# Large Eddy Simulation of Diesel Spray Flame using KIVA-LES with Flamelet Model and CIP Scheme

30th International Energy Association Task Leaders Meeting

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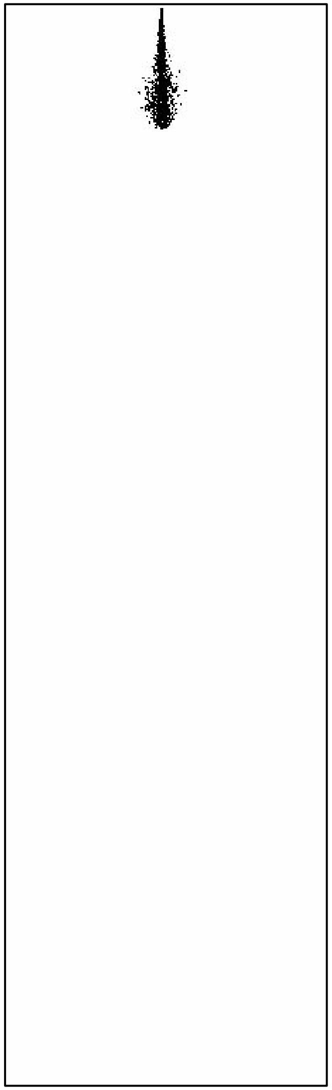
# Diesel spray simulation



Conventional spray simulation

1.Computational code (KIVA, Star-CD, Fire, etc.)

(1)DDM

(2)Two way coupling

(3)RANS approach for turbulent analysis

2. Improvement approach

(1)Spray model(droplet breakup model, evaporation model)

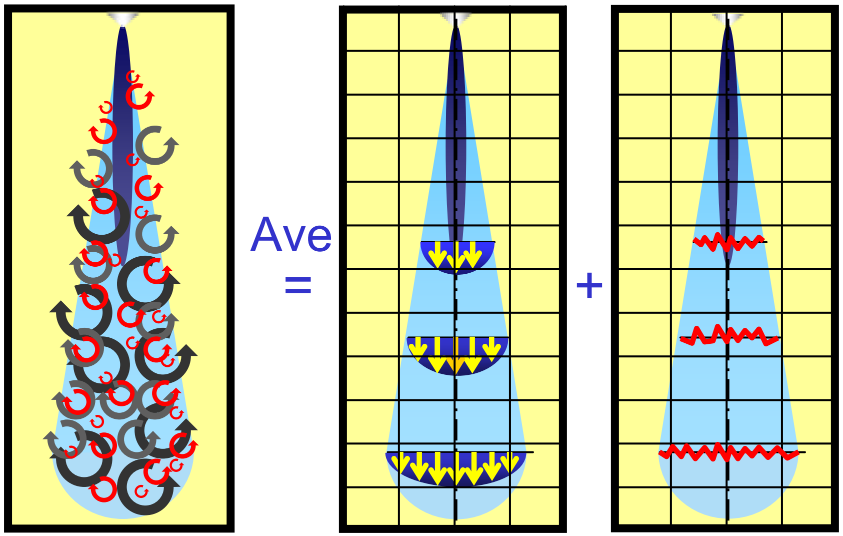
(2)Interaction between turbulent flow and chemical reaction

(3)Detailed chemical mechanism

(4) RANS → Large Eddy Simulation(LES)

# Difference between RANS and LES in diesel spray simulation

## RANS approach (Conventional method ex.KIVA code)

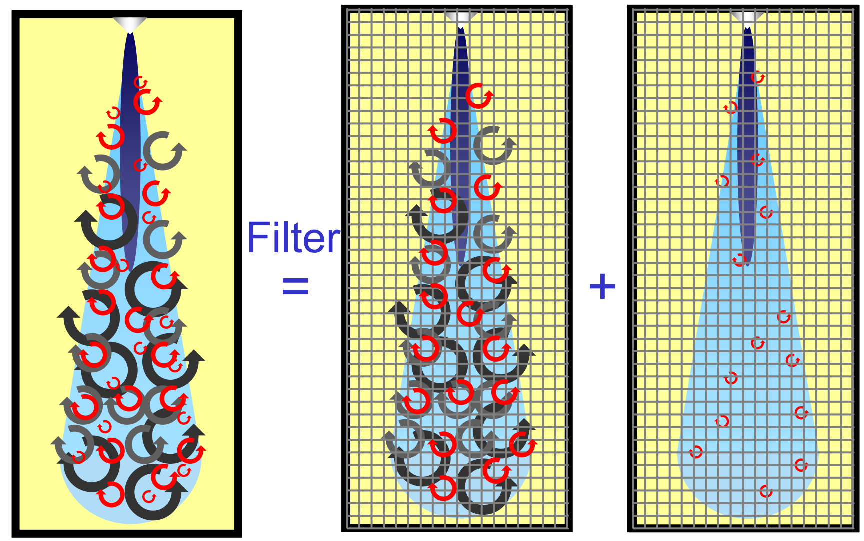



DNS or Experiment — Averaged (Resolved) — Fluctuation (Modeled)

