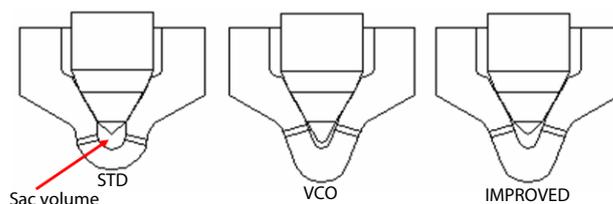


Figure 9. Three types of nozzle with different sac volume

The orifice of STD type is under the needle valve seat with a large sac volume, and the orifice of VCO type nozzle is above the needle valve seat nearly without sac volume, and also the orifice of IMPROVED type is above the needle valve seat, but it has a sac volume a bit smaller than the STD type.

For these three different models, they had the same boundary conditions and orifice geometry. Injection pressure was 50 MPa and the back pressure was 0.5 MPa. The calculation results were shown in fig. 10. At the early stage of the injection, the tip penetration of the three different types were similar, while at the end stage of injection, the VCO nozzle had the longest penetration and the smallest value of SMD. Considering of nozzle cavitating flow comprehensively, from the aspect of spray tip penetration and SMD, IMPROVED nozzle could acquire better spray characteristics.

#### Summary and conclusions

- In this paper, a 3-D high-precision structure model of nozzle geometry was obtained using the X-ray phase contrast imaging measurement, which was helpful to establish the CFD model of nozzle more exactly.

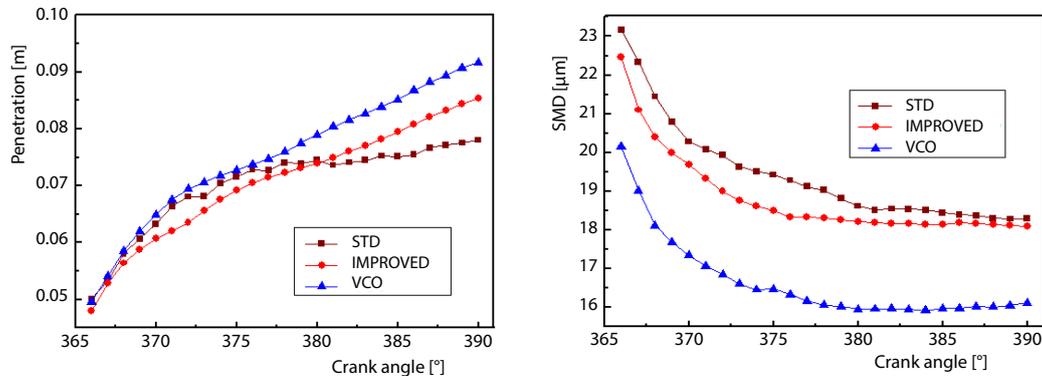


Figure 10. Spray tip penetration and SMD of three different types of nozzle

- The model proposed in this paper adopted the VOF method to simulate the internal nozzle flow and the near-field dense spray, then used the original position of the traditional LDEF method for the nozzle downstream. The velocity (magnitude and direction) and density of the upstream Euler flow were made as the initial conditions of the downstream applying the conventional Lagrangian approach. Comparing the visual spray experiment data and numerical results, it was verified that the spray model coupled with cavitating flow in nozzles was more accurate than the traditional spray model widely used nowadays.
- The multi-scheme numerical simulations indicated that the nozzle structure has an important effect on the spray characteristics. The spray tip penetration is increased with the ratio of length to diameter increased, and the SMD would increase. The existence of entrance curvature radius may reduce the cavitation inside the orifice, and causing a larger value of the tip penetration and the SMD. Considering of nozzle cavitating flow comprehensively, from the aspect of spray tip penetration and SMD, IMPROVED nozzle could acquire better spray characteristics. The simulation results supply the theoretical foundation for the optimization design of the injector.

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### Nomenclature

$C_{s1}, C_{s2}$  – empirical coefficient

$D$  – diameter of orifice, [m]

$D_d$  – droplet diameter, [m]

$L$  – length of orifice, [m]

$L/D$  – length to diameter of orifice

$l$  – liquid phase

$N_{bub}$  – number of vapor bubbles

$P_{sat}$  – saturation pressure, [Pa]

$P_{\infty}$  – surrounding pressure, [Pa]

$R$  – average vapor bubble radius

$r$  – curvature radius, [m]

$R_a, R_b$  – orifice inlet top and bottom curvature radius, [m]

Re – Reynolds number

S – total turbulence energy source

$T_b$  – characteristic time scale

$u$  – average velocity

$u_d$  – instantaneous velocity

$V$  – volume, [m<sup>3</sup>]

$V_{tot}$  – total cells volume

$v$  – fuel vapor phase

We – Weber number

#### Greek symbols

$\alpha$  – volume fraction

$\theta$  – spray angle, [°]

$\mu$  – dynamic viscosity, [Pa·s]

$\mu_l$  – liquid viscosity

$\rho$  – density, [kgm<sup>-3</sup>]

$\sigma$  – surface tension coefficient, [Nm<sup>-1</sup>]

$\tau_b$  – characteristic time scale, [s]

#### Acronyms

CCD – charge coupled device

CFD – computational fluid dynamics

DNS – direct numerical simulation

IMPROVED – improved

LDEF – Lagrangian-droplet-eulerian-fluid

SMD – sauter mean diameter, [m]

SRF – synchrotron radiation facility

STD – standard

VOF – volume of fluid

#### Subscript

d – instantaneous droplet diameter

in – upstream location of a nozzle

l – liquid

out – nozzle hole outlet

s – turbulence energy source term

v – vapor

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