REAL SIZE CALCULATION OF HIGH PRESSURE HYDROGEN FLOW AND ITS AUTO-IGNITION IN CYLINDRICAL TUBE

ASAHARA, Makoto : Aoyama Gakuin University
YOKOYAMA, Akinori : Aoyama Gakuin University
TATSUMI, Yuto : Aoyama Gakuin University
KATO, Suguru : Aoyama Gakuin University
YAMADA, Eisuke : Aoyama Gakuin University
Hayashi, A.Koichi : Aoyama Gakuin University

5th International Conference on Hydrogen Safety
September 9-11, 2013
Brussels, Bergium

Background (1)

Why do we study H2 ignition?

- **Development of Fuel Cell system.**
- **Accidents at factories.**

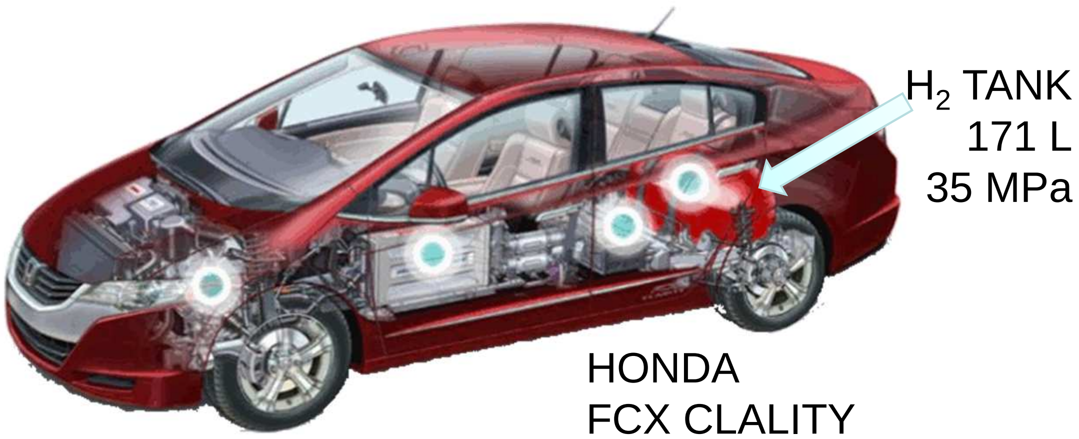
Recent accidents

- **Increase of unknown H2 explosions due to an development of fuel cell car.**

Auto-ignition by diffusion is reported.

Mechanism and conditions of such diffusion ignition are not much known so far.

Needs safety standard for auto-ignition of high pressure hydrogen.



Background (2) **Passed Studies**

Wolański and Wójcicki (1973)

Investigate the mechanism of the diffusion ignition of a combustible gas flowing into an oxidizing atmosphere.

Tanaka et al. (1979)

Uejima et al. (1998)

Liu et al. (2005), Bazhenova et al. (2005)

Calculate the hydrogen jet coming out to air at the room temperature.

Dryer et al. (2007), Pinto et al. (2007)

Show the unique ignition potentials for pressurized releases of hydrogen.

Golub et al. (2008), Mogi et al. (2008), Yamada et al. (2008)

Show the relationship between the pressure and the length of tube.

Xu et al. (2008)

Discuss an auto-ignition would initiate inside the tube at the contact surface due to mass and energy exchange.

Mogi et al. (2009), Yamada et al.(2011), Kitabayashi et al.(2012)

Kim et al. (2013)

Sandia National Laboratories (2003~)

Investigate the hydrogen Release behavior

Background (3) **AGU Passed Studies**

Liu et al. (2005)

Numerical study (DNS) on high pressure hydrogen jet spouting from a small hole.

Aizawa, Pinto, et al. (2007)

Experimental study on high pressure hydrogen jet: different length and diameters.

Kitabayashi et al. , Yamada et al. (2008)

Experimental and numerical studies on high pressure hydrogen jet:
Auto- ignition inside tube (Numerical Analysis).
Different size of tubes (Experiments)

Kitabayashi et al., Yamada et al. (2009-2012)

Experimental and numerical studies on high pressure hydrogen jet:.

Auto-ignition for different tube length (Experiments and Numerical Analysis)

Tatsumi et al., Yamada et al. (2011-)

Experimental and numerical studies on high pressure hydrogen jet:.

Different tube size (Numerical analysis)

Purpose

Numerical Analysis of High Pressure H_2 Ignition

- **Auto-ignition has not simulated at a real size level.**
  - **We do not know what happens in a real size tube numerically.**

Mogi et al. (2008)

A real size numerical analysis

- **Comparison with experiments.**
- **Validity of calculation using a detailed chemistry.**
- **Clarification of detailed auto-ignition mechanism.**

Numerical Method

◎Governing equations

- 2D axisymmetric and compressible Navier-Stokes equations with species conservation equations
- 9 species (H_2,O_2,O,H,OH,HO_2,H_2O_2,H_2O,N_2)

◎Discretization methods

- Time integration：Strang type fractional step method
- Convective term：2nd-order explicit Harten-Yee non-MUSCL modified flux type TVD scheme
- Production term：Point implicit method

◎Detailed chemical reaction model

- Petersen and Hanson model (1999)
  (P-H model)

Numerical Conditions

◎Boundary conditions

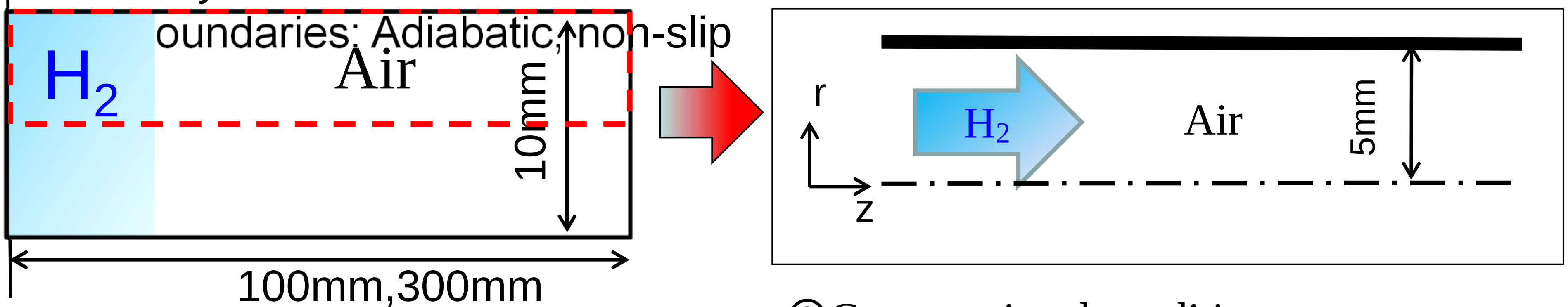
Left boundary: Inflow

Righ and their numbers are t boundary: Outflow

oundaries: Adiabatic, non-slip

2D Axisymmetric

Half of computational region



◎Initial conditions (Hydrogen)

Burst pressure, MPa	**2.0～14.6**
Temperature, K	**300**

◎Initial conditions (Air)

Burst pressure, MPa	**0.1**
Temperature, K	**300**

◎Computational conditions

Grid shape: square grids

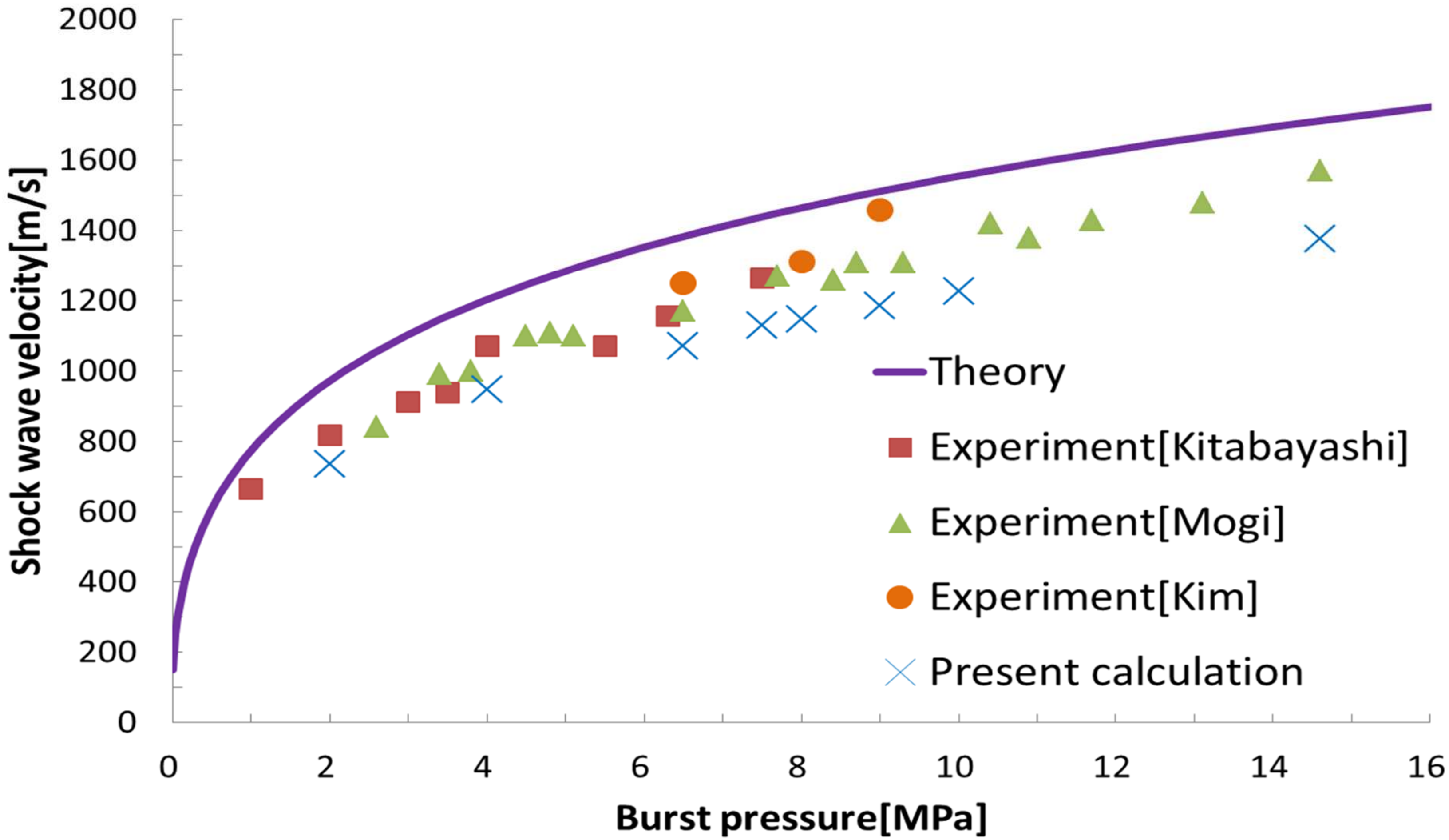
Grid points: 20001×1001, 30001×501, 15001×251

Grid sizes: 5μm, 10μm, 20μm

These values are decided based on the experimental conditions by Kitabayashi, Mogi, and Kim et al.

