

# **3-D Simulation of Non-Evaporating Diesel Spray by Means of LES Task 1.5F**

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and their Control of Combustion and Emissions (21-22 Aug. 06)**



# CONTENTS

- Background
- Way of Calculation
- Numerical results and Discussion
- Conclusion

# Diesel spray structure



Sectional image  
(Experiment)

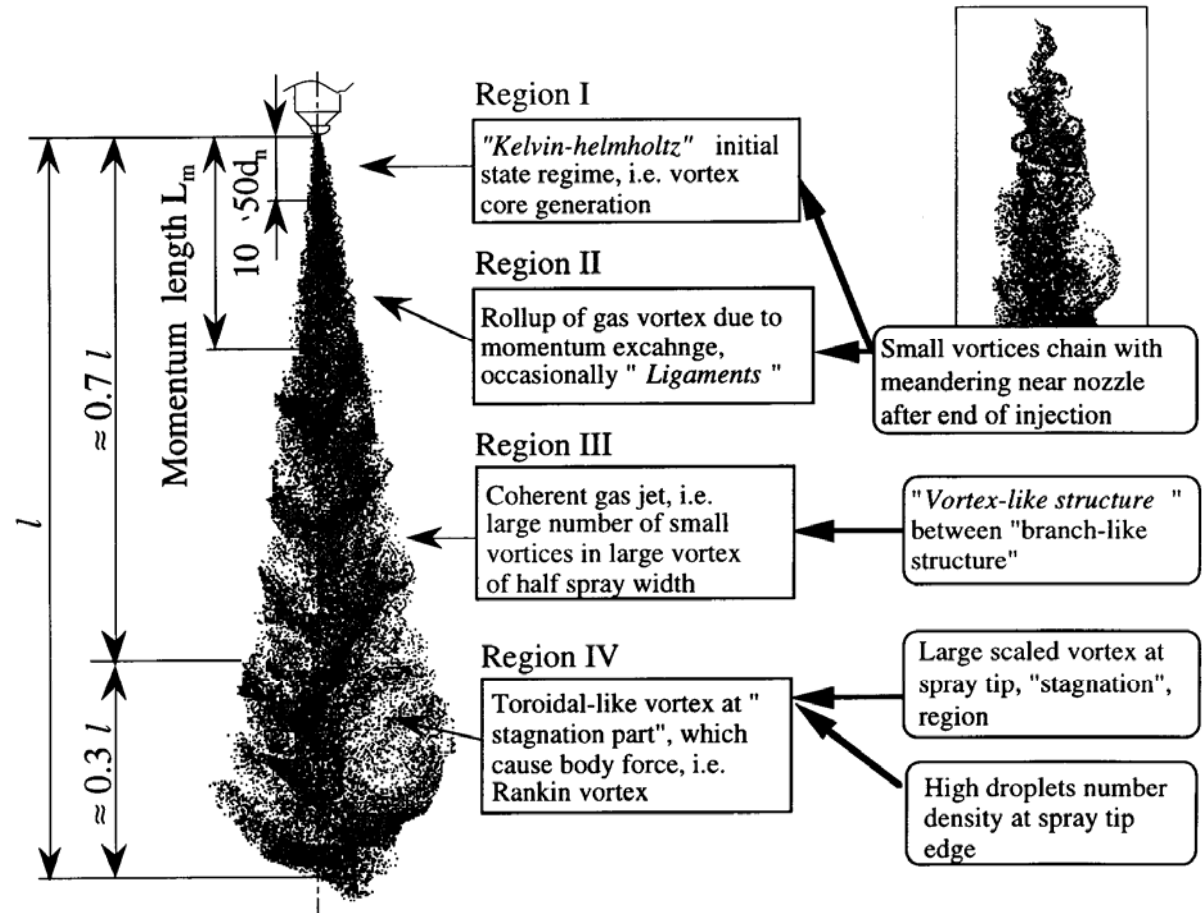
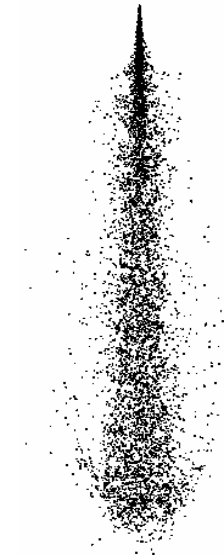


Fig.3 Model of inner structure of diesel spray

T. Dan et al., "Effect of Ambient Gas Properties for Characteristics of Non-Reacting Diesel Fuel Spray", SAE paper 970352, pp.219-221 (1997).

# Diesel spray simulation

- RANS approach
  - KIVA, Star-CD, Fire, Fluent
  - DDM+RANS
    - Low CPU time + Robustness
    - Cycle averaged velocity
- LES approach
  - KIVALES, Sone, Menon  
( Computational Combustion Laboratory, 2000)
  - DDM+LES
    - High accuracy
    - Instantaneous flow field
    - Coherent vortex

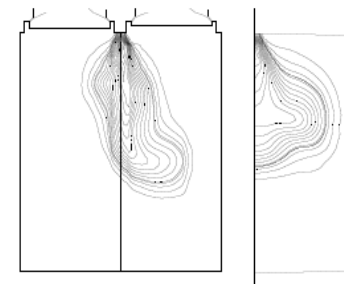


KIVA3V(RANS)

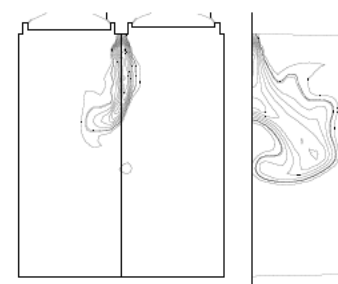


Exp.

Sectional image



(a)KIVA3V



(b)KIVALES

Sone et al., "KIVALES: Large-Eddy Simulations of Internal Combustion Engines. Part I: Theory and Formulation", Computational Combustion Laboratory (2000)



# Purpose of this study

The objective is the numerical simulation of a non-evaporative diesel spray in constant volume vessel using LES

- (1) KIVALES code was constructed to build in LES to KIVA code.
- (2) The simulated results compared with the experimental results, such as spray shape, spray tip penetration and sauter mean diameter.
- (3) 3-D flow of the surroundings around the spray was visualized by means of the laplacian pressure and examined the effect of this flow on the process of the formation of diesel spray.