$u \;=\; \bar{u} \;+\; u'$

(1) CPU cost is low
(2) Vortex information is lost in the averaged process

## LES approach (Present way)



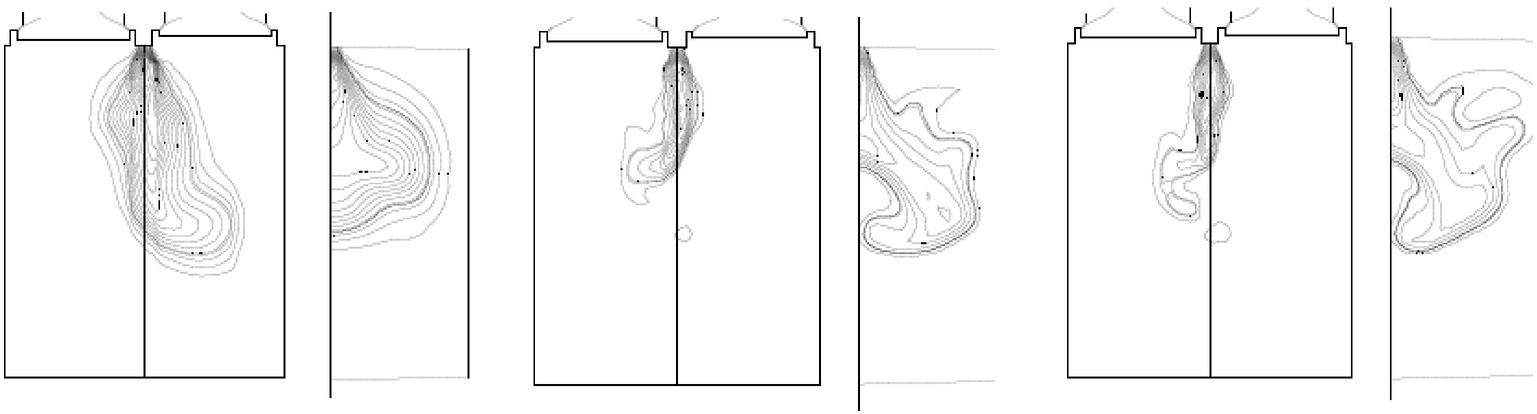

DNS or Experiment — GS (Resolved) — SGS (Modeled)

$u \;=\; u^{gs} \;+\; u^{sgs}$

(1) CPU cost is high
(2) Vortex of GS is predicted on the resolved field

# KIVALES

LES approach is incorporated into KIVA3V res.2 according to Sone and Menon paper



(a)KIVA3V (b)KIVALES (c)KIVALES-LEM

Refference

* Sone, K. and Menon, S., "KIVALES: A New Large-Eddy Simulation Approach Based on the Kiva-3V Code. Part II: User's Manual ," Georgia Tech, CCL Technical Report, CCL-00-009, 2000

* Sone, K. and Menon, S., "KIVALES: A New Large-Eddy Simulation Approach Based on the Kiva-3V Code. Part I: Formulation and Validation Studies ," Georgia Tech, CCL Technical Report, CCL-00-008, 2000

CCL(Computational Combustion Lab) , http://www.ccl.gatech.edu/home_html

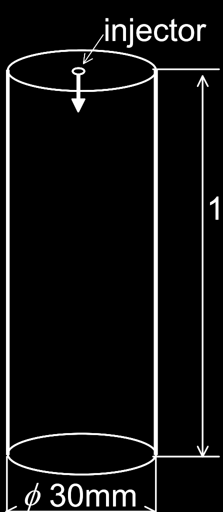
# LES of Diesel Spray Flame with FTS model

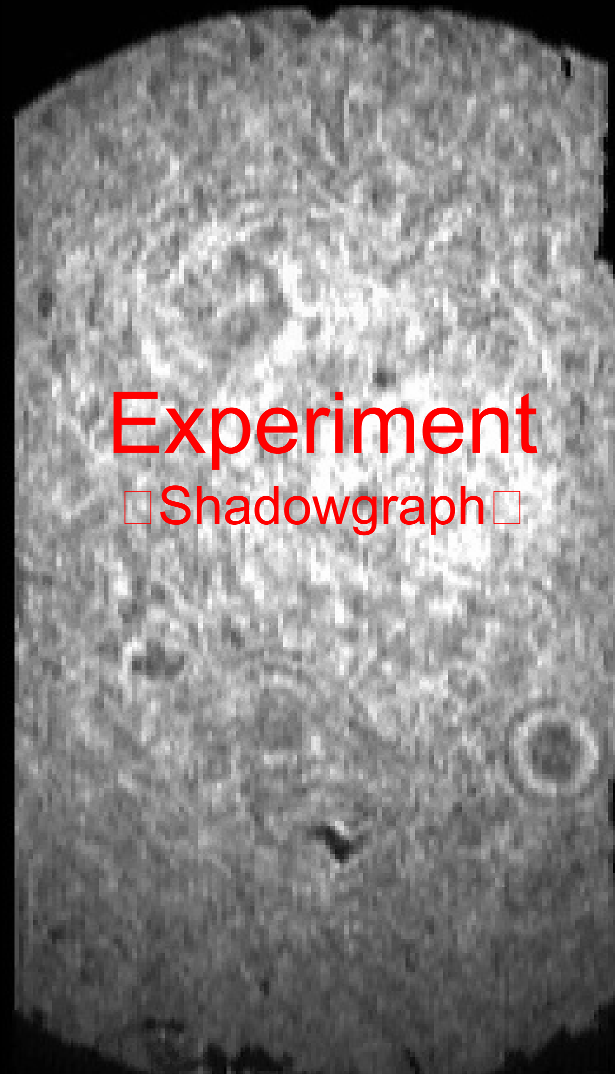
| | | |
|---|---|---|
| Code | KIVA-LES | |
| Temporal accuacy | Spatial □secand order□Temporal: first order | |
| Convective scheme | Momentum equation | CIP method |
| | Others | QSOU (KIVA standard scheme) |
| SGS stress model | $k$-$\Delta$ model | |
| SGS scalar model | Gradient diffusion model | |
| Injection model | Blobs model | |
| Break up model | KHRT or Modified TAB model | |
| Droplet evaporation | KIVA original model | |
| Collision and coallecence model | W/O | |
| Reaction mechanism for fuel | One step reaction | |
| Low temperature oxidation model | Shell model ; $T_a$ <1000K | |
| High temperature oxidation model | Flamelet model (FTS model) ; $T_a$ >1000K | |