NUMERICAL RESULTS

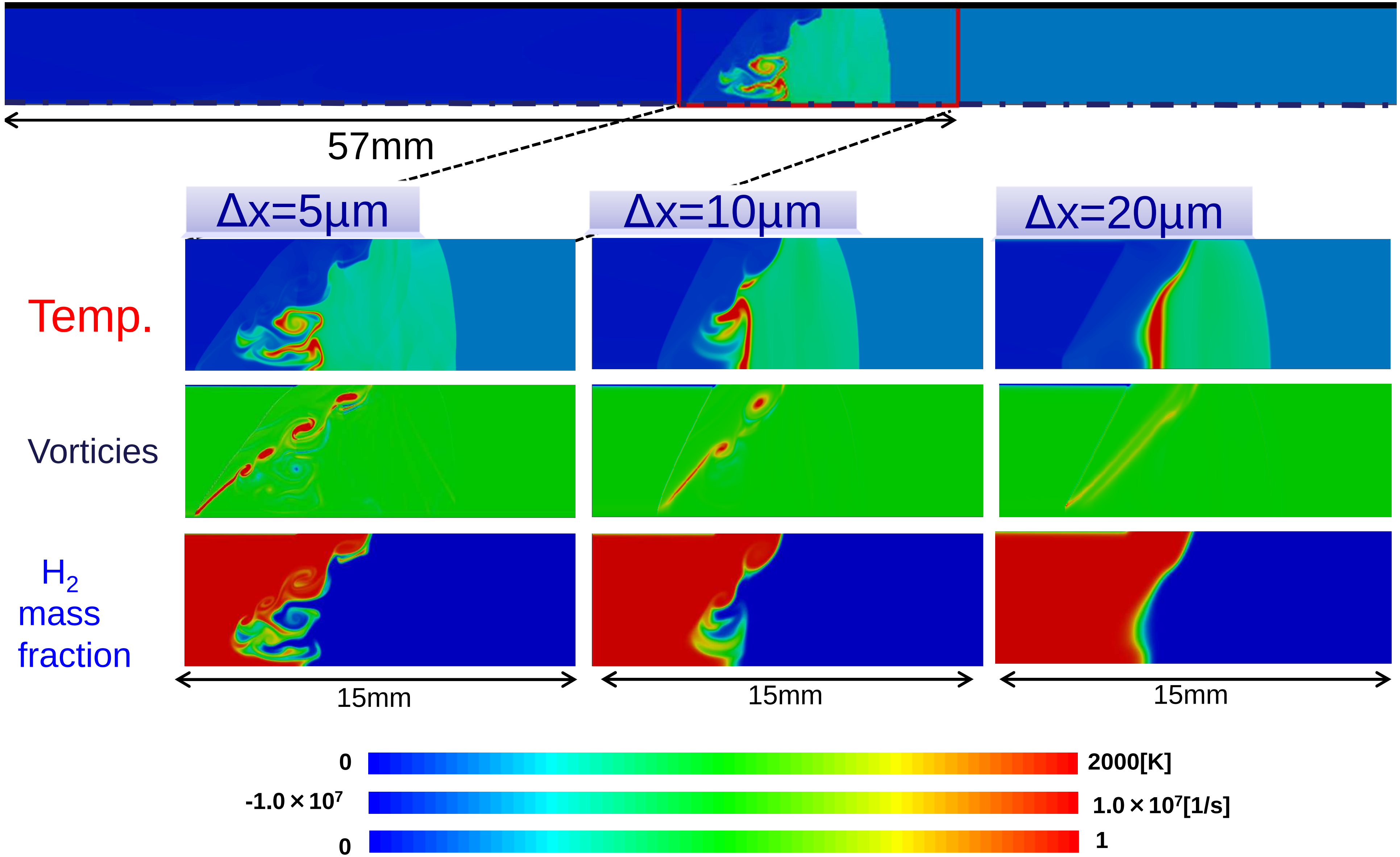
Shock Wave Velocity



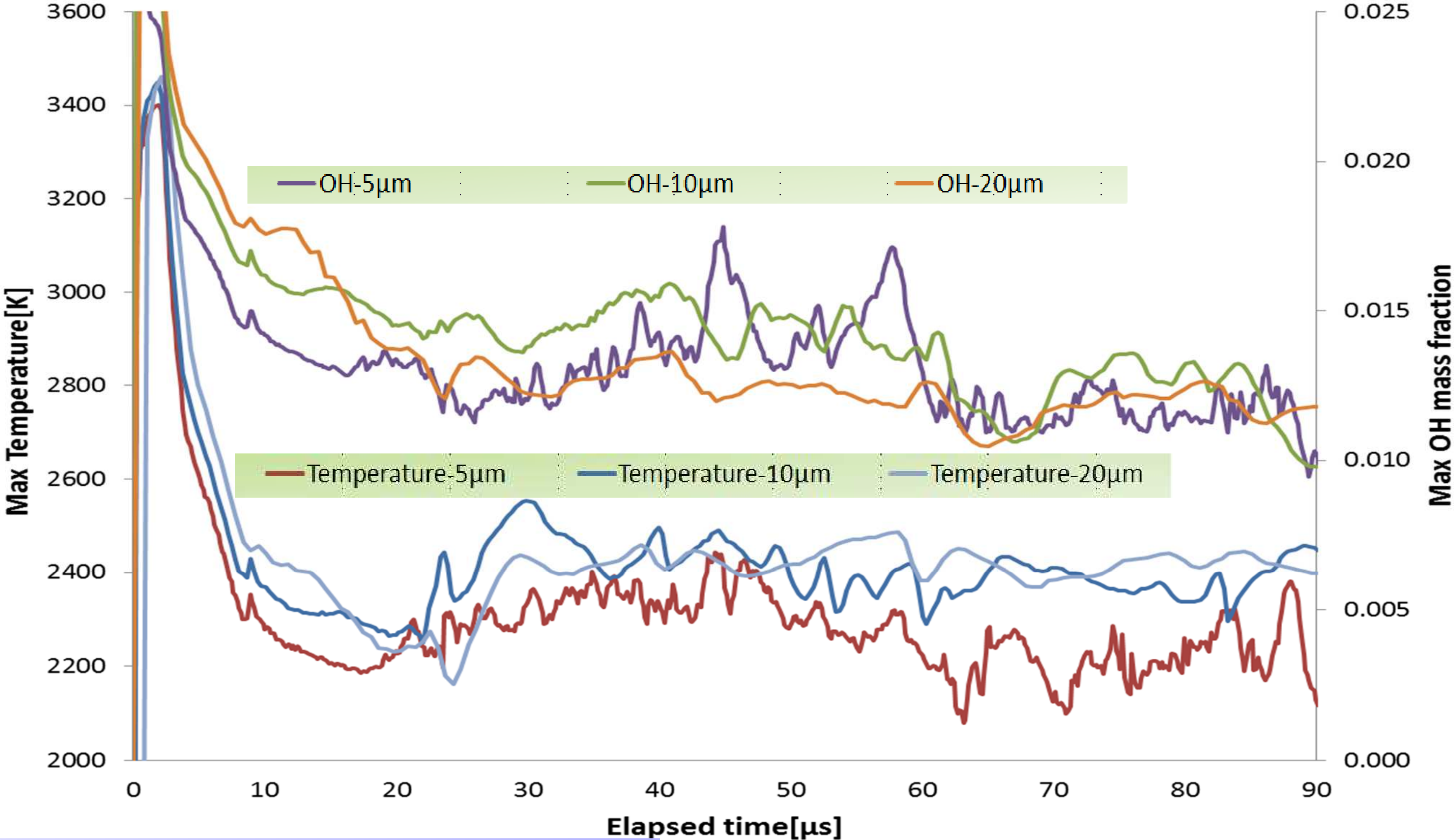
Agreement on shock wave velocity is in 20-30 % difference with the theoretical values and within 10 % with experimental values. This should certify the present numerical results.

Dependency of grid size on the results

Initial burst pressure: 14.6MPa



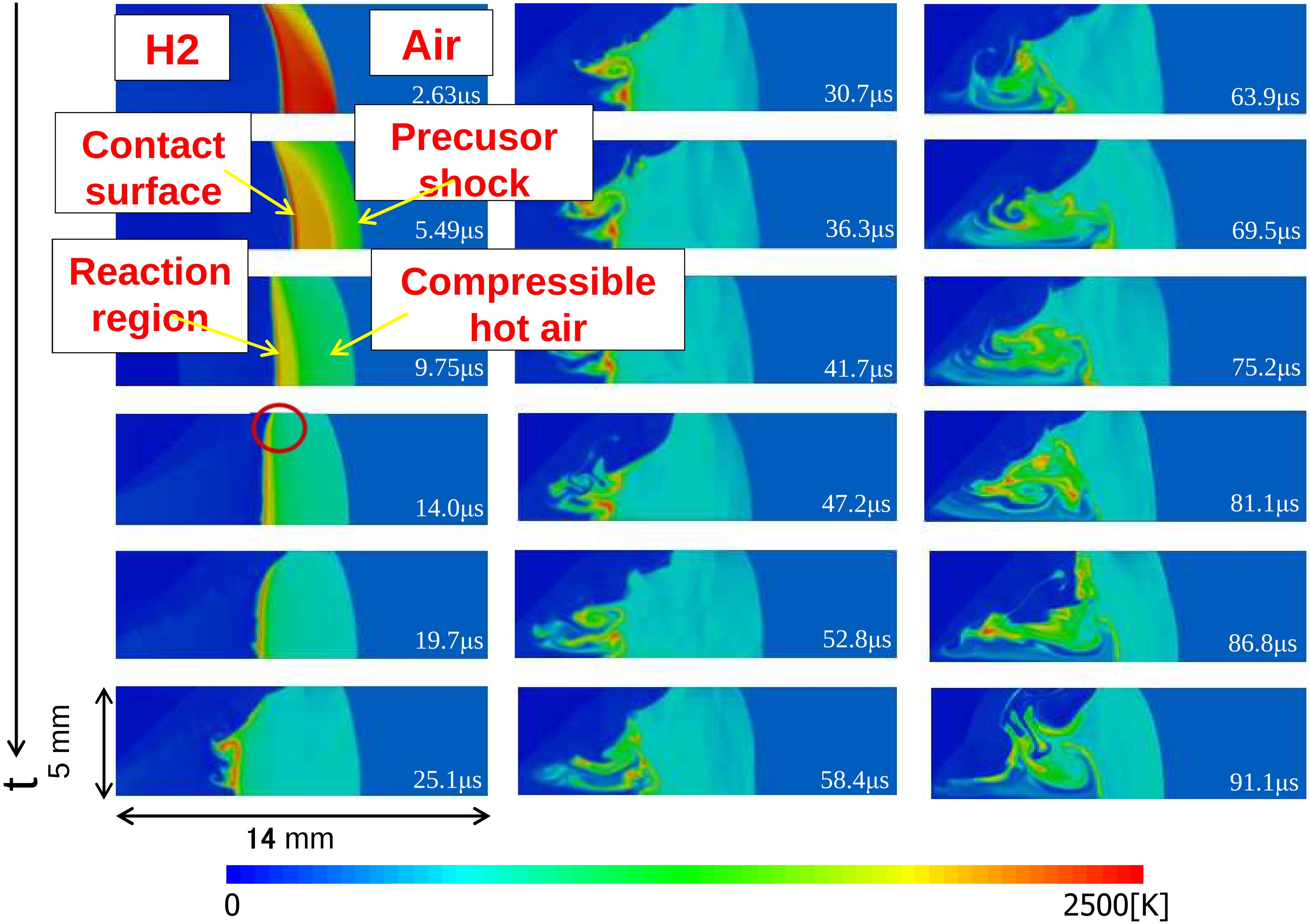
Time History of Temperature and OH Mass Fraction (Maximum values in the total numerical region)