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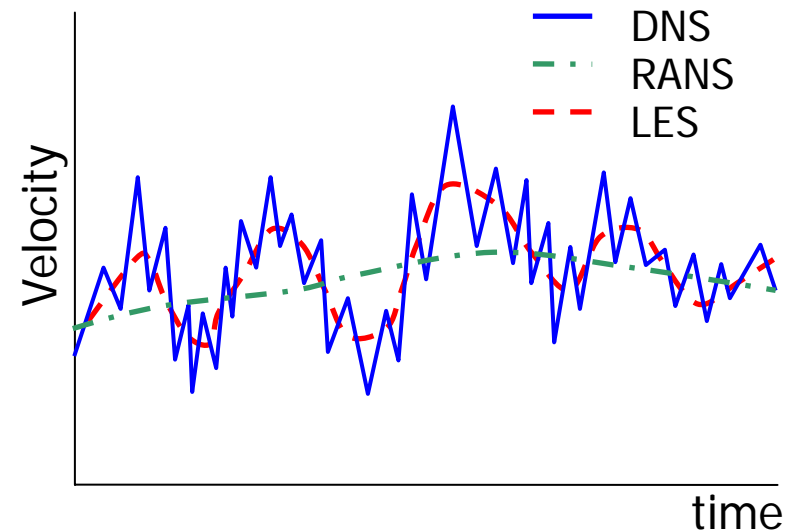
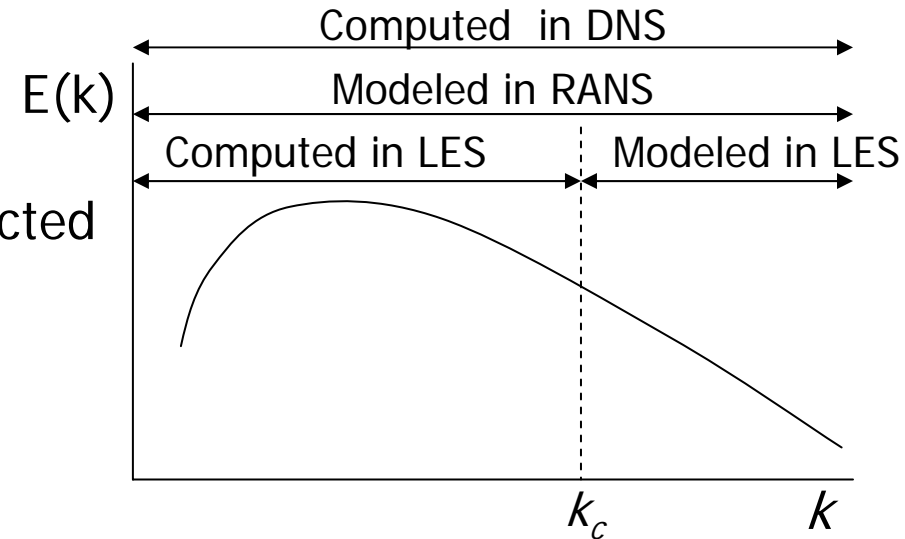
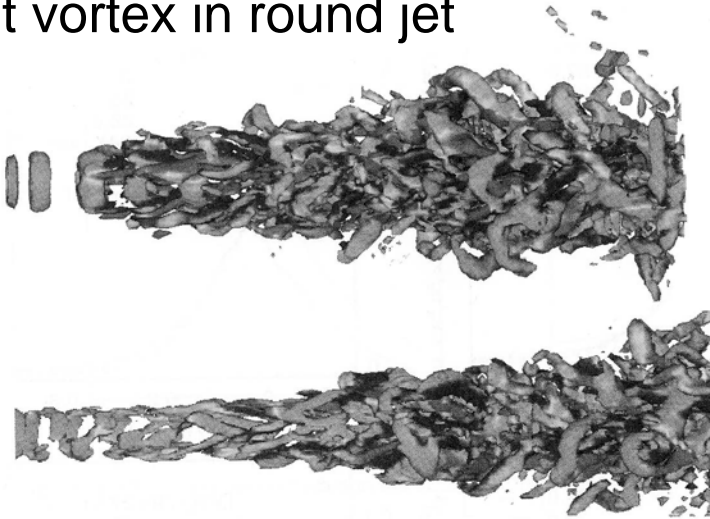
- Background
- Way of Calculation
  - LES and RANS
  - Governing equation
  - SGS modeling
  - Computational conditions
- Numerical results and Discussion
- Conclusion

# LES and RANS

## LES(Large Eddy Simulation)

- High Accuracy for turbulent flow
- Instantaneous and 3D flow are predicted
- Coherent vortex

### Coherent vortex in round jet



“Large Eddy Simulations of Turbulence”, MARCEL LESIEUR et.al..

# Governing equations

Continue equation

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j}{\partial x_j} = \overline{\dot{\rho}^s}$$

Momentum equation

$$\frac{\partial \bar{\rho} \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{\rho} \tilde{u}_i \tilde{u}_j - \bar{\tau}_{ij} + \tau_{ij}^{sgs} \right) = \overline{F_i^s}$$

Internal energy equation

$$\begin{aligned} \frac{\partial \bar{\rho} \tilde{e}}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j \tilde{e}}{\partial x_j} = & -\bar{\rho} \frac{\partial \tilde{u}_j}{\partial x_j} - \frac{\partial h_j^{sgs}}{\partial x_j} - \frac{\partial \tilde{q}_j}{\partial x_j} \\ & + \bar{\sigma}_{ij} \frac{\partial \tilde{u}_j}{\partial x_j} + \Theta^{sgs} + \Pi^{sgs} + \overline{\dot{Q}^s} \end{aligned}$$

Chemical species equation

$$\frac{\partial \bar{\rho} \tilde{Y}_m}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{\rho} \tilde{u}_j \tilde{Y}_m - \bar{\rho} \bar{D}_m \frac{\partial \tilde{Y}_m}{\partial x_j} + \Phi_{j,m}^{sgs} \right) = \overline{\dot{\rho}_m^s}$$



# SGS modeling

## SGS stress model

$$\tau^{sgs} = 2\bar{\rho}v_t \left( \tilde{S}_{ij} - \frac{1}{3} \tilde{S}_{kk} \delta_{ij} \right) + \frac{2}{3} \bar{\rho} k^{sgs} \delta_{ij}$$

## $k$ - $\Delta$ model

$$v_t = C_v k^{sgs 1/2} / \bar{\Delta}$$

$$\bar{\Delta} = V_{cell}^{1/3}$$

$$\frac{\partial (\bar{\rho} k^{sgs})}{\partial t} + \frac{\partial \bar{\rho} \tilde{u}_j k^{sgs}}{\partial x_j}$$

$$= -\tau_{ij}^{sgs} \frac{\partial \tilde{u}_i}{\partial x_j} - D^{sgs} + \frac{\partial}{\partial x_j} \left( \bar{\rho} \frac{v_t}{Pr_t} \frac{\partial k^{sgs}}{\partial x_j} \right) + \dot{W}^s$$

## SGS model: gradient diffusion model

$$h_{i,m}^{sgs} = -\bar{\rho} \frac{v_t C_p}{Pr_t} \frac{\partial \tilde{T}}{\partial x_j}$$

$$\Phi_{i,m}^{sgs} = -\bar{\rho} \frac{v_t}{Sc_t} \frac{\partial \tilde{Y}_m}{\partial x_i}$$

$$\begin{aligned} \Theta^{sgs} &= D^{sgs} \\ &= \frac{C_\varepsilon \bar{\rho} k^{sgs 3/2}}{\bar{\Delta}} \end{aligned}$$



# Computational model

| Computational code       | KIVALES  | KIVA                                   |
|--------------------------|--|--|
| Turbulent model          | LES<br>with $k-\Delta$ model   | RANS<br>with RNG $k-\varepsilon$ model |
| Gas phase                | Finite Volume method based on ALE  |  |
| Convective term          | Interpolated-donor cell differencing scheme                              |  |
| Spray model              | Droplet Discrete Method (DDM)  |  |
| Droplet                  | Rigid sphere   |  |
| Breakup                  | Modified TAB model ( $K=10/3 \rightarrow 8/9$ , $\phi=2 \rightarrow 6$ ) |  |
| Velocity interpolation   | Nordin model ( $n=2$ )   |  |
| Collesion and coalecence | O'Rourke model   |  |



# Computational conditions

\*Dan, T., Takagishi, S., Senda and J., Fujimoto, H., SAE technical paper 970352, pp.219-234, (1997) .

