MECHANISM OF HIGH PRESSURE HYDROGEN AUTO-IGNITION WHEN SPOUTING INTO AIR

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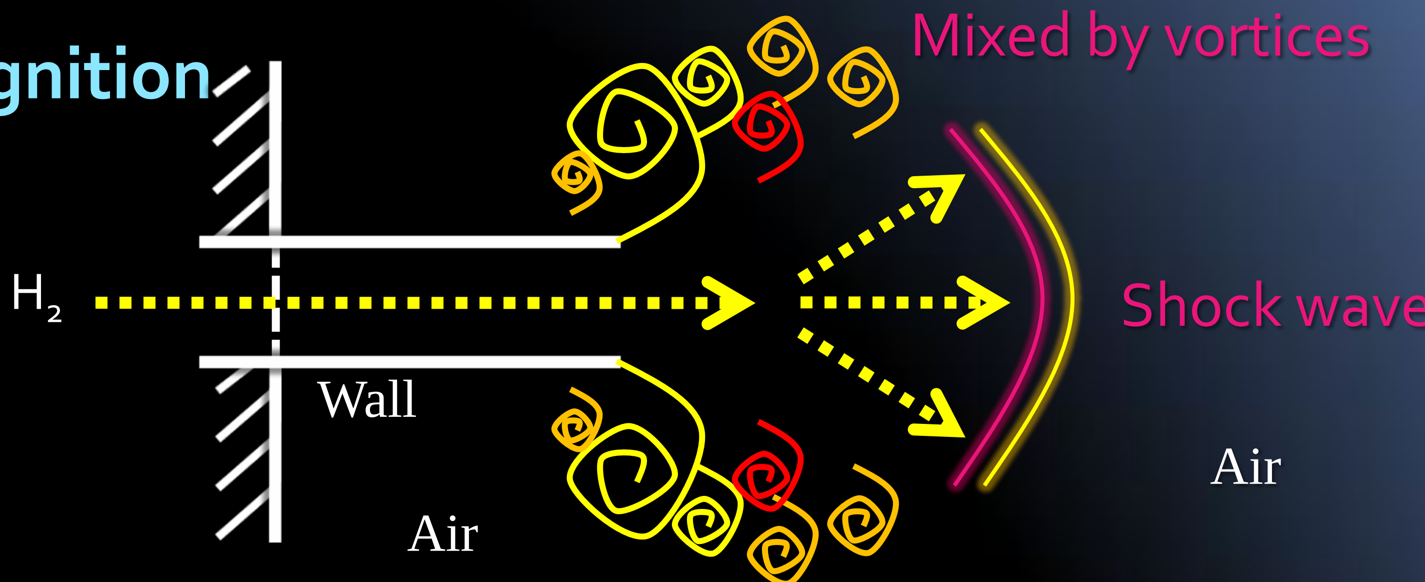
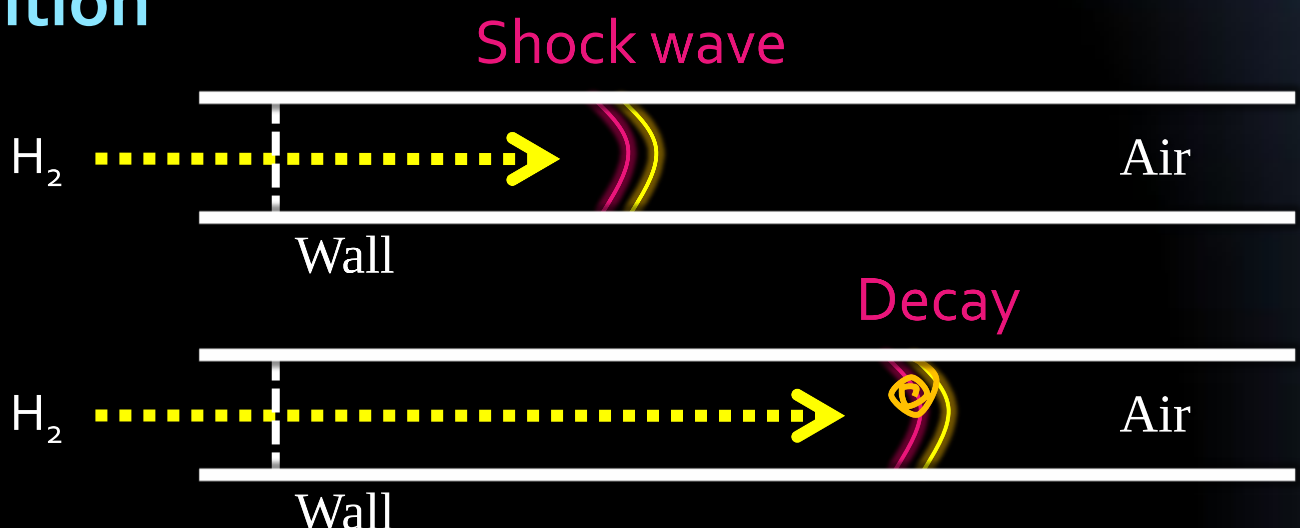
Ignition type

Outside ignition



Some researchers have reported.