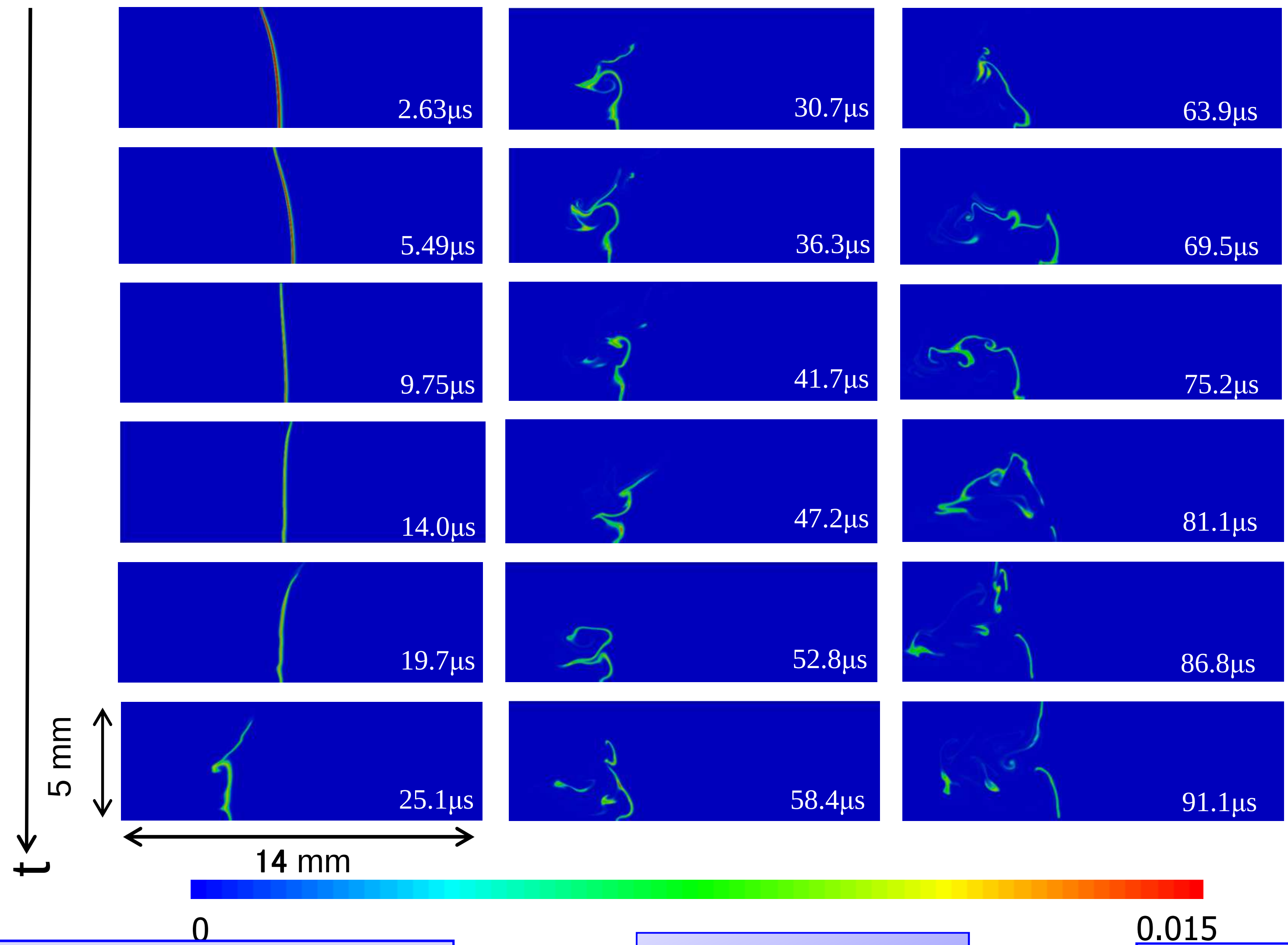
Captured the phenomena in detail when grid size is smaller.

5μm grid gives the better results.

Time History of Temperature Profiles: 5μm grid



Time History of OH Mass Fraction: 5μm



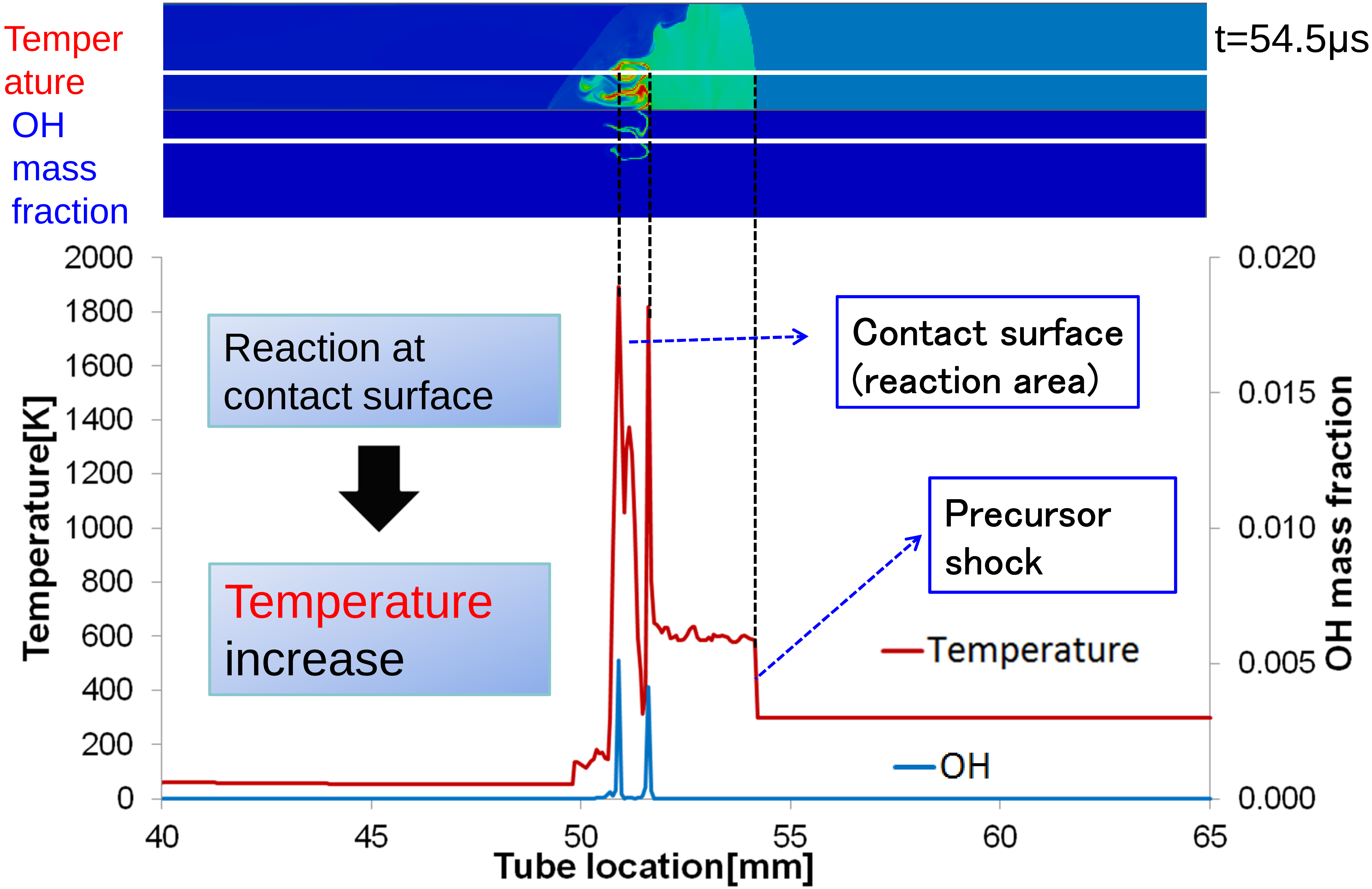
Vortices provide the contact surface fluctuation.

Expansion of reaction area.