# Comparison of evaporative diesel spray between LES and RANS

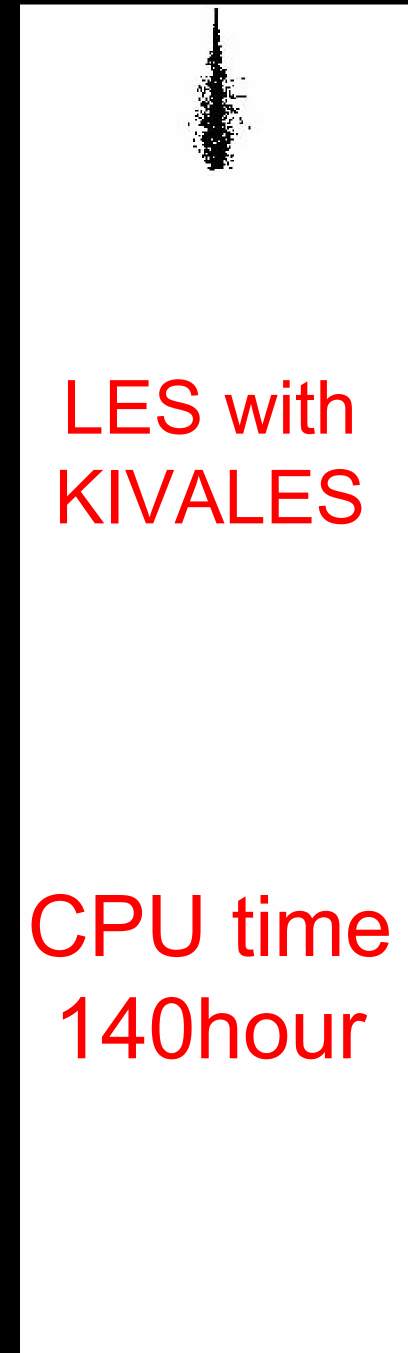
$t$ = 0.0-5.0 ms
$p_{inj}$ 77 MPa
$\rho_a$ 15 kg/m$^3$
$t_{inj}$ 1.8 ms

Computational grid
60x60x200
(720,000)
Computational cost
140 hour



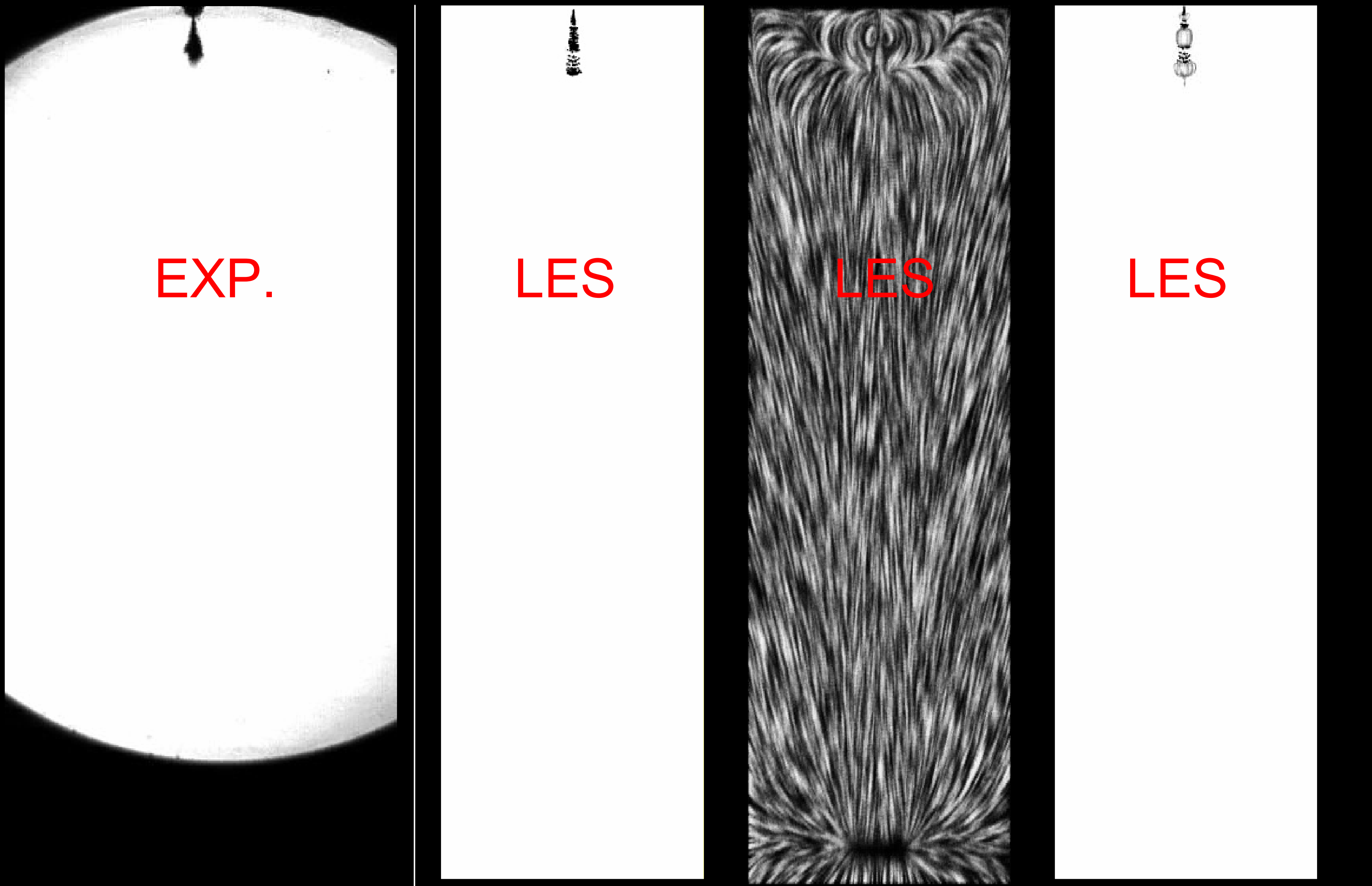




↑ Exp. (Shadowgraph)