|                     |                      |                |
|---------------------|----------------------|----------------|
| Hole diameter       | [mm]                 | 0.20           |
| Injection pressure  | [MPa]                | 77             |
| Injection duration  | [ms]                 | 1.8            |
| Fuel                |                      | n-tridecane    |
| Fuel amount         | [mg]                 | 12             |
| Fuel temperature    | [K]                  | 300            |
| Ambient gas         |                      | N <sub>2</sub> |
| Ambient pressure    | [MPa]                | 1.5            |
| Ambient density     | [kg/m <sup>3</sup> ] | 17.3           |
| Ambient temperature | [K]                  | 300            |



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# Diesel spray simulation (L)LES (R)RANS

$t = 0.0 \text{ ms} - 3.0 \text{ ms}$

$\rho_{inj}$  77 MPa

$\rho_a$  17.3 kg/m<sup>3</sup>

$t_{inj}$  1.8 ms

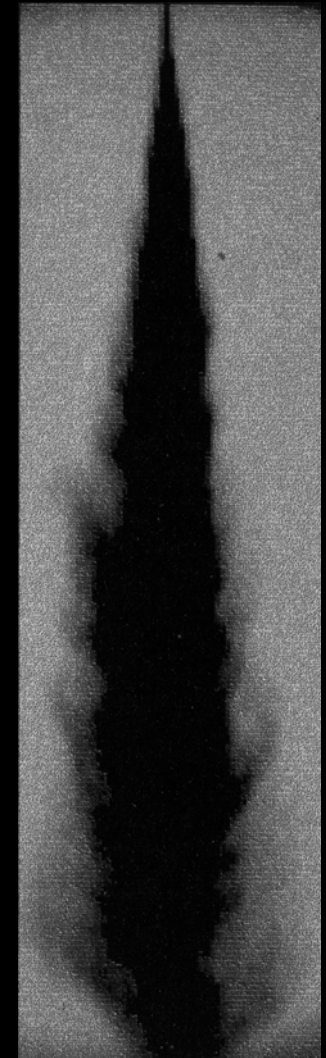
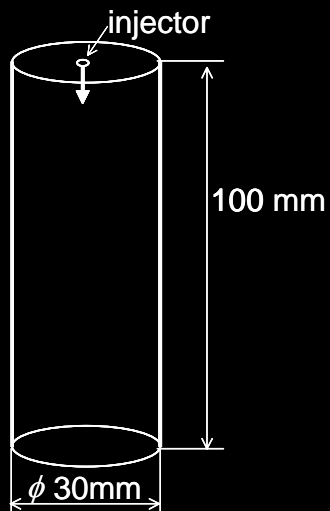
Computational grid

60x60x200

(720,000)