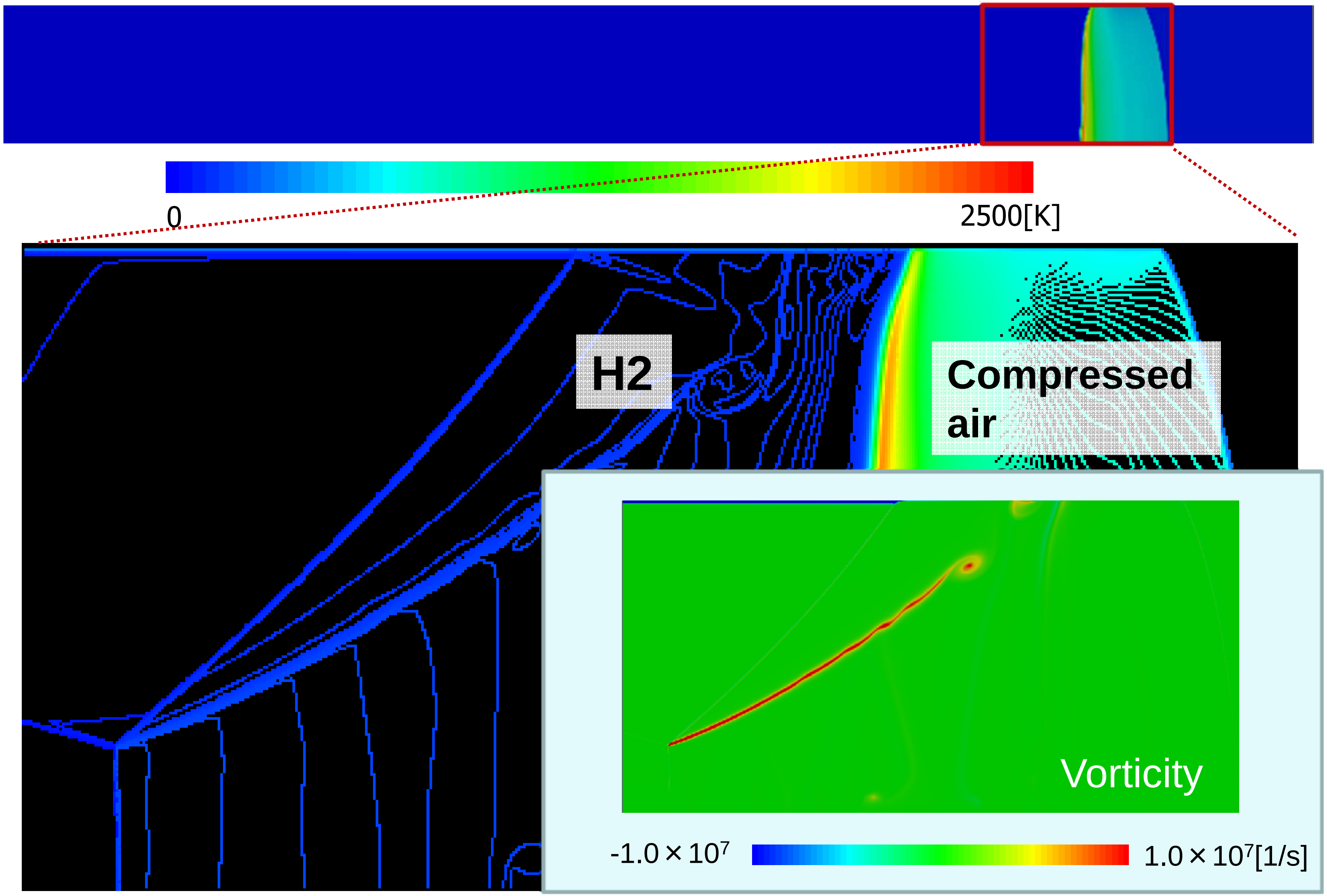
Maintenance of autoignition

Temperature and OH Profiles at certain radial position

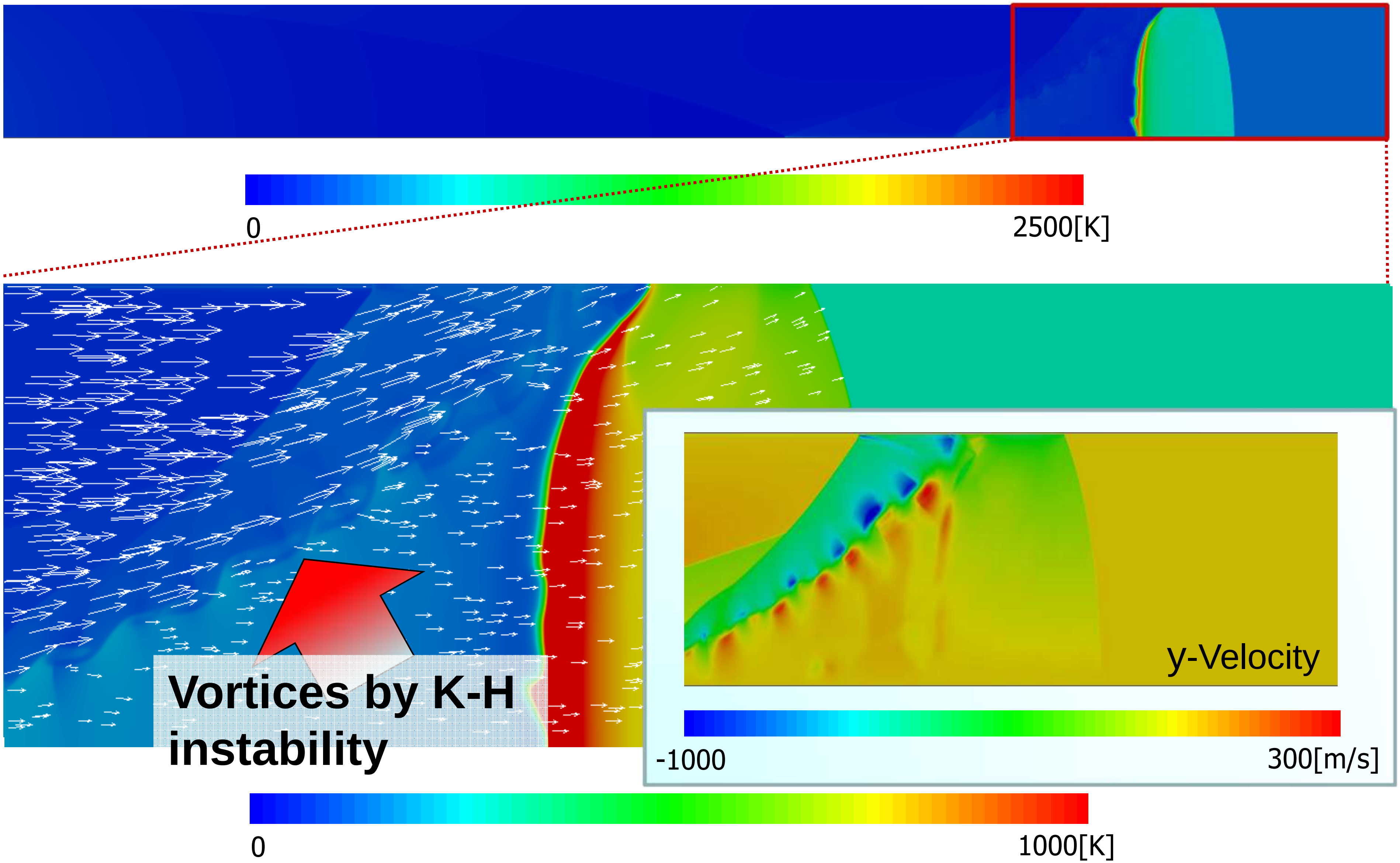
dx=dy=5μm. r=2.0mm



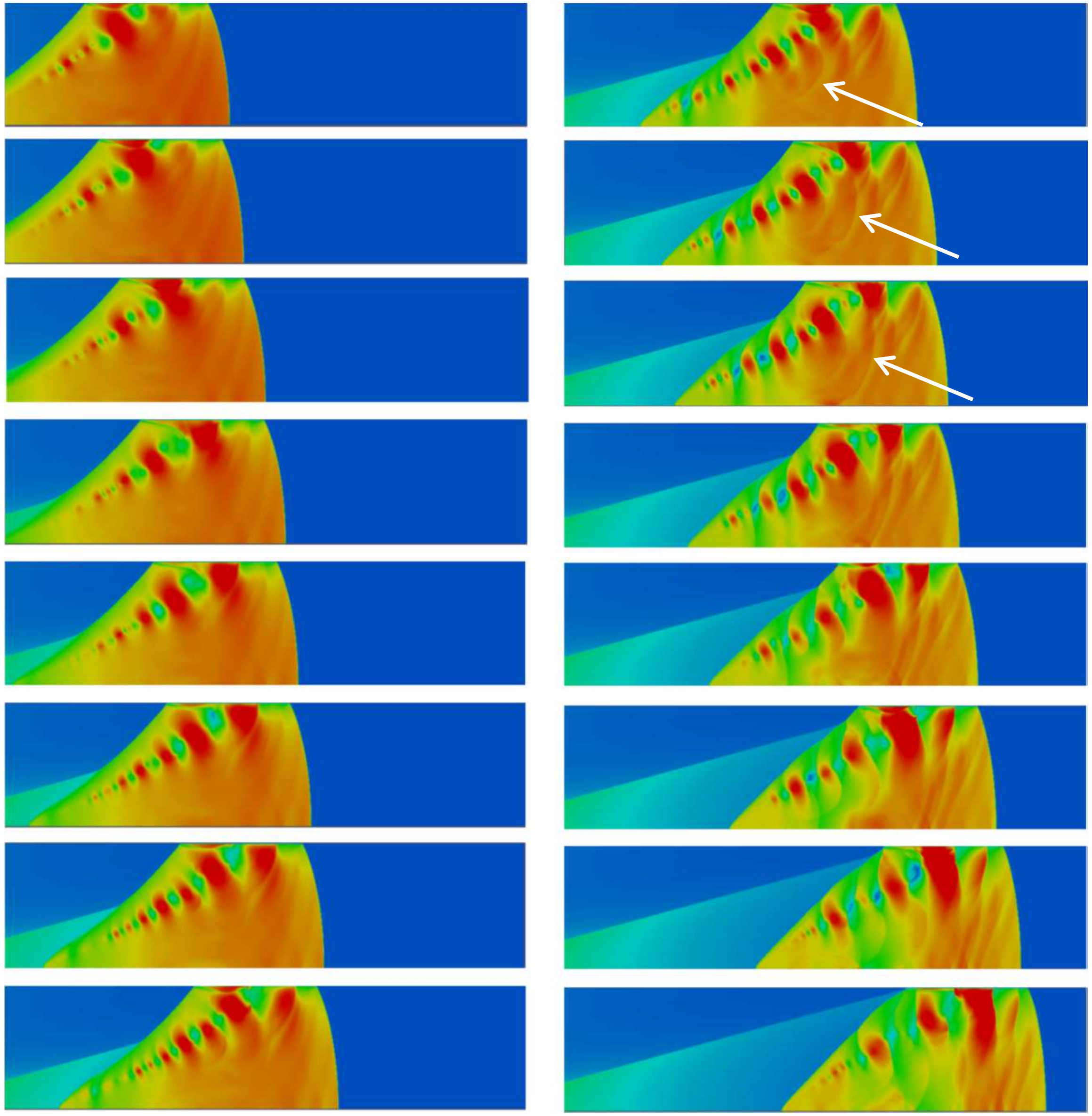
Temperature Profiles at14.0μs



Temperature Profiles at 19.7μs



Pressure Profiles at 6.9～22.5μs



Production of compressible waves by vortices

Proceeding the deformation of contact surface

Conclusions

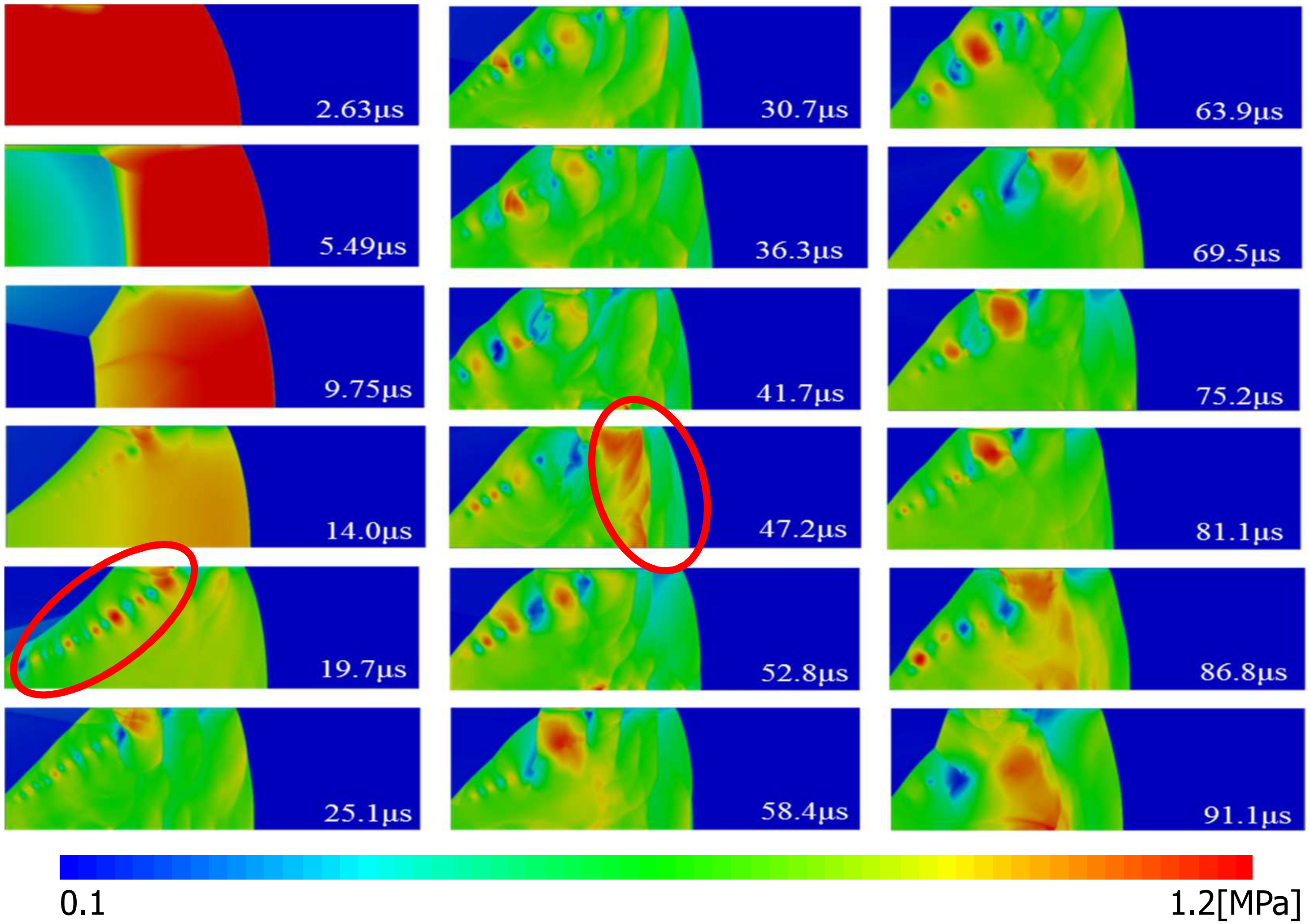
The following results are obtained by calculating high pressure hydrogen auto-ignition in a tube:

- ➢ The validity of the present numerical analysis was certified by comparing the computed results with the passed experimental results since the numerical results agree with the experimental ones within 10 % differences.
- ➢ The fluctuation at the contact surface proceeds the mixing of hydrogen with air to yield auto-ignition.
- ➢ One of the causes of contact surface fluctuation is due to vortcies produced by K･H instability.