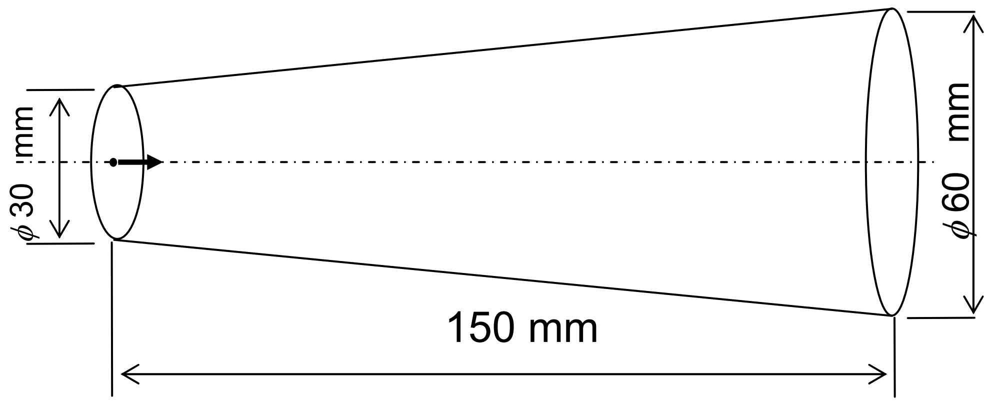

Hori, T., Senda, J., Kuge T. and H. Gen Fujimoto,
SAE paper 2006-01-3334, 2006.

# LES results of a non-evaporative spray ($p_{inj}$=80MPa, $\rho$=17kg/m$^3$)




Exp.(Shadowgraph) | 3D spray | 2D flow line | 3D spray + vortex

# Validation of LES results using experimental data of ECN(Engine Combustion Network)

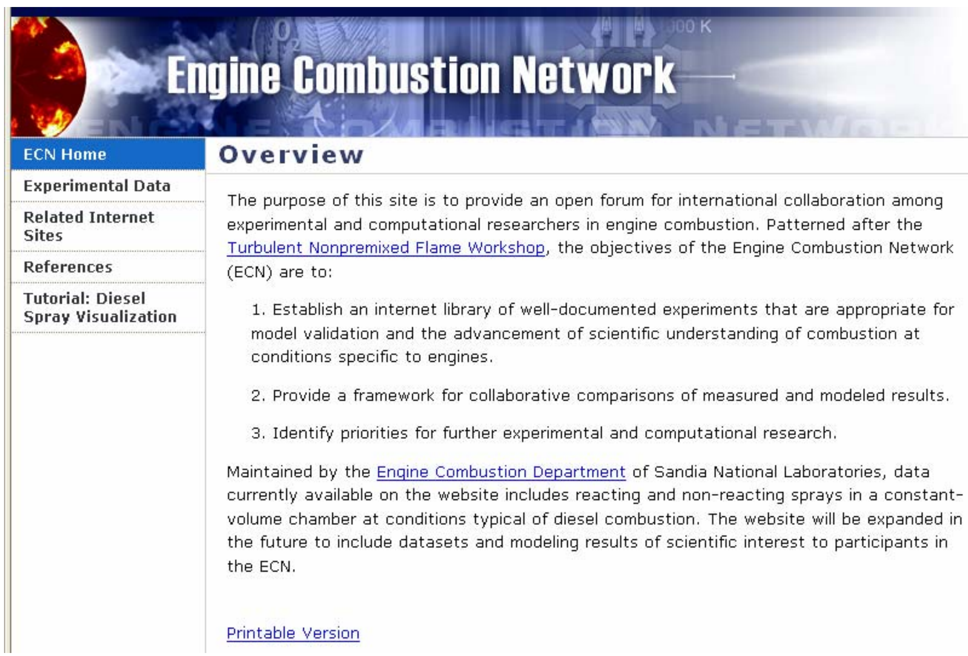



Grid□($r$□$\theta$□$z$□□□120,60,300□
= 2,160,000

Computational time□55 day□5.5ms□

Computational device :

CPU=Xeon, memory=32GB



Engine Combustion Network

ECN Home
Experimental Data
Related Internet Sites
References
Tutorial: Diesel Spray Visualization

**Overview**

The purpose of this site is to provide an open forum for international collaboration among experimental and computational researchers in engine combustion. Patterned after the Turbulent Nonpremixed Flame Workshop, the objectives of the Engine Combustion Network (ECN) are to:

1. Establish an internet library of well-documented experiments that are appropriate for model validation and the advancement of scientific understanding of combustion at conditions specific to engines.
2. Provide a framework for collaborative comparisons of measured and modeled results.
3. Identify priorities for further experimental and computational research.

Maintained by the Engine Combustion Department of Sandia National Laboratories, data currently available on the website includes reacting and non-reacting sprays in a constant-volume chamber at conditions typical of diesel combustion. The website will be expanded in the future to include datasets and modeling results of scientific interest to participants in the ECN.