CPU time

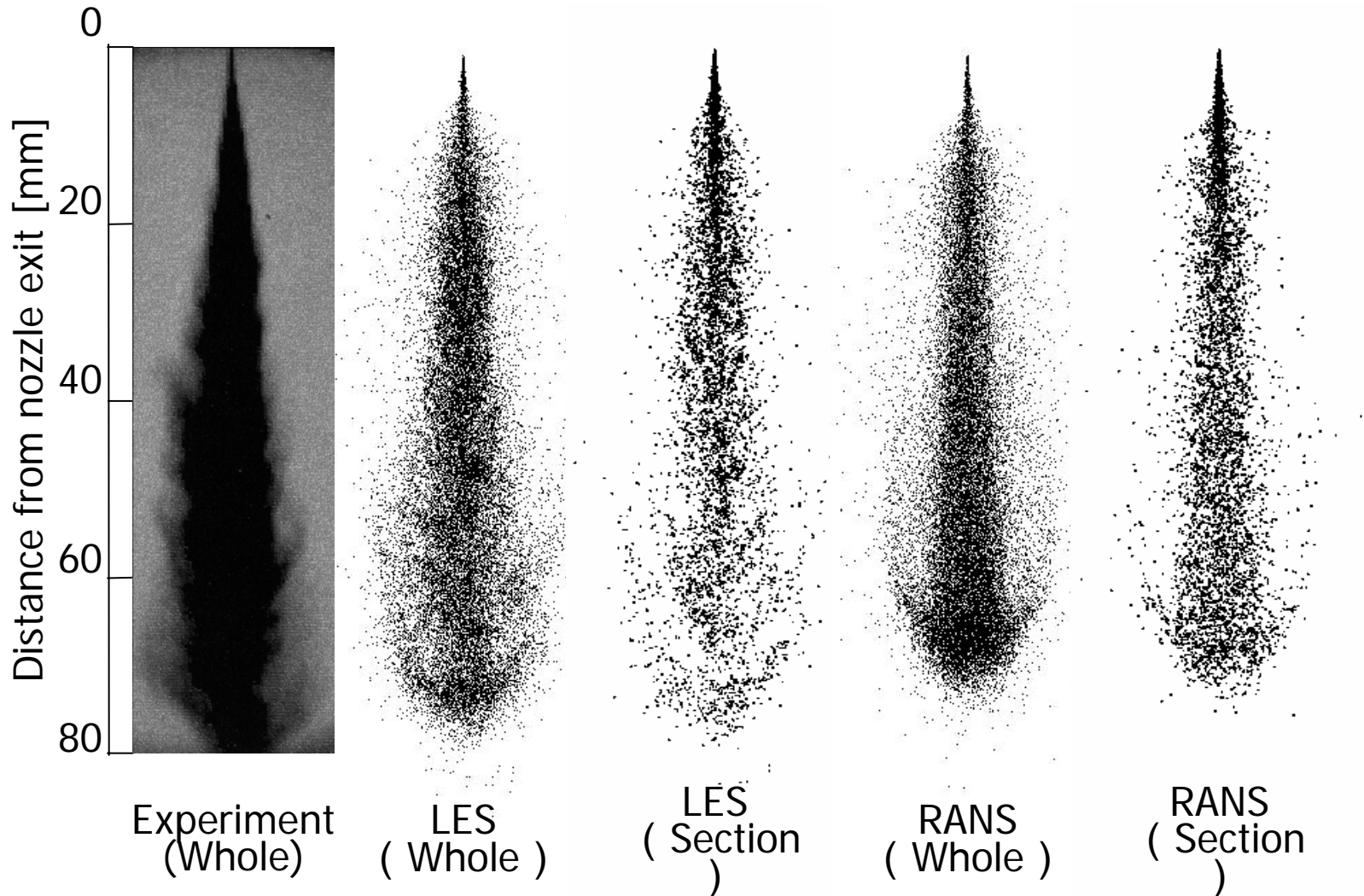
140 hour



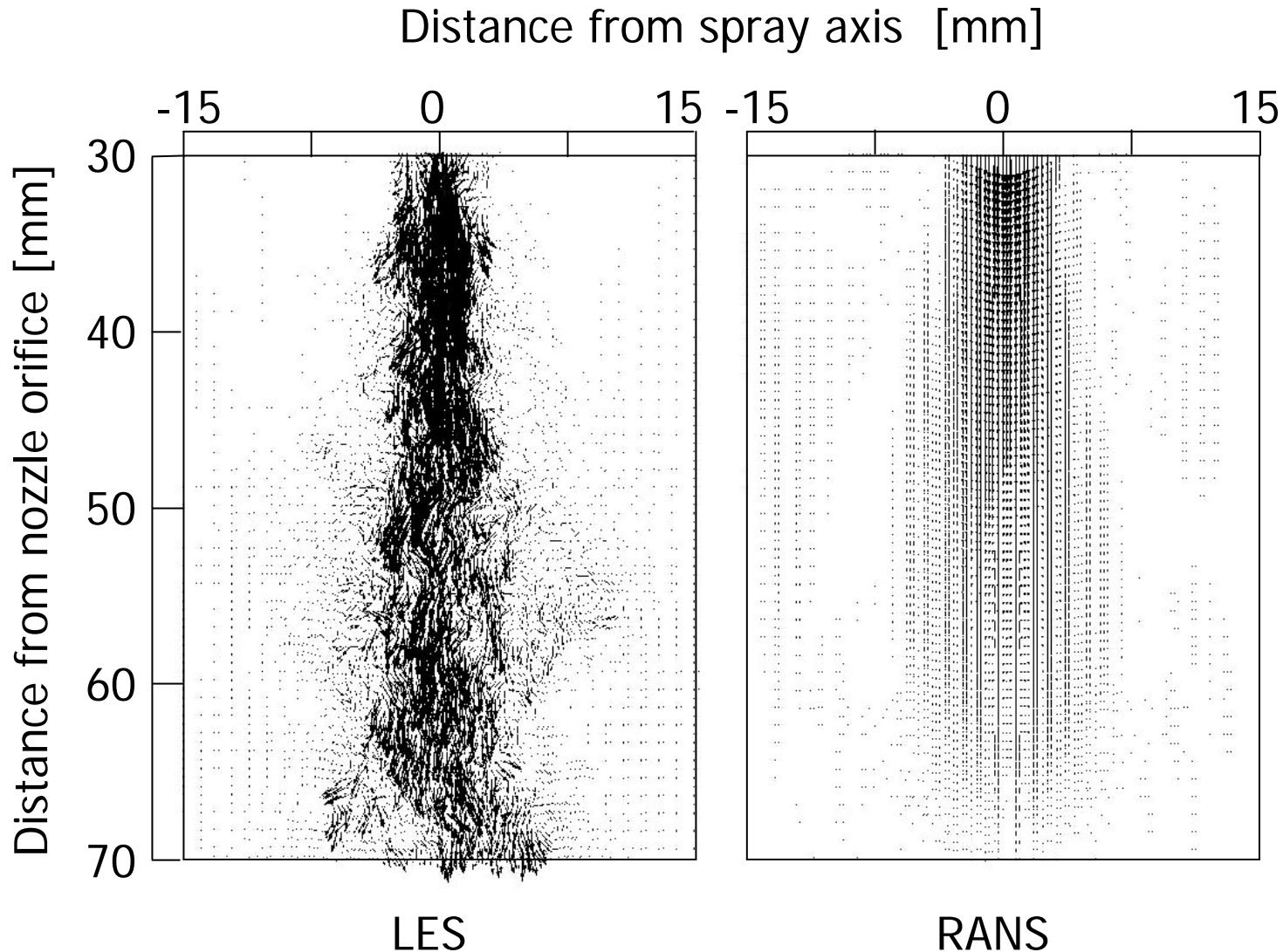
Experiment ※  
(  $t = 1,8\text{ms}$  )

※Takagishi, S.,  
master's thesis,  
Doshisha University ( 1996

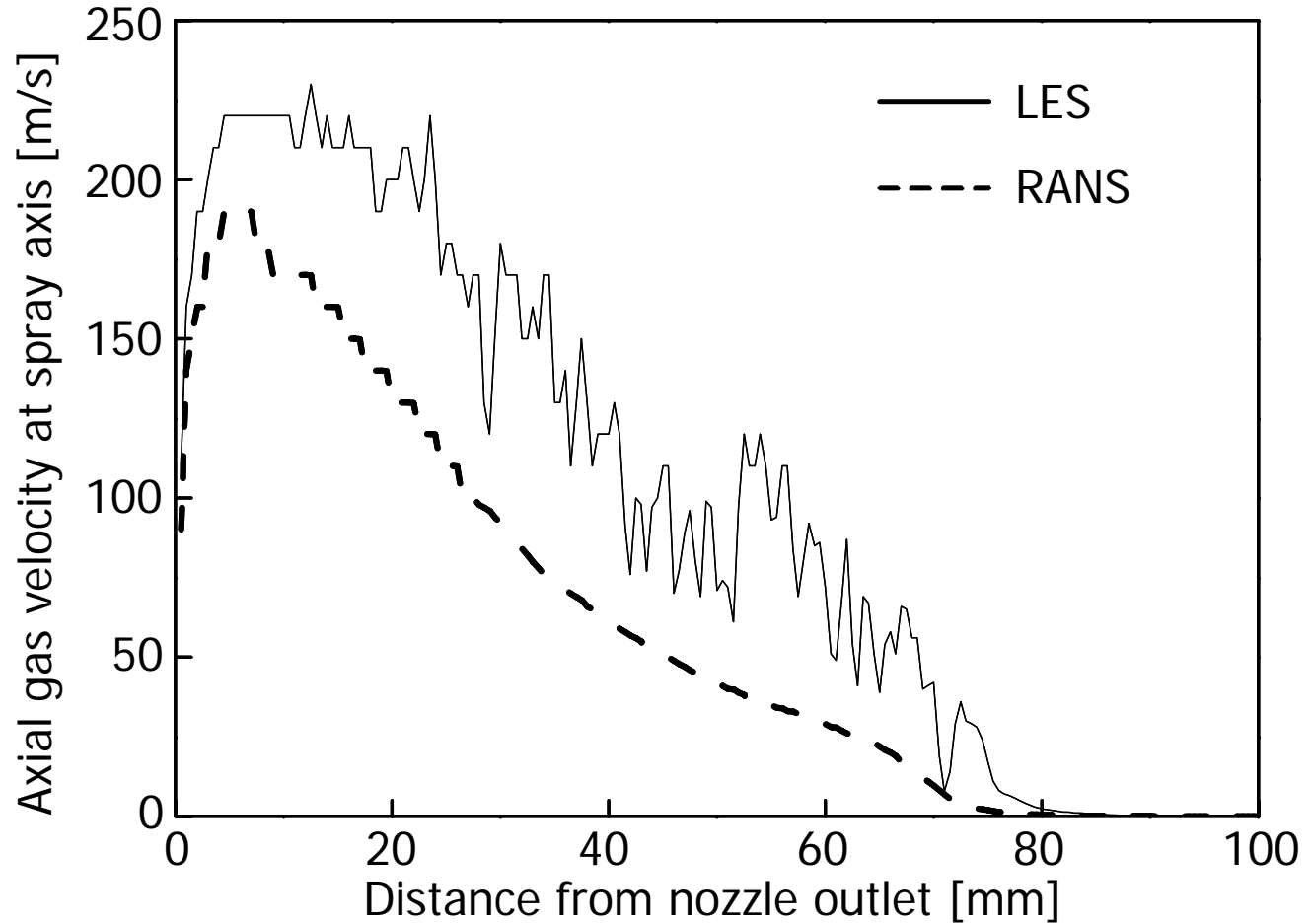
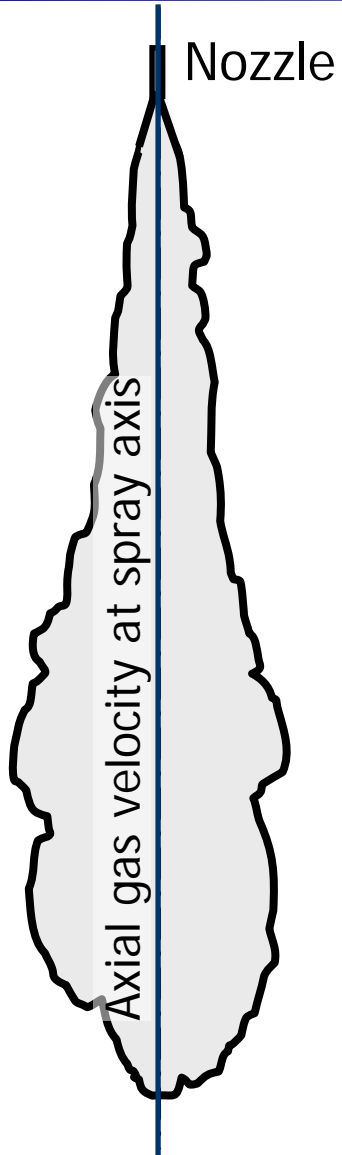
# Spray shape obtained by LES and RANS