･It is necessary to calculate the cases changing tube length and diameter.

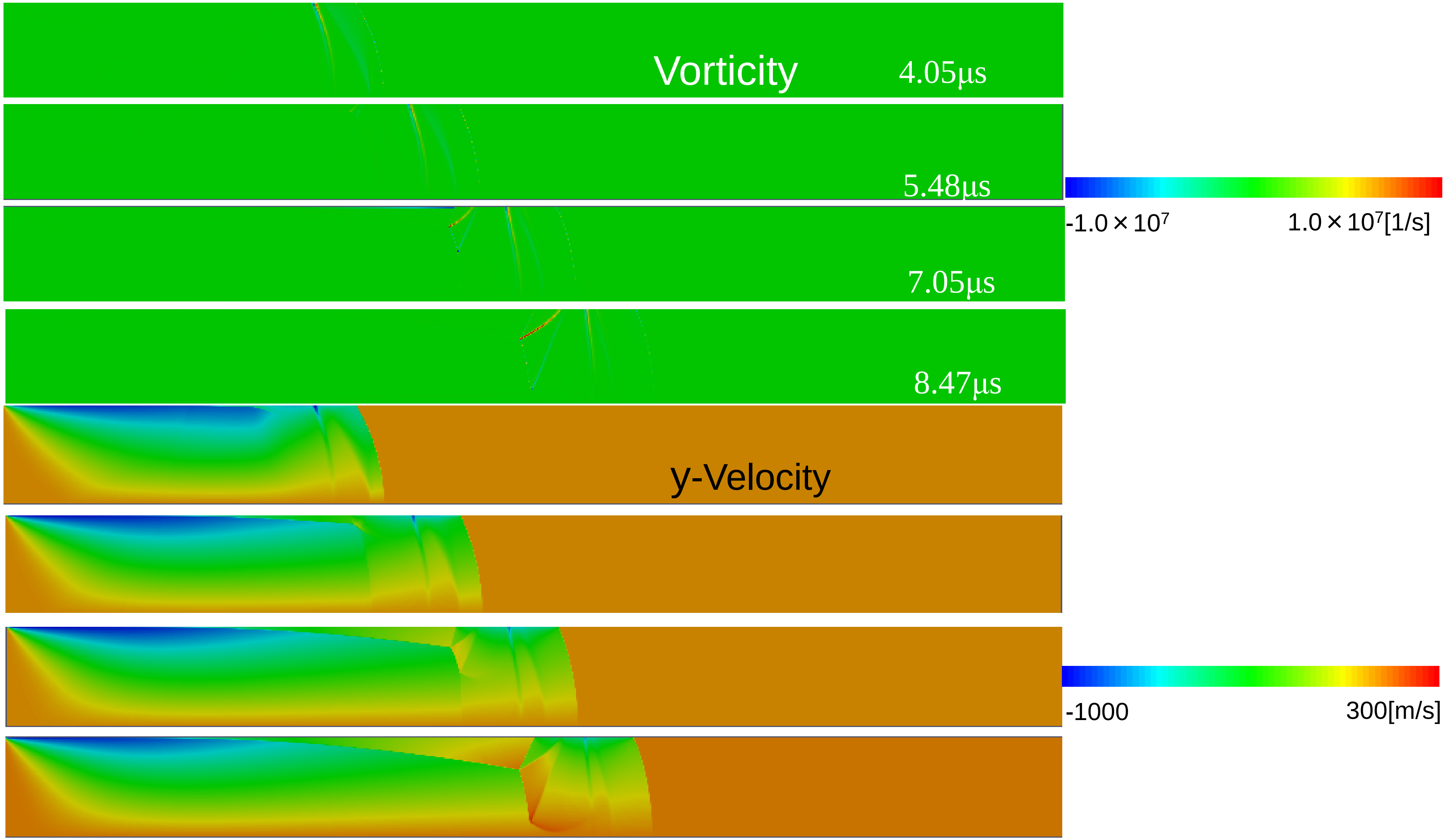
･3D calculation must be done to see the real physics in detail.

圧力分布履歴



渦によって生じた圧縮波による干渉 ⇒ 管出口まで高圧・高温を維持

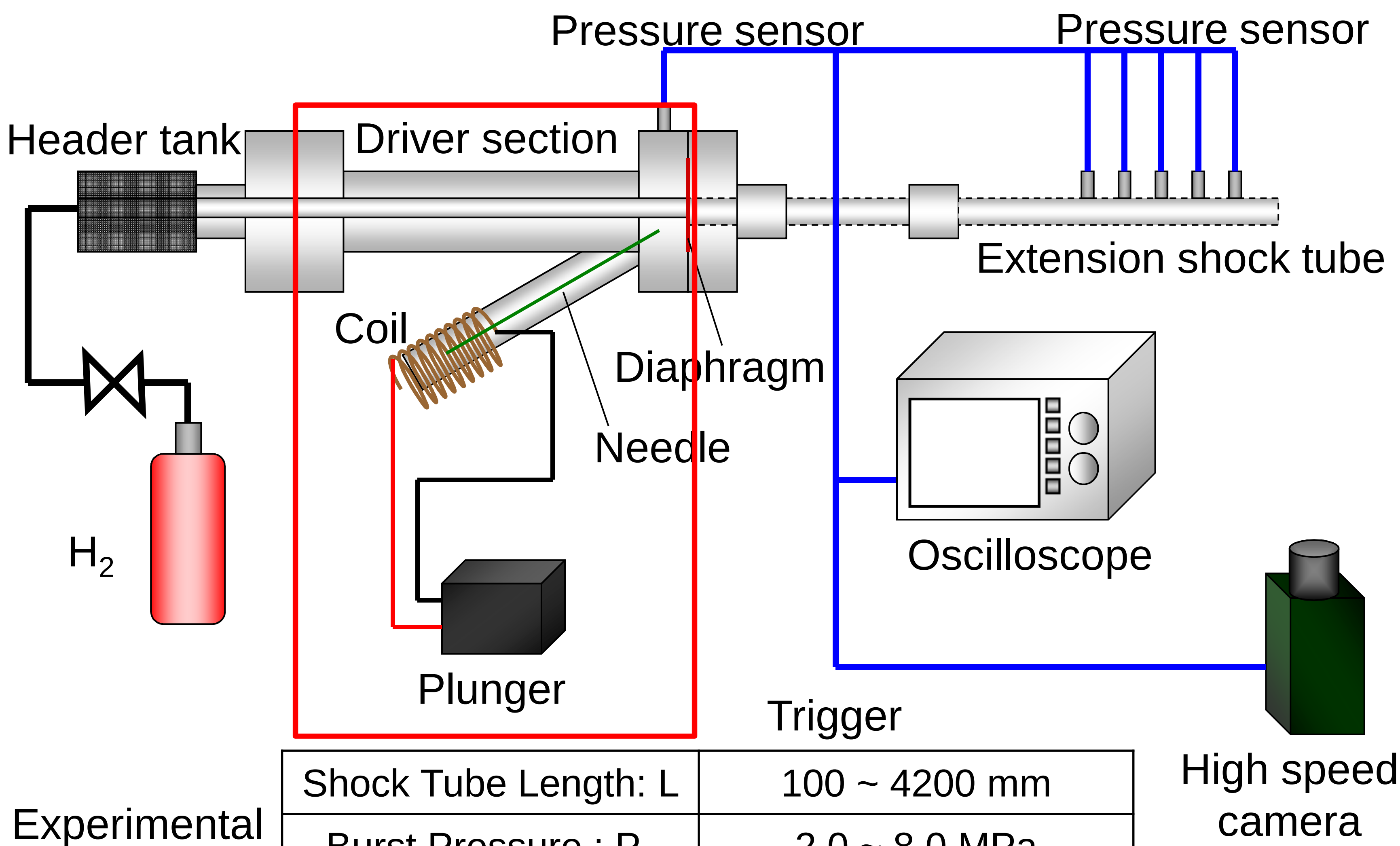
速度せん断層



Vorticity
4.05μs
5.48μs
7.05μs
8.47μs
-1.0×10⁷
1.0×10⁷[1/s]
y-Velocity
-1000
300[m/s]