Printable Version

http://www.ca.sandia.gov/ecn/

## Experimental conditions

| | | |
|---|---|---|
| Hole diameter | [mm] | 0.10 |
| Injection pressure | [MPa] | 150 |
| Injection duration | [ms] | 6.8 |
| Fuel | [-] | C7H16 |
| Fuel amount | [mg] | 17.8 |
| Fuel temperature | [K] | 357 |
| Ambient gas oxygen concentration | [-] | 0.0 vol.% |
| Ambient density | [kg/m$^3$] | 14.8 |
| Ambient pressure | [MPa] | 4.2 |
| Ambient temperature | [K] | 1000 |

LES

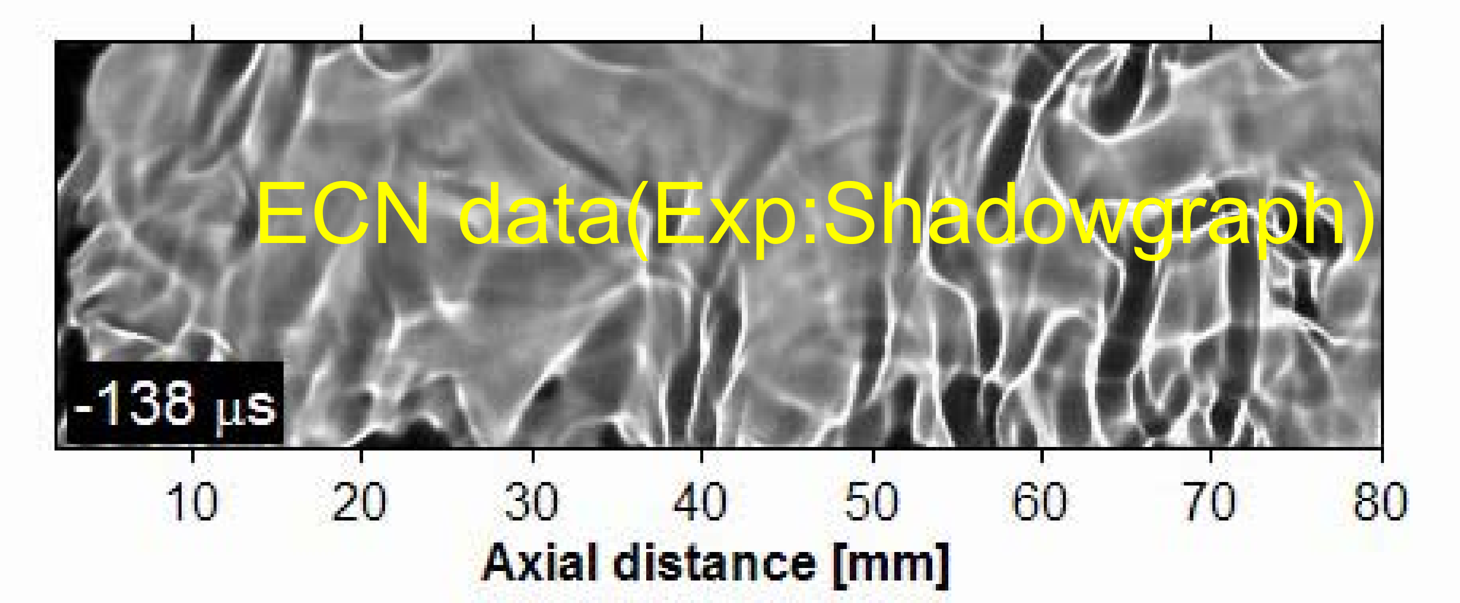
2,160,000 mesh

CPU time: 60days(-7.0ms)

LES

2,160,000 mesh

CPU time: 30days(-3.5ms)



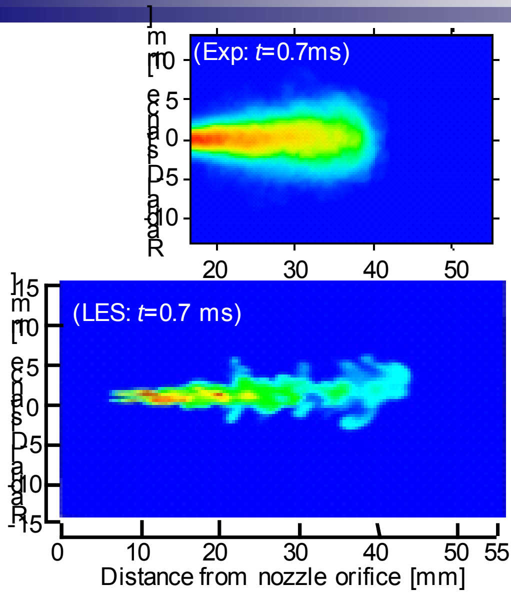

Exp.

(Shadowgraph, ECN data )

http://www.ca.sandia.gov/ecn/

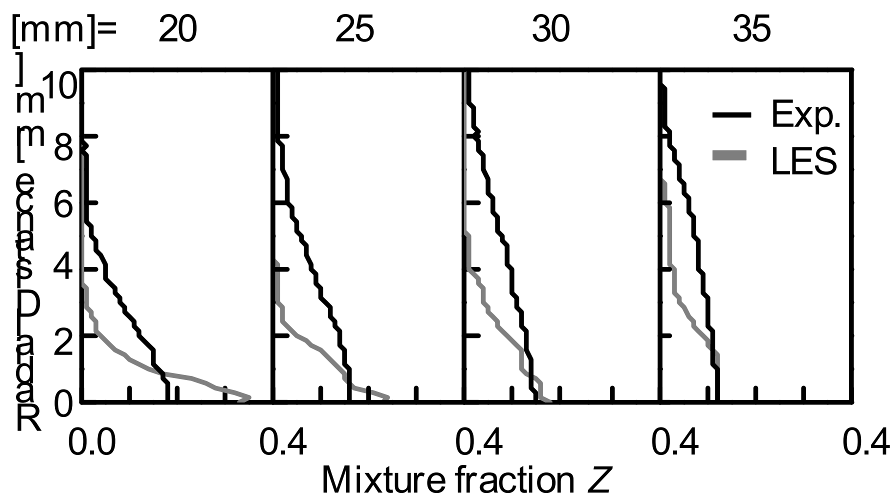
# Validation of LES result of evaporative spray using ECN data of Rayleigh scattering method ($p_{inj}$=150MPa, $\rho_a$=14.8kg/m$^3$)