# Instantaneous velocity distribution at cross section at 1.8ms

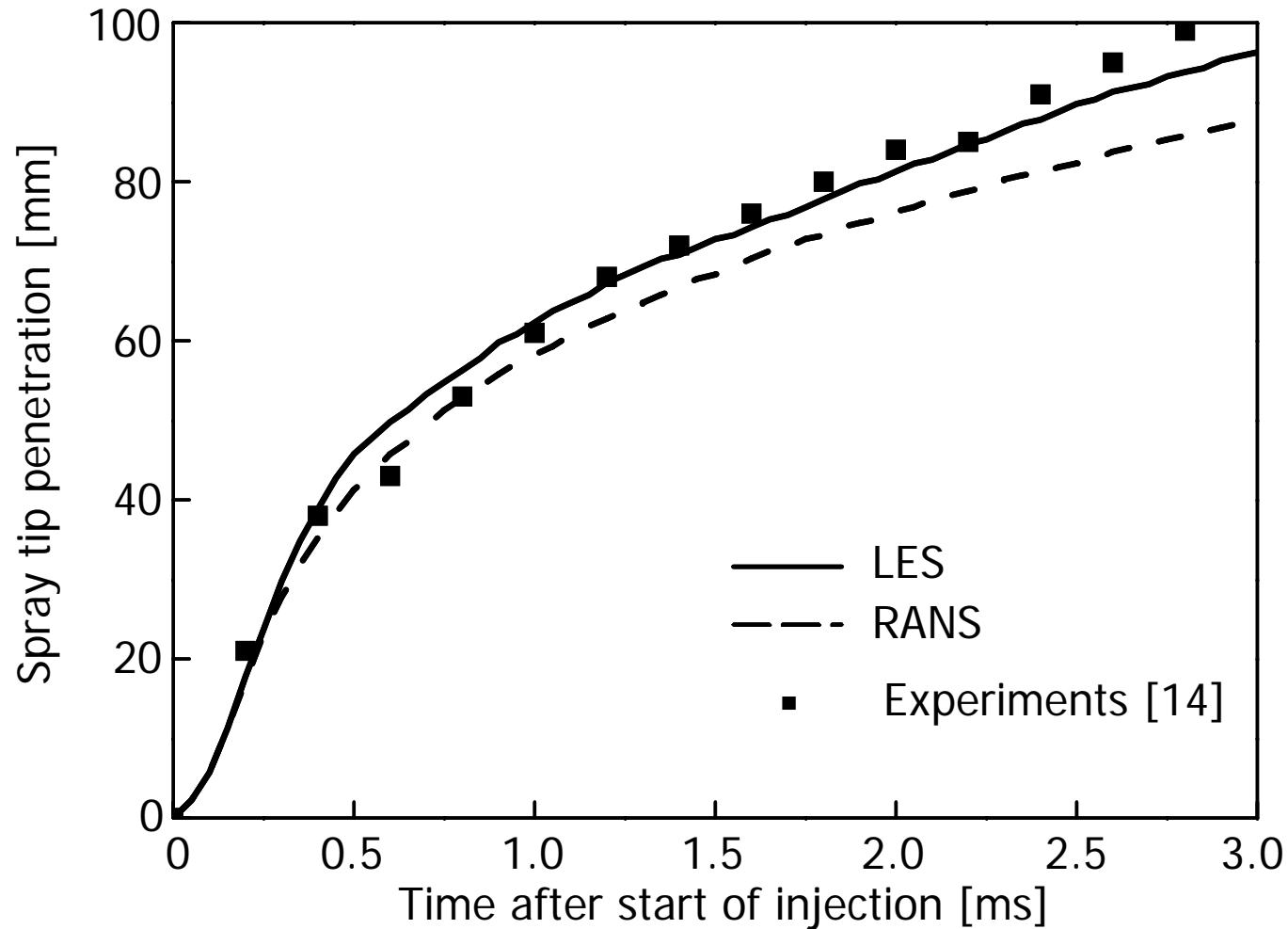
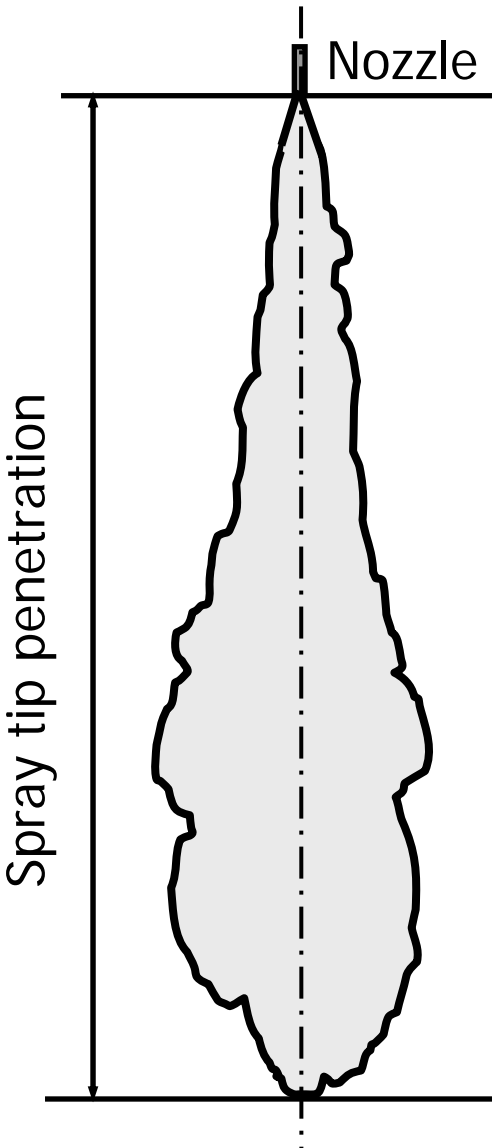