Numerical Analyses of Auto-Ignition using a Shock Tube with a plunger system

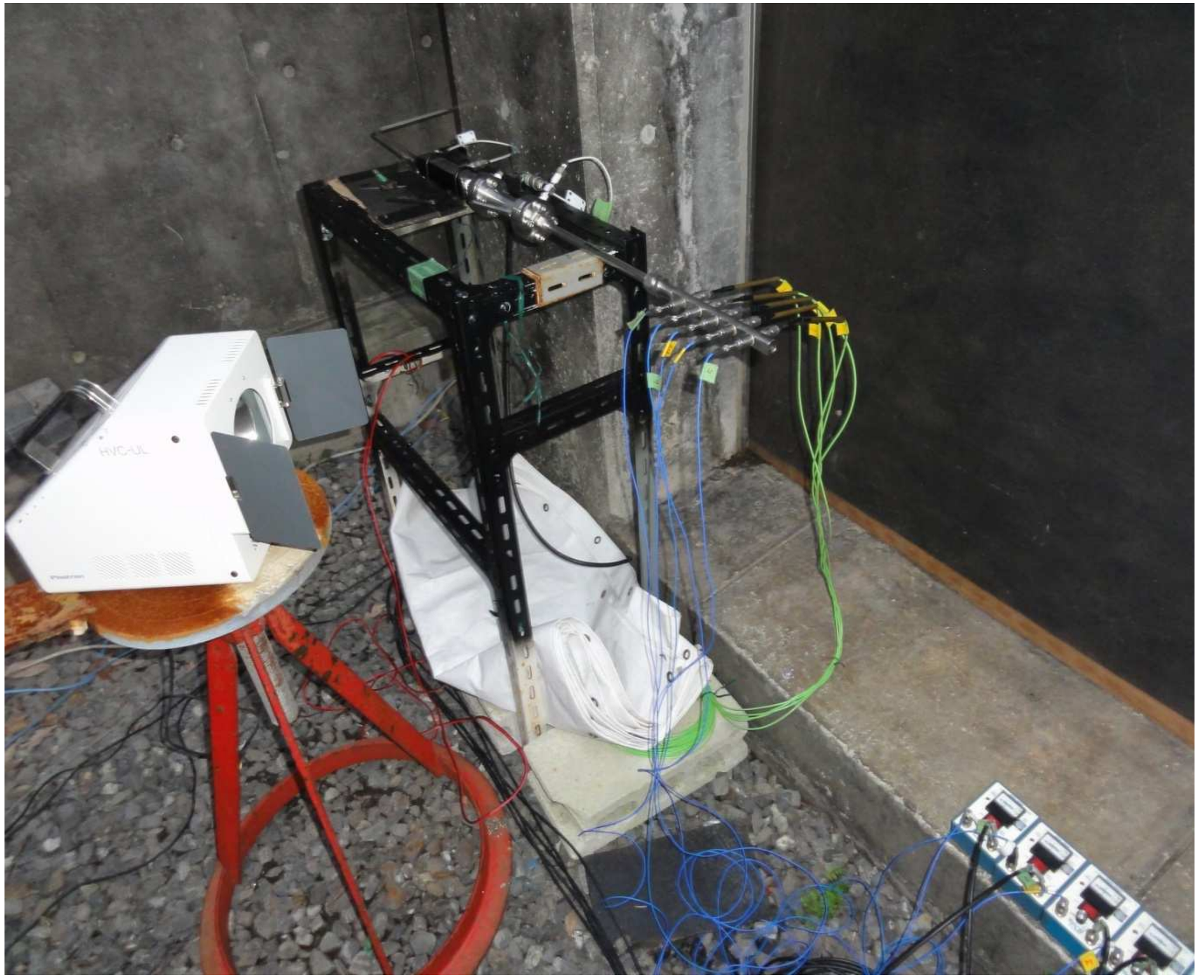
Experimental Setup



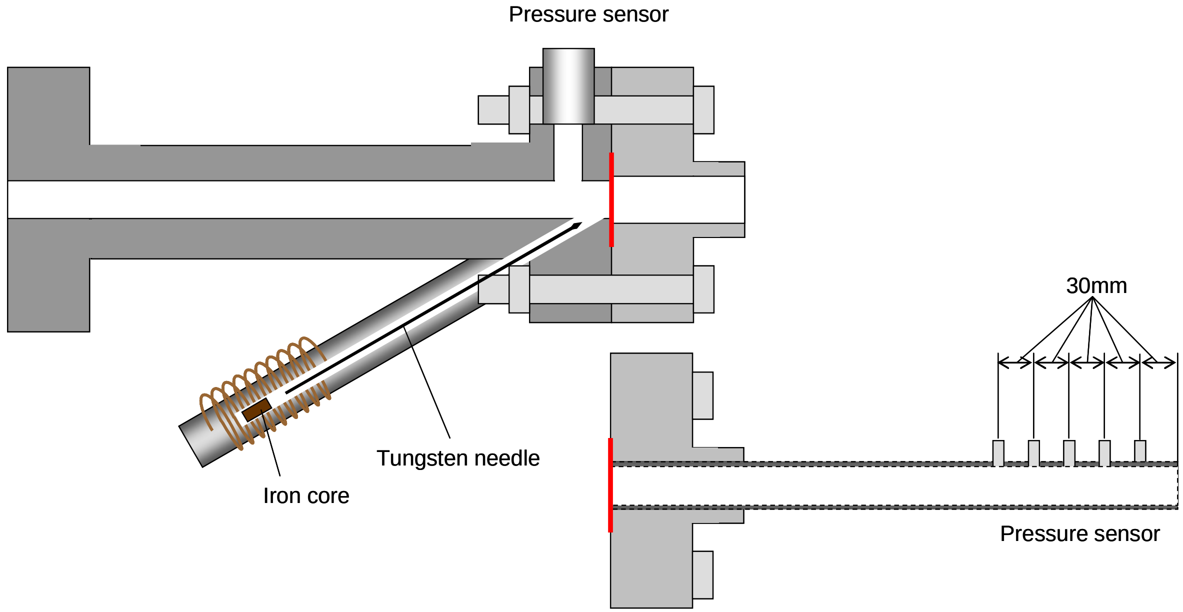
Experimental Conditions

Shock Tube Length: L	100 ~ 4200 mm
Burst Pressure : P_b	2.0 ~ 8.0 MPa
Tube Diameter: D	10 mm

Shock Tube



Shock Tube with a Plunger System

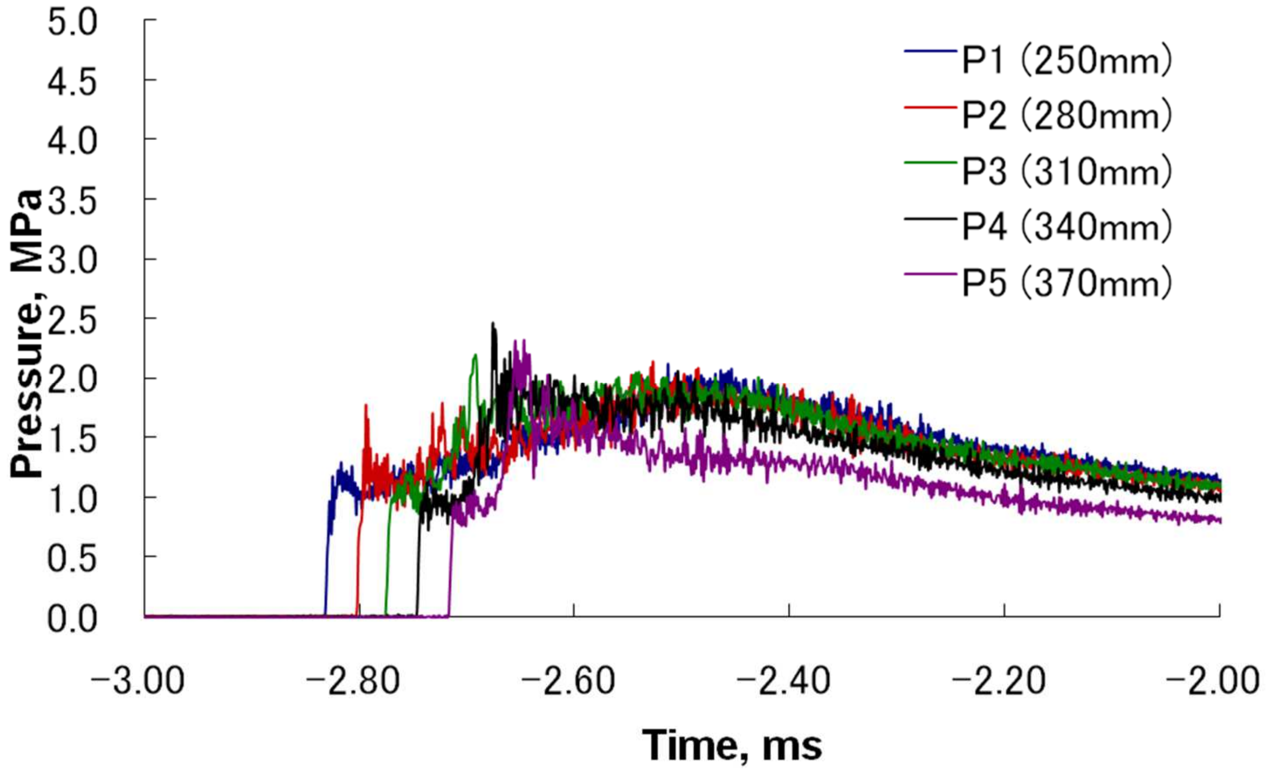


High Speed Camera

Pressure Profiles for Pb=4.8MPa Case

Pb=4.8MPa
L=400mm

No Auto-Ignition



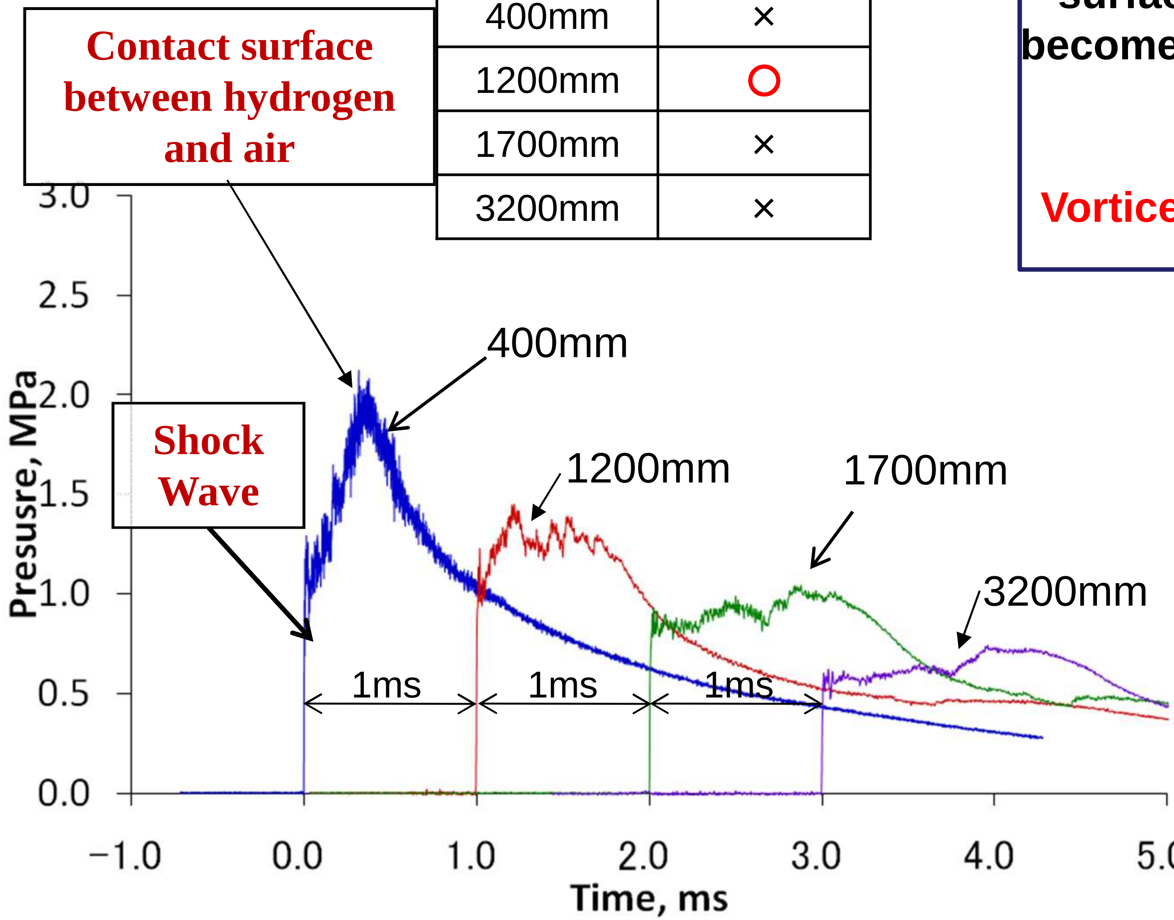
Pressure Wave Profiles

Comparison pressure profiles at the pressure transducer located at 150 mm inside from the tube exit for four different tube length cases at the condition of P_b=4.8MPa.

Tube length	Auto-ignition
400mm	×
1200mm	○
1700mm	×
3200mm	×

The pressure profile at the contact surface between air and hydrogen becomes collapse for the longer tube.