*http://www.icel.tkk.fi/FSWS2008/SprayWorkshopDetroit2008_Pickett.pdf

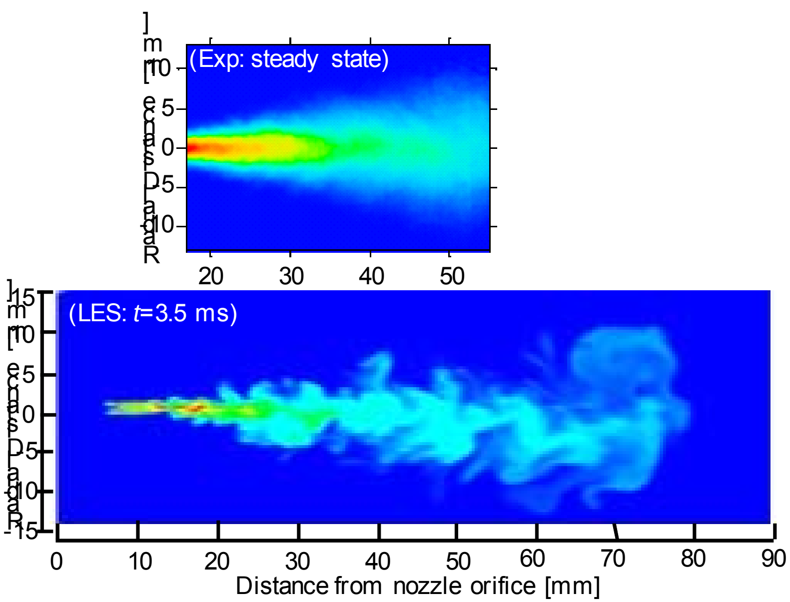


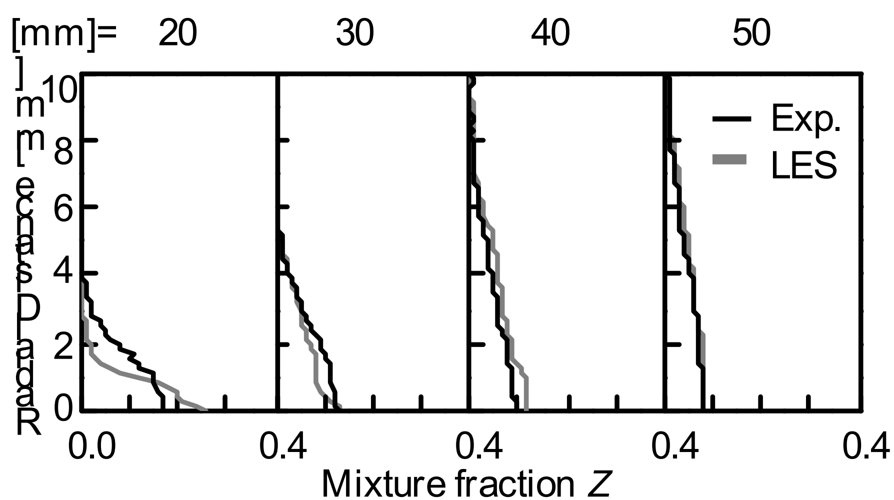

Exp.
(Mean)

LES.
(Instantaneous)