# Distribution of instantaneous axial gas velocity at spray axis (1.8ms)

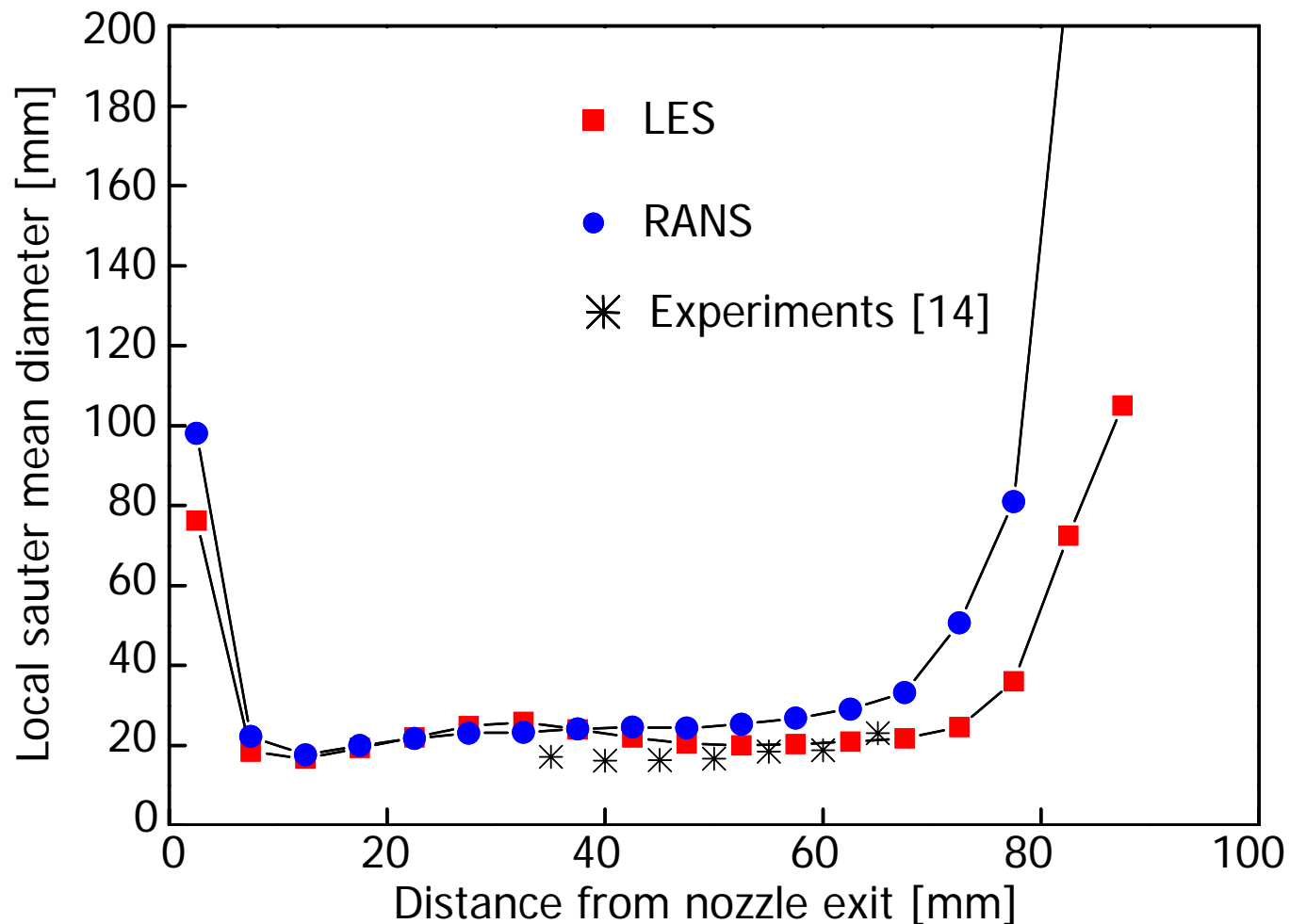
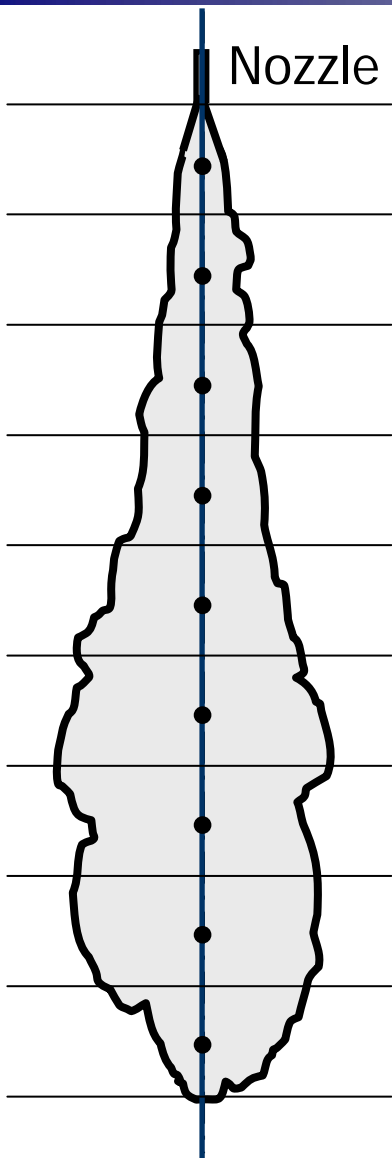