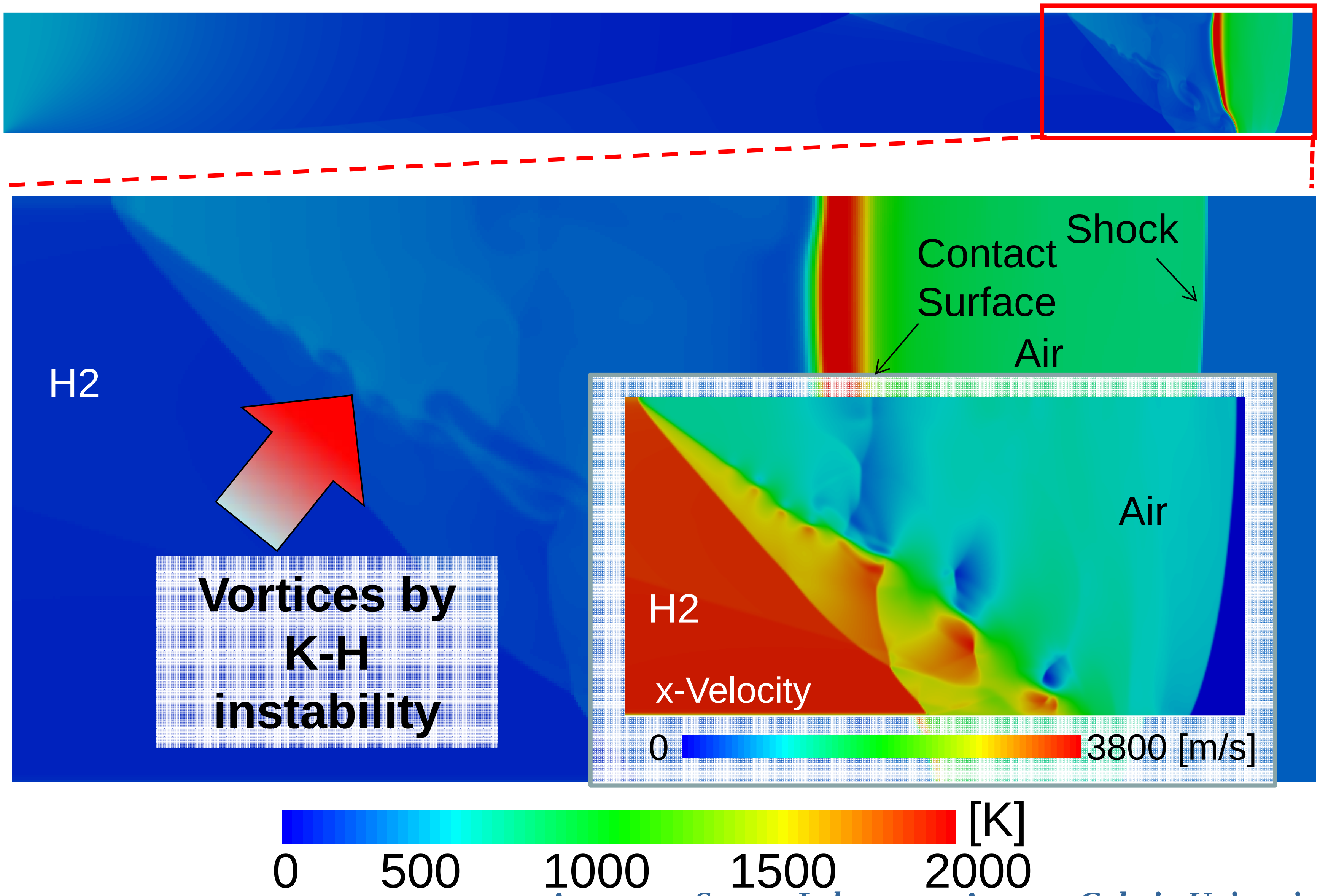
Vortices exist at the contact surface



Auto-ignition occurred at the case of 1200 mm tube only.

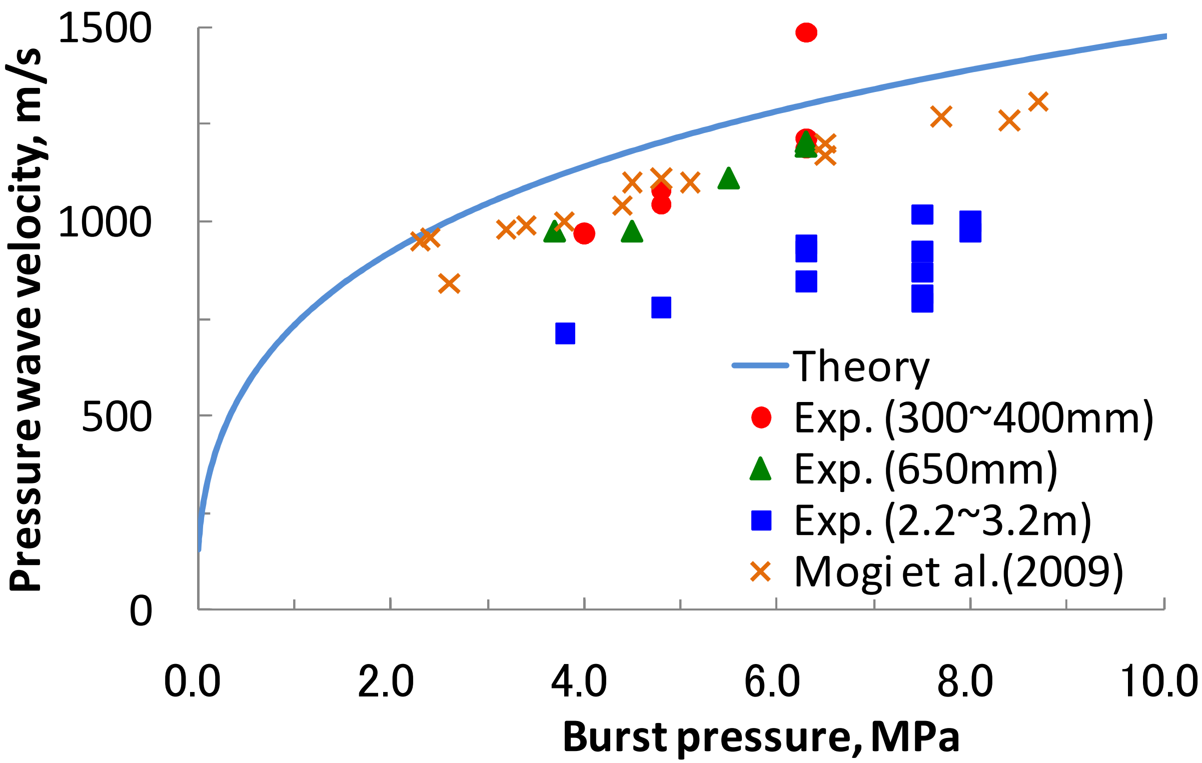
There is a relation between the vortex and the shock wave strength.

Numerical Temperature Profiles (14.8 ms)



Shock Velocity

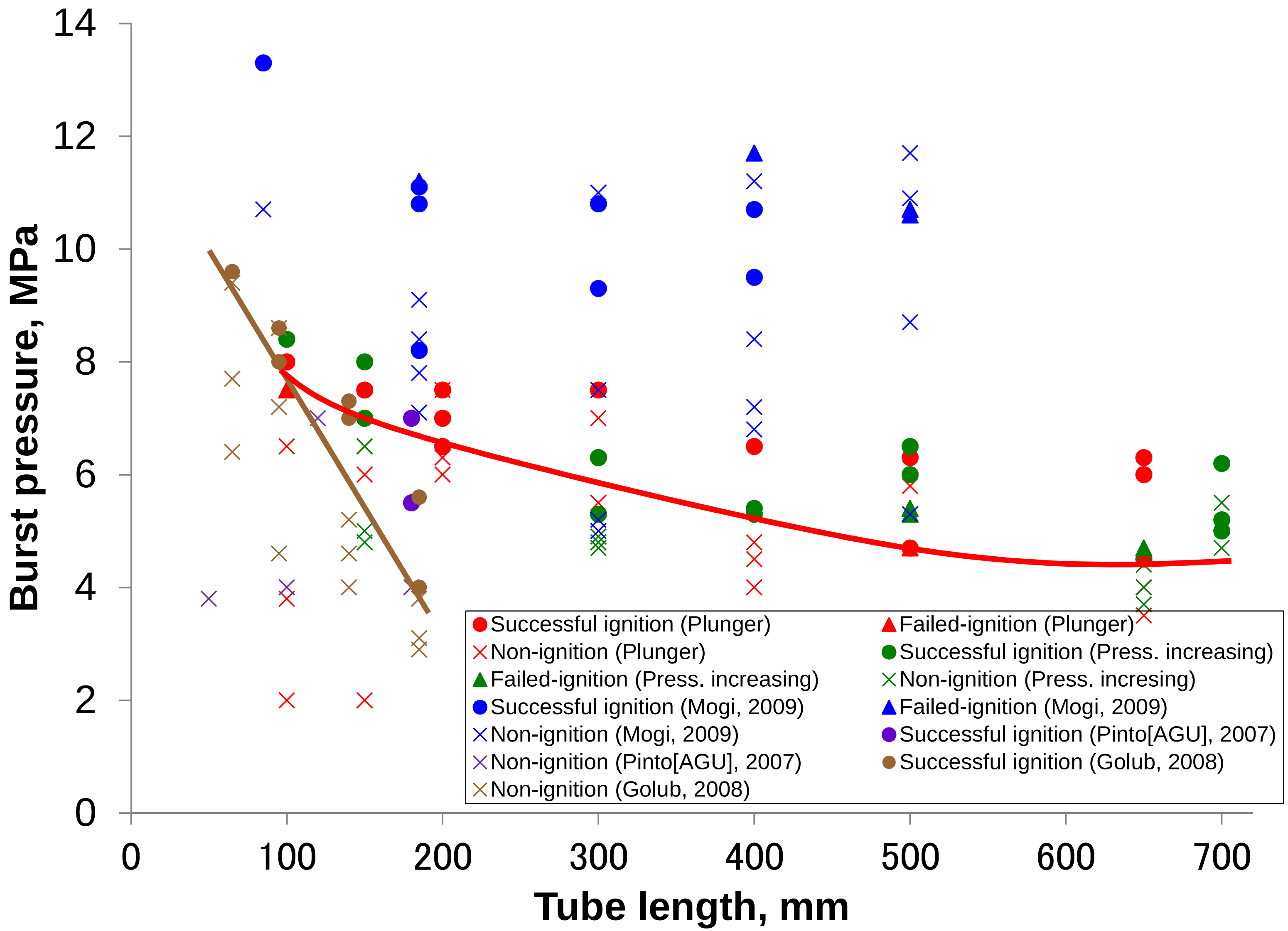
The relation between burst pressure and shock velocity at the tube length of 300, 400, 650 mm and 2.2, 3.2 m.