(a) $t$=0.7ms

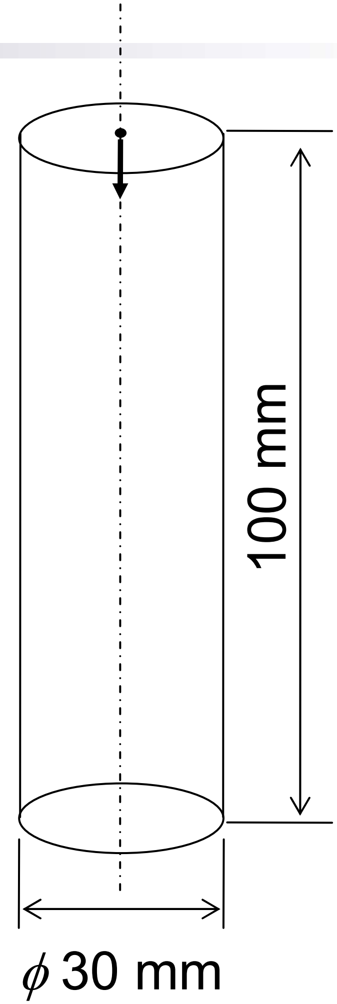



(b) $t$=3.5ms

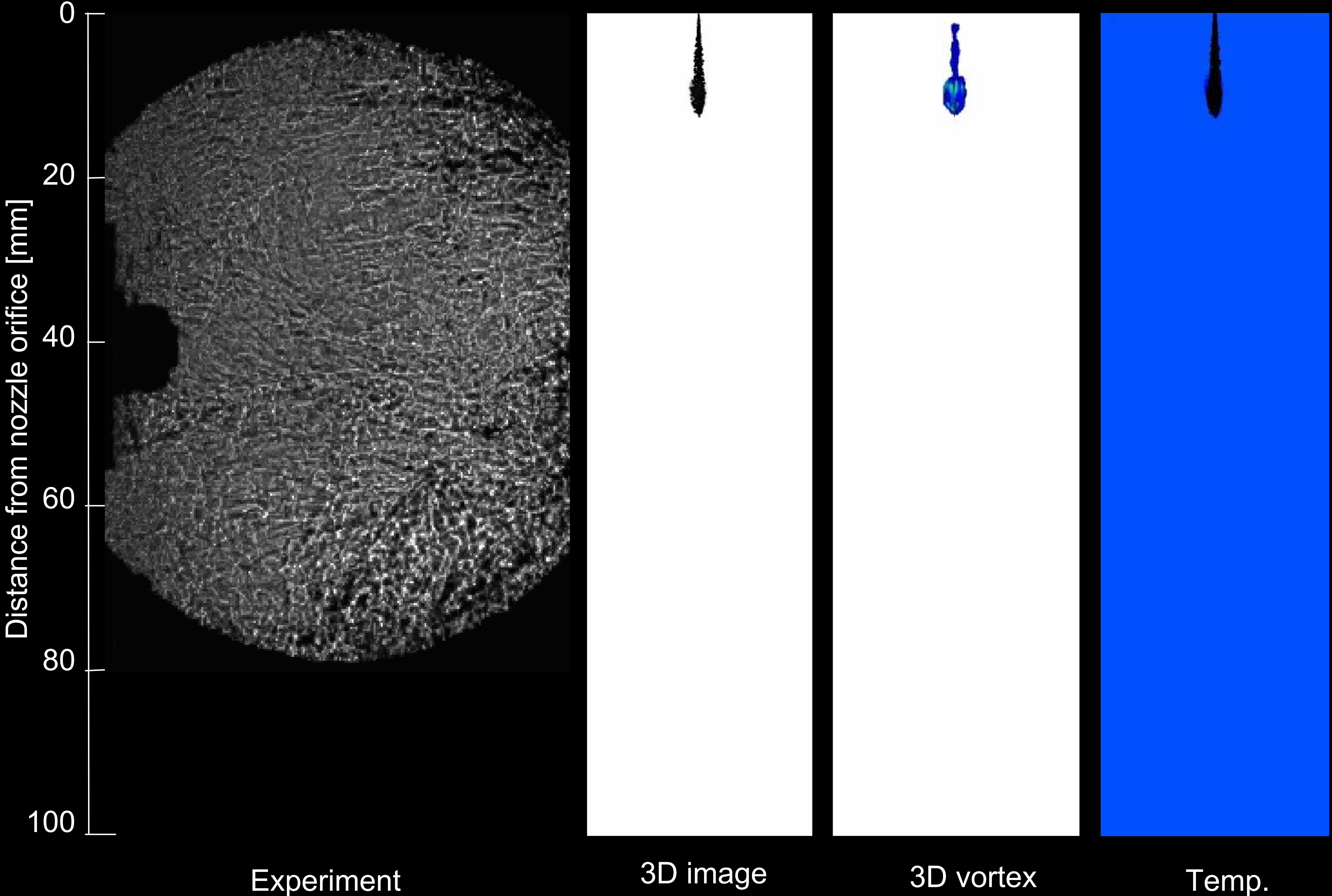
# Computational conditions of diesel spray flame simulation

| | | |
|---|---|---|
| Hole diameter | [mm] | 0.20 |
| Injection pressure | [MPa] | 70 |
| Injection duration | [ms] | 2.2 |
| Fuel | | C12H26 |
| Fuel amount | [mg] | 20.0 |
| Fuel temperature | [K] | 300 |
| Ambient gas oxygen concentration | | 21 vol.% |
| Ambient pressure | [MPa] | 4.1 |
| Ambient temperature | [K] | 900 |