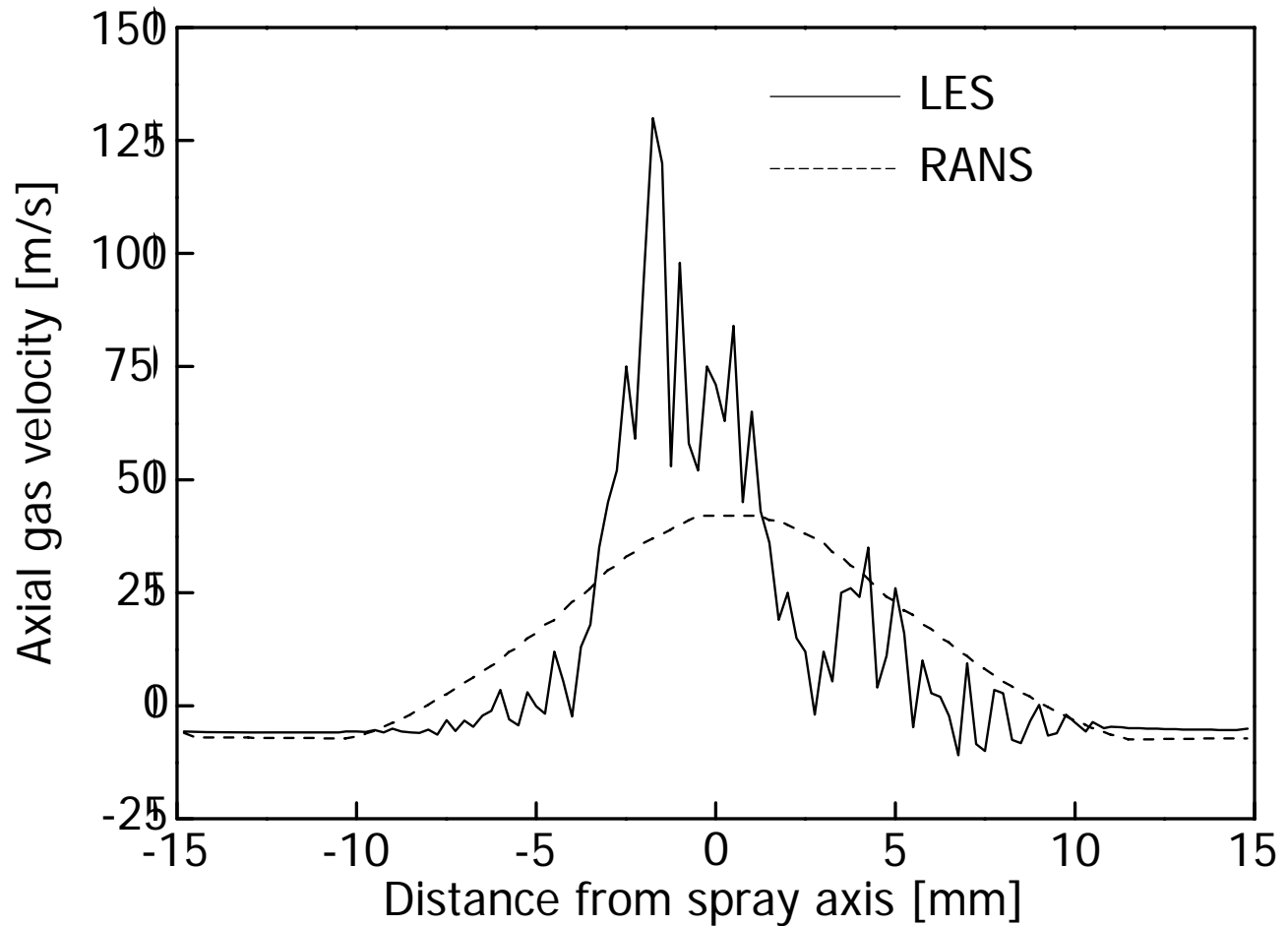
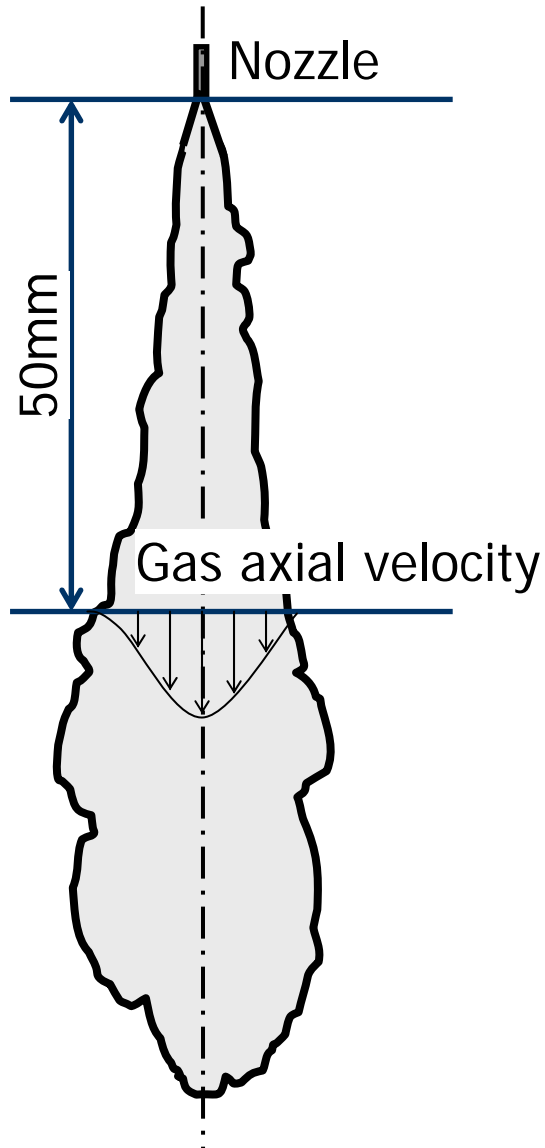
# Comparison of spray tip penetration obtained by LES and RANS with that of experiments



# Comparison of SMD obtained by LES and RANS with that of experiments at 1.8 ms



# Radial distribution of instantaneous axial velocity (50 [mm] from nozzle exit)



# Coherent vortex (RANS)

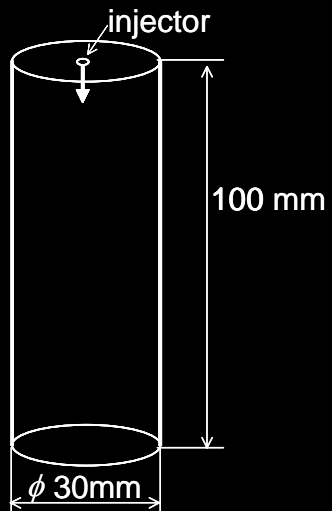
$\rho_{inj}$  77 MPa

$\rho_a$  17.3 kg/m<sup>3</sup>

$t_{inj}$  1.8 ms

Computational  
grid  
60x60x200  
(720,000)

CPU time  
140 hour



0.10ms

# Coherent vortex (LES)

$p_{inj}$  77 MPa

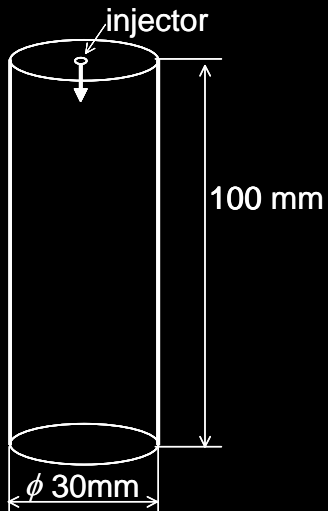
$\rho_a$  17.3 kg/m<sup>3</sup>

$t_{inj}$  1.8 ms

Computational  
grid

60x60x200  
(720,000)