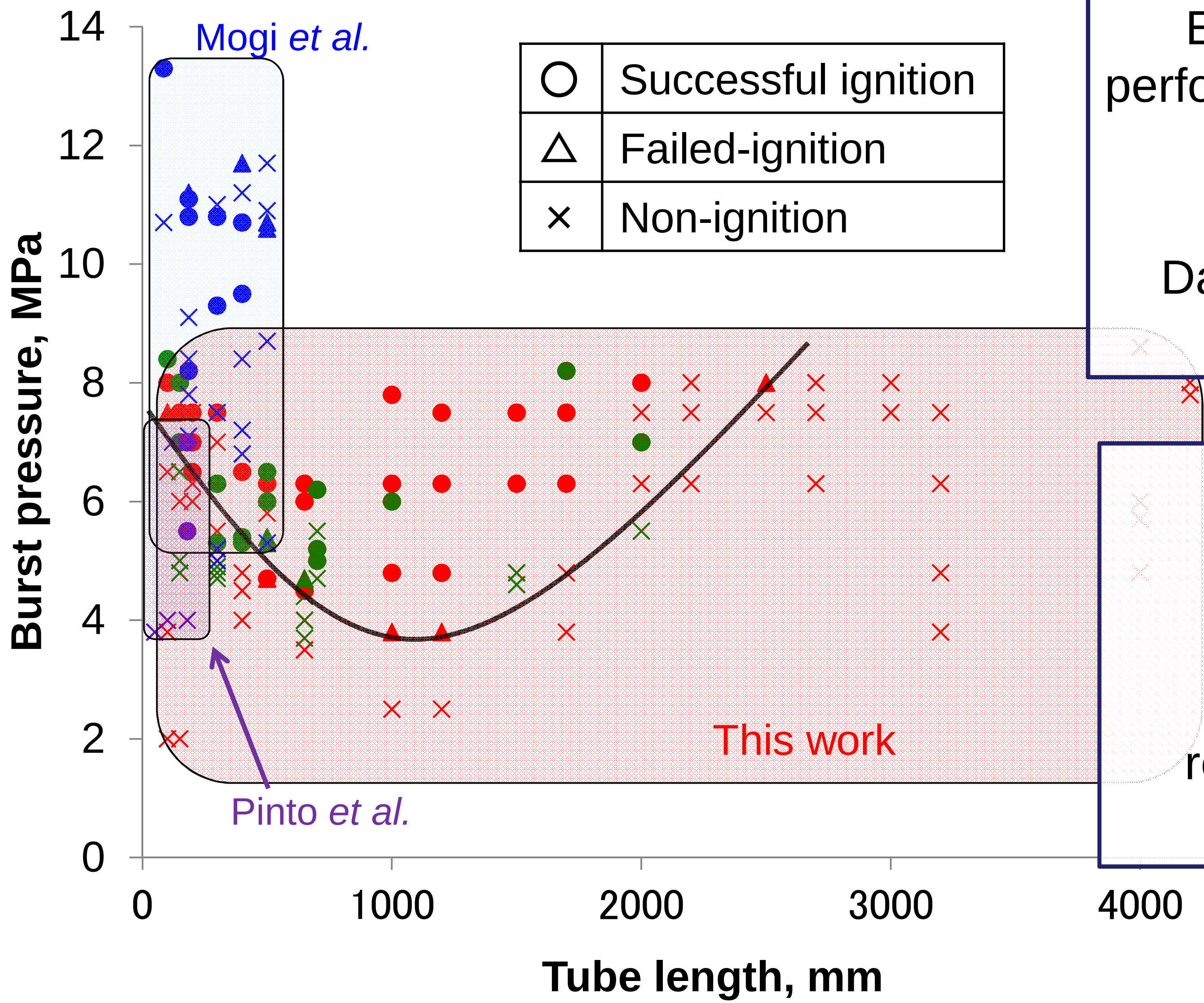
- The similar tendency as theory. (200 m/s below)
- The same results as the old study for the short tube (300-600 mm)
- The 400 m/s lower than theory for the long tube (2.2-3.2 m)

- The theory and experiments are in the same tendency.
- The diaphragm breaks in a finite time and 3D way.
- The boundary layer effect.

Auto-Ignition Limit Curve(Tube Length of up to 700mm)



Auto-Ignition Limit Curve



Experiments were performed at the constant burst pressure

Data were obtained repeatedly.

Auto-ignition curve has a minimum.

Hydrogen can be released safely using a long tube.

High-Speed Movie Data

Focus Distance	100 mm
F-Number	3.5
Frame Speed	60000 fps
Tube Diameter	500 mm
Burst Pressure	4.8 MPa

Sustainable and Non-Sustainable Auto-Ignition

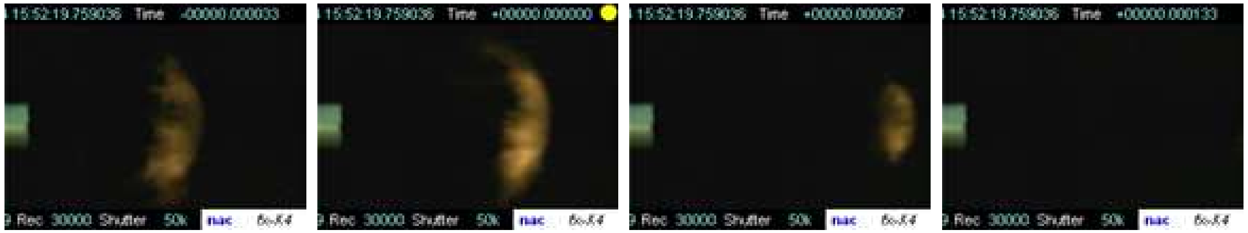
Mogi *et al.* (2008)

D=5 mm
L=185 mm
P_b=14.5 MPa

0 µs 50 µs 100 µs 300 µs

(a) Sustainable combustion case

D=5 mm
L=185 mm
P_b=11.6 MPa



0 µs 33 µs 100 µs 166 µs

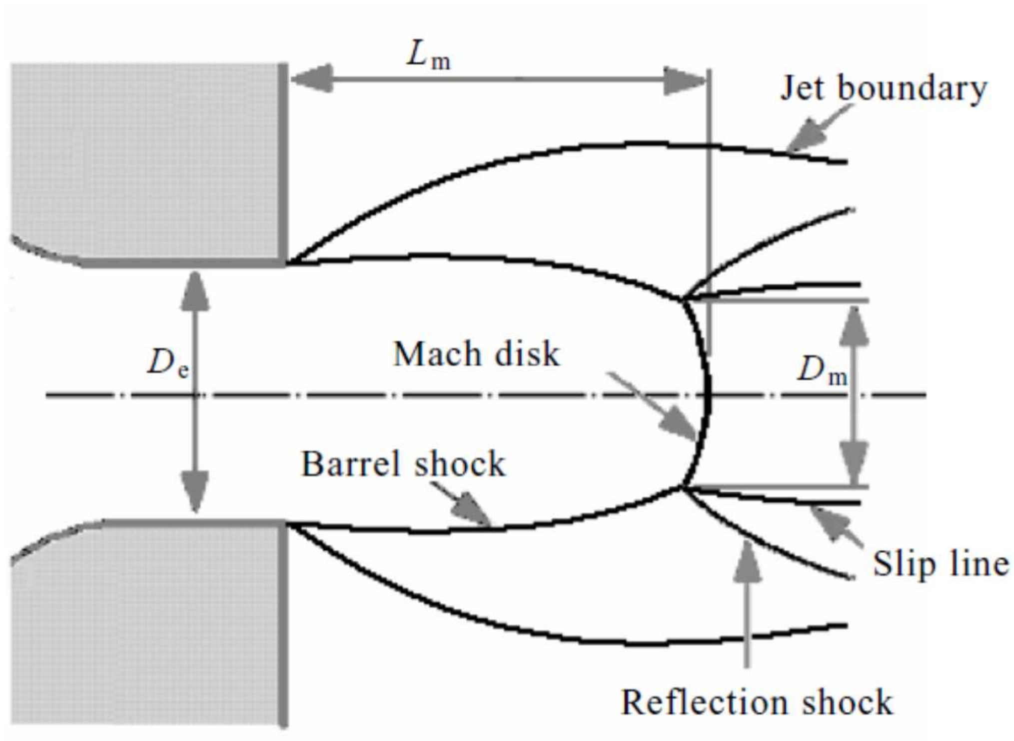
(b) Non-sustainable combustion case

- **High pressure**
- **Long Tube**

→ **Easier to ignite**

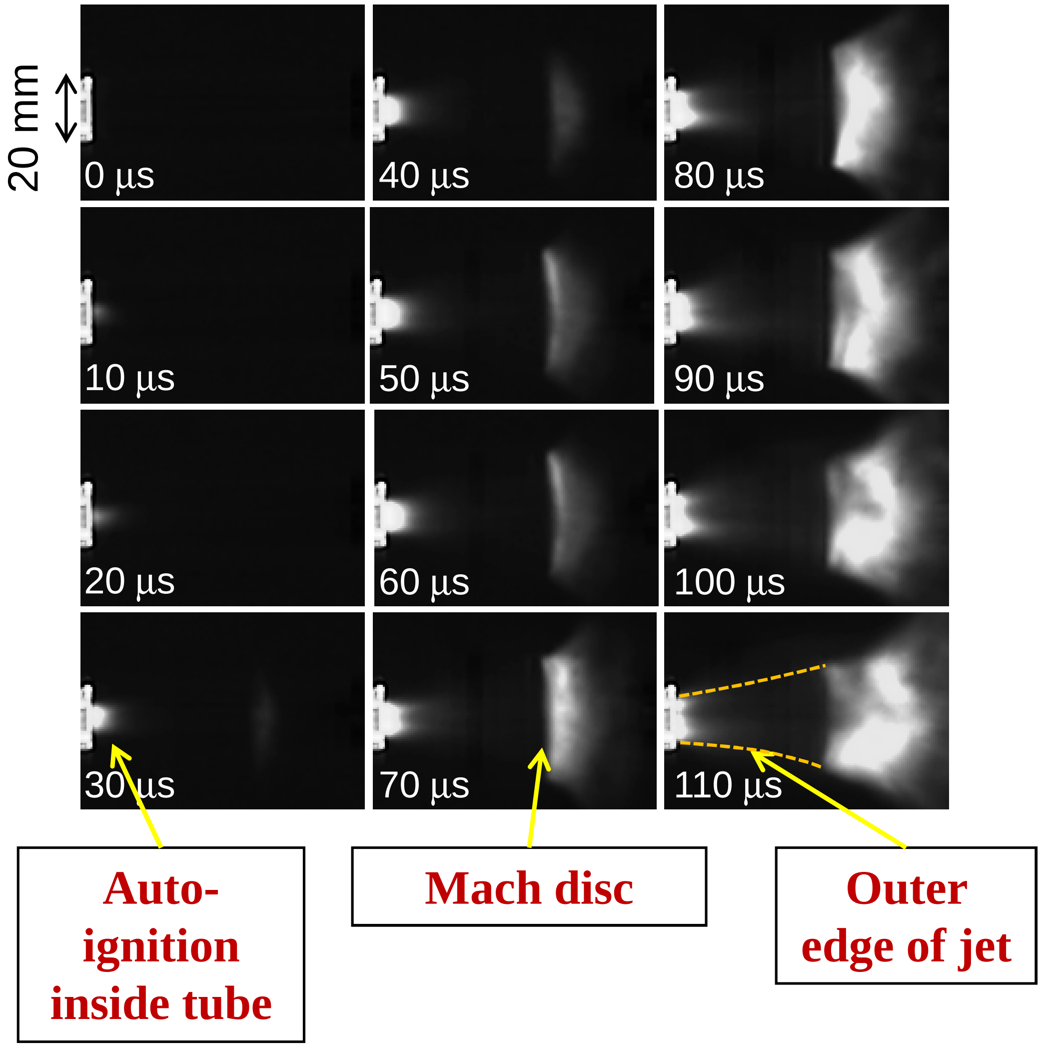
(2008)

Mach Disc in Under-Expansion Supersonic Nozzle



Detailed Photos

- Took a high speed movie near the tube exit



Focal length	105 mm
Focal number	2.8
Shutter speed	100000 fps
Tube length	650 mm
Burst pressure	5.0 MPa

- Saw the auto-ignition inside of the tube.
- Recognized the phenomena of supersonic jet.

Conclusion

- Experiments of Auto-Ignition using a Shock Tube with a plunger system

  - Obtained the clear auto-ignition limit curve by experimenting the shock wave with a control of burst pressure.
  - Found that no auto-ignition with an enough length of tube.
  - Observed auto-ignition in tube.