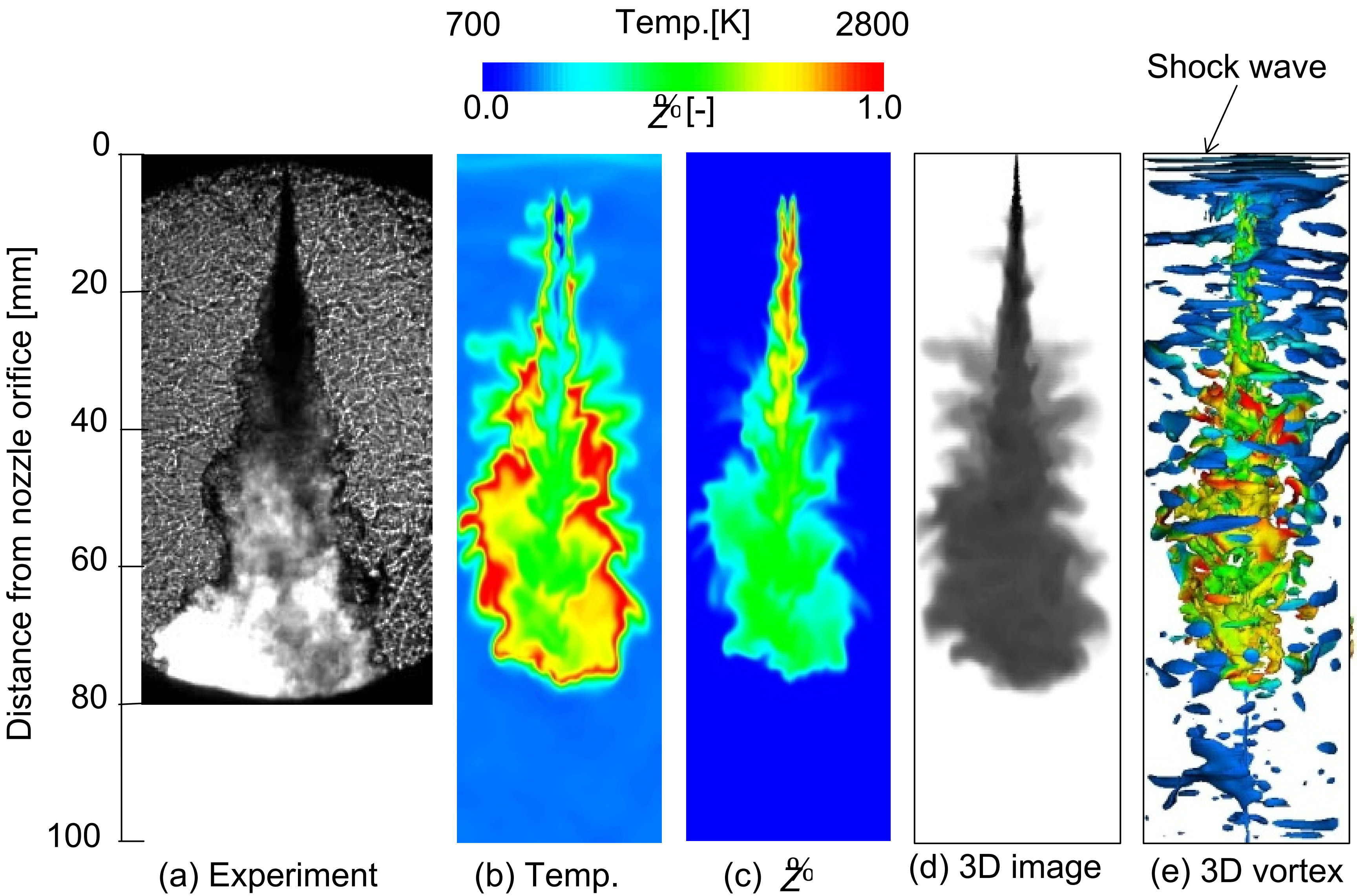



Computational grid□60x60x200
CPU time□333h
(cycle=48,000,5.0ms)

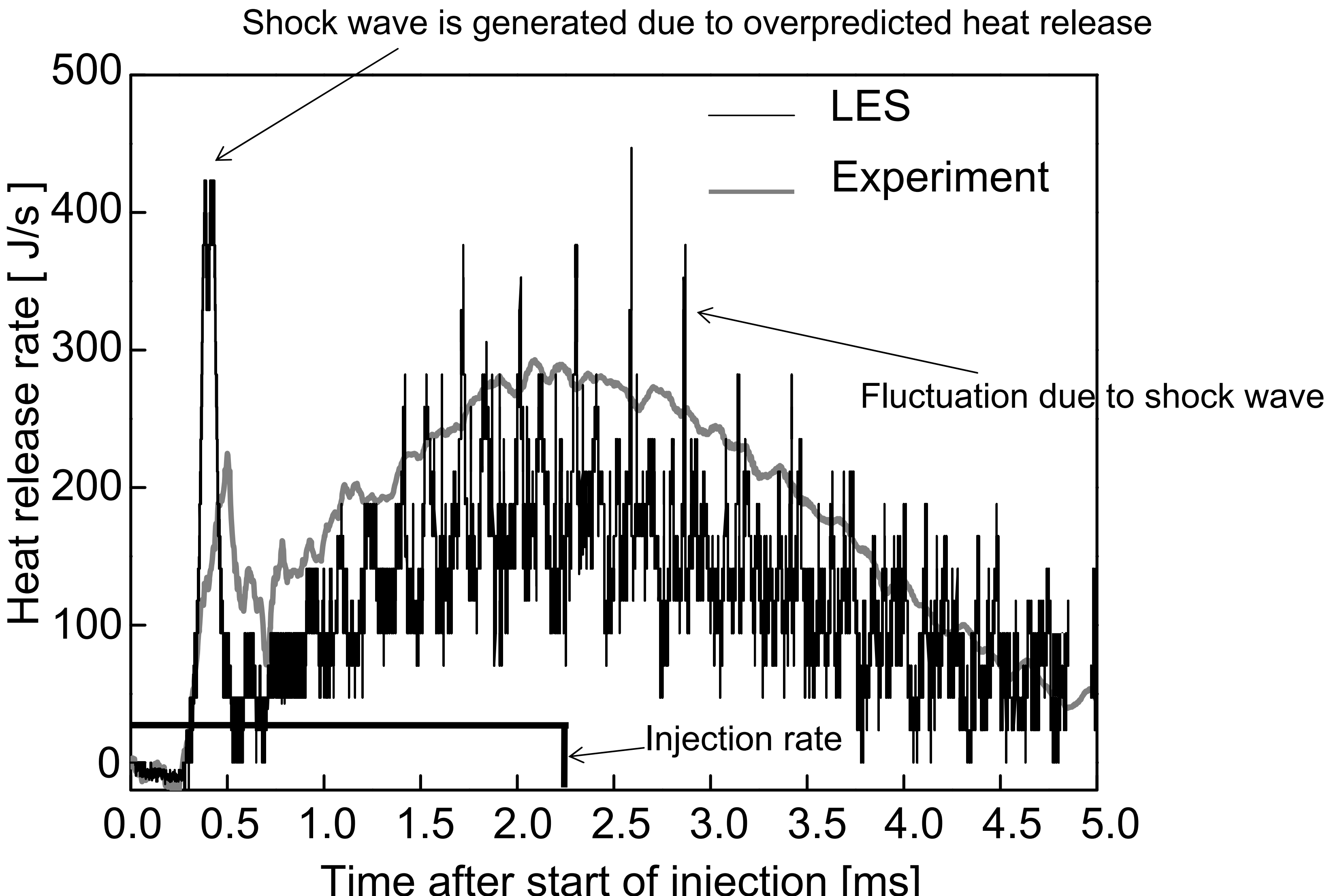
# Time evolution of diesel spray flame



# Instantaneous spray shape at 2.2 ms



# Comparison of heat release rate between LES and experimental result



# Summary and Conclusion

Diesel spray simulation using LES has been developed to describe the unsteady formation process of diesel spray.

1. In LES approach, the unsteady formation process of a diesel spray is able to be predicted, because the vortex in the gas phase is simulated. This vortex is not predicted in conventional RANS approach.
2. The good agreement of mixture distribution in evaporative diesel spray between LES and Rayleigh scattering method is obtained at the steady state.
3. Diesel spray flame simulation using LES is able to be captured the shock wave in addition to the unsteady spray formation process.