CPU time  
140 hour



0.10ms



Top View

0.10ms



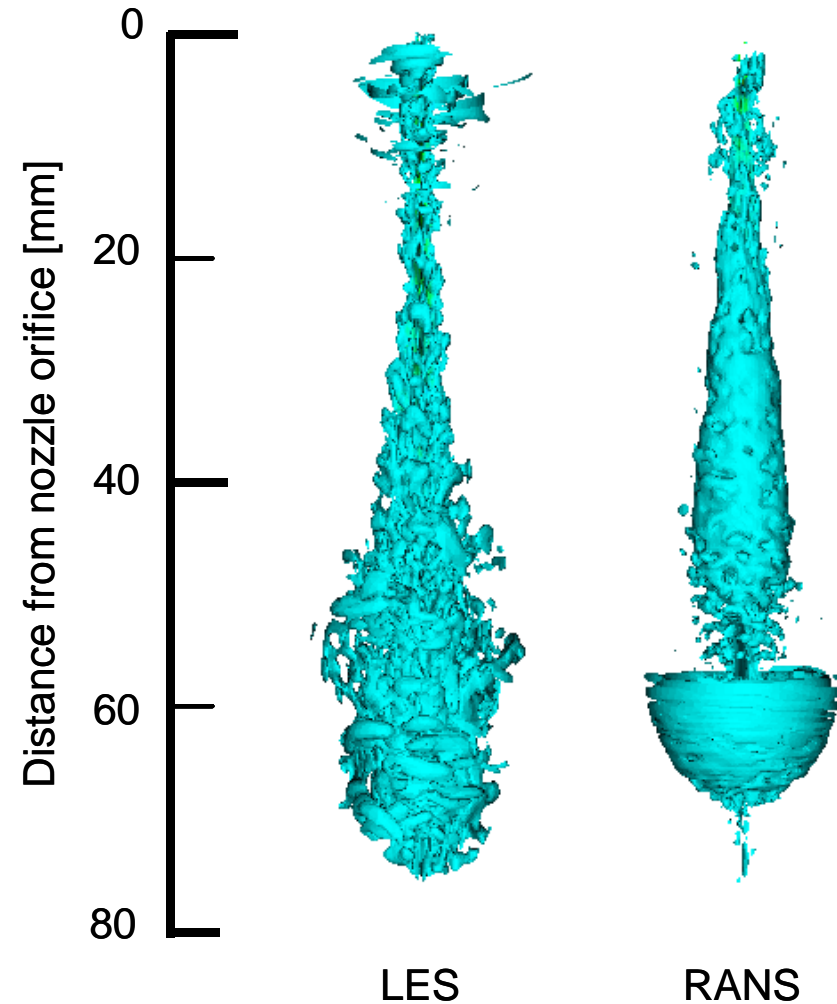
Bottom View

0.10ms

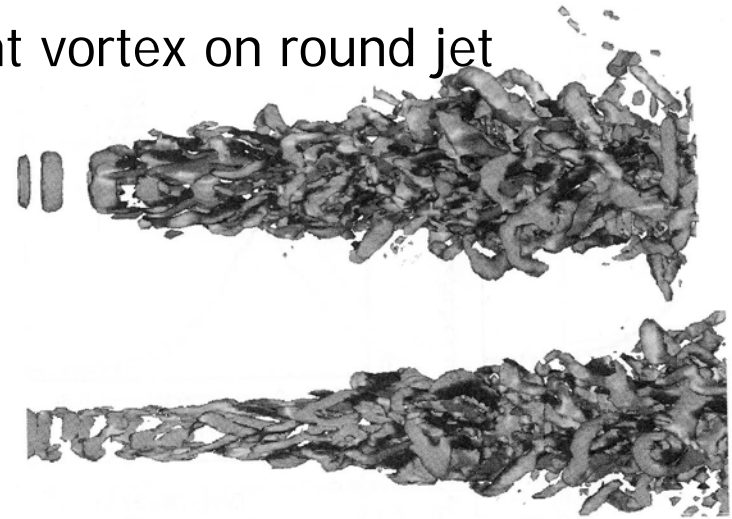


# Coherent Vortex

$t = 1.8 \text{ ms}$

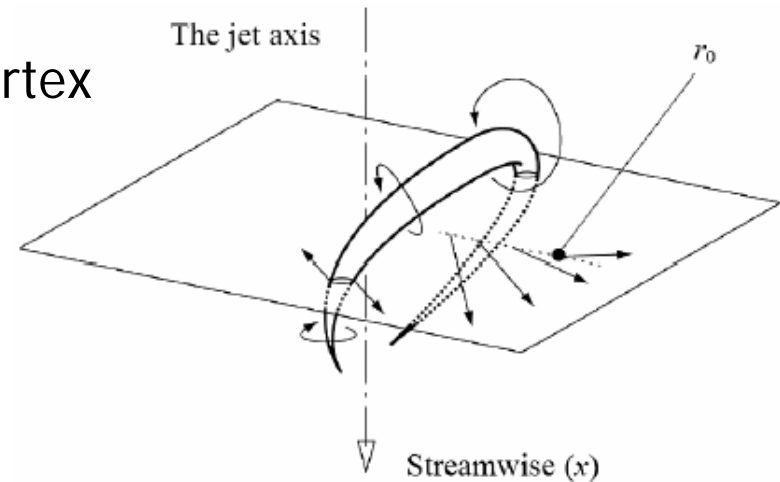


Coherent vortex on round jet



"Large Eddy Simulations of Turbulence", MARCEL LESIEUR et.al..

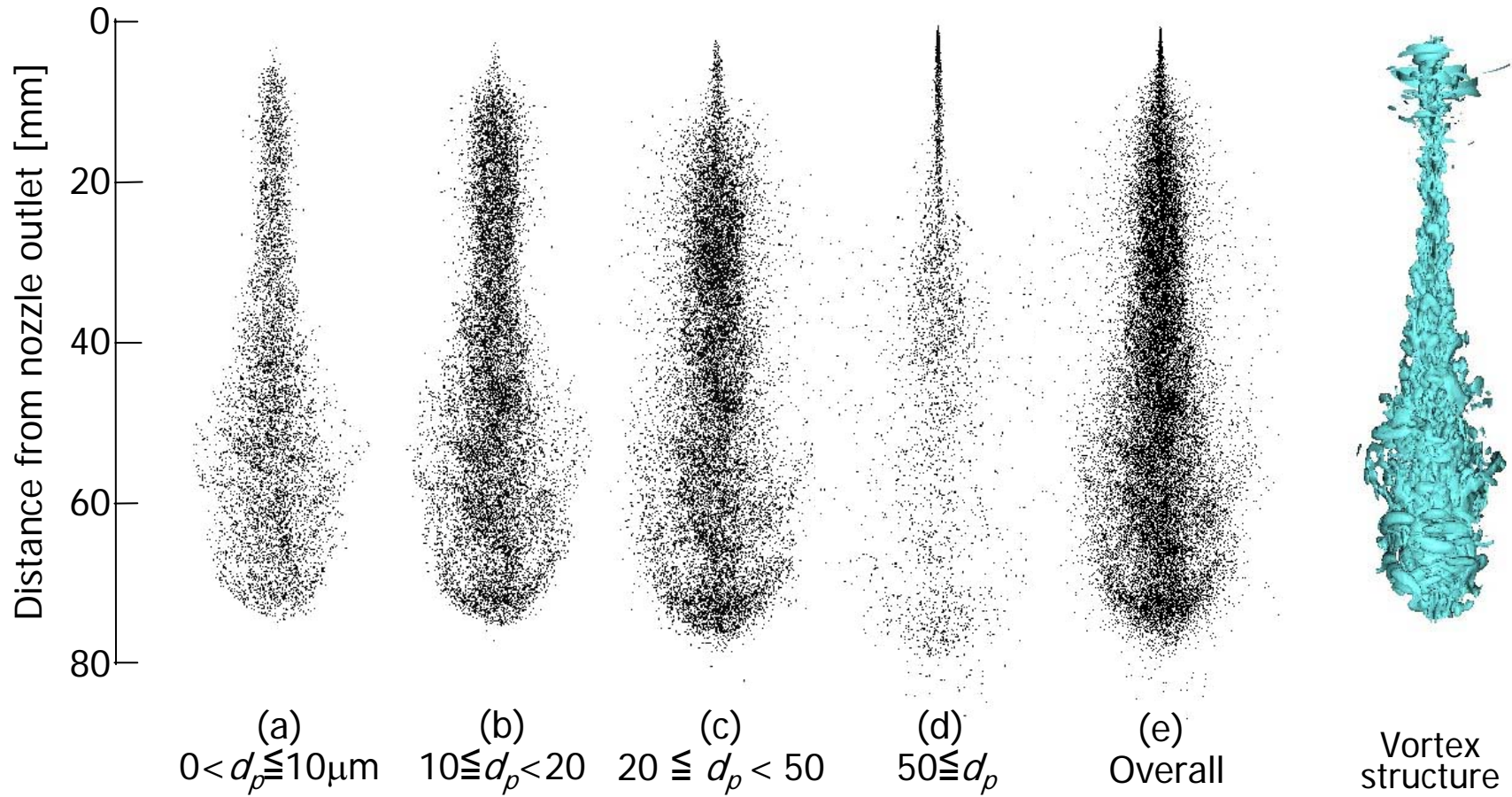
Hairpin vortex



"On the vortical structure in a round jet", Matsuda et.al..

# Droplet dispersion by Coherent vortex

$t = 1.8\text{ms}$





# Conclusion

1. It is possible to simulate the heterogeneous structure of a diesel spray by the method proposed in this work.
2. The spray tip penetration and SMD obtained through the simulation agree well with that shown through the experiments.
3. It is able to simulate the detailed 3-D structure of vortex in a diesel spray. The structure is almost the same as that of a coaxial jet.
4. It is capable of explaining the actual phenomena in a diesel spray by the simulated result.
5. There is the capability of the application of LES to not only an evaporating diesel spray but also a burning diesel spray.





Thank you for your kind attention!