Inside ignition



Not enough discussion.

Research history

Wolański and Wójcicki (1973)

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

Tanaka et al. (1979)

Confirm the similar ignition.

Uejima et al. (1998)

Discuss the turbulent effects on the ignition.

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

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

Dryer 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.

Sandia National Laboratories (2003~)

Investigate the hydrogen Release behavior.

Background and object

High pressure tanks are often used to store hydrogen in many practical cases (e.g. fuel cell vehicle). If an accidental release of high pressure hydrogen occurs, a strong shock wave would be generated and might lead to an explosion.

High pressure hydrogen leaks are one of the top safety issues. The object is to clarify the physics and mechanism of high pressure hydrogen jet ignition.

H_2 TANK
171 L
35 MPa

HONDA
FCX CLALITY

Numerical method

An auto-ignition of hydrogen from a tube attached to a high pressure reservoir tank is calculated with the direct numerical simulation (DNS).

Governing equations

Two dimensional compressible Navier-Stokes equations

Conservation of mass, momentum, energy and chemical species

Equation of state

Discrete form

Finite different method on the cylindrical coordinate system

Scheme for convection term

second-order Explicit Harten-Yee Non-MUSCL modified-flux type TVD

Chemical reaction

9 chemical species (H_2, O_2, O, H, OH, HO_2, H_2O_2, H_2O, and N_2)

18 elementary reactions (Petersen and Hanson, 1999)

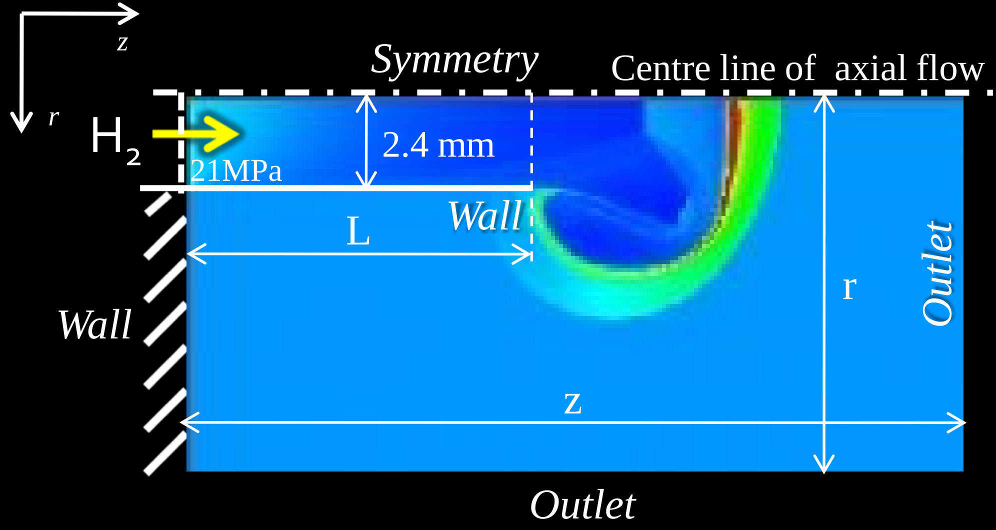
Transport coefficient

Lennard-Jones intermolecular potential model

Wilke's empirical rule for the mixture

Condition

Outside ignition $\Delta r = \Delta z = 20\ \mu m$

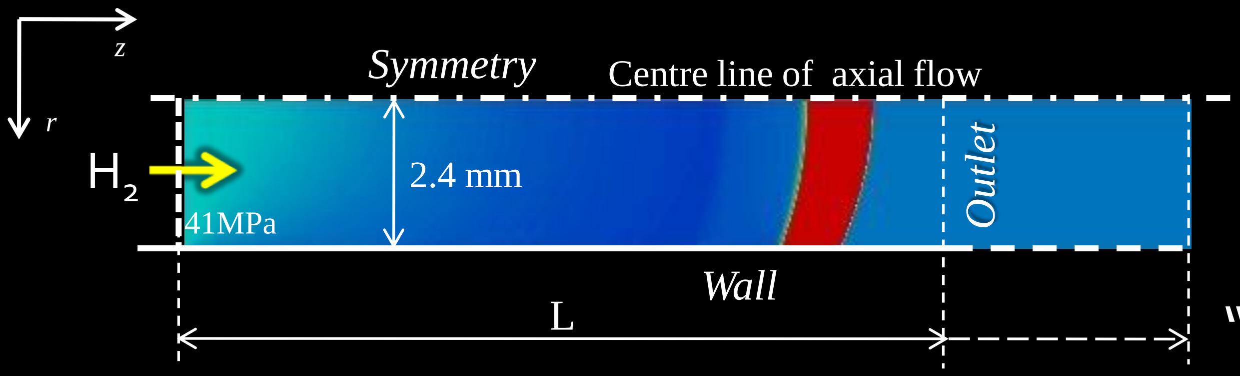


Grid condition

#	L [mm]	r x z [mm]	Grid
1	0	40 × 36	3,600,000
2	2	40 × 38	3,800,000
3	10	40 × 46	4,600,000
4	20	40 × 56	5,600,000

Investigate the effect of tube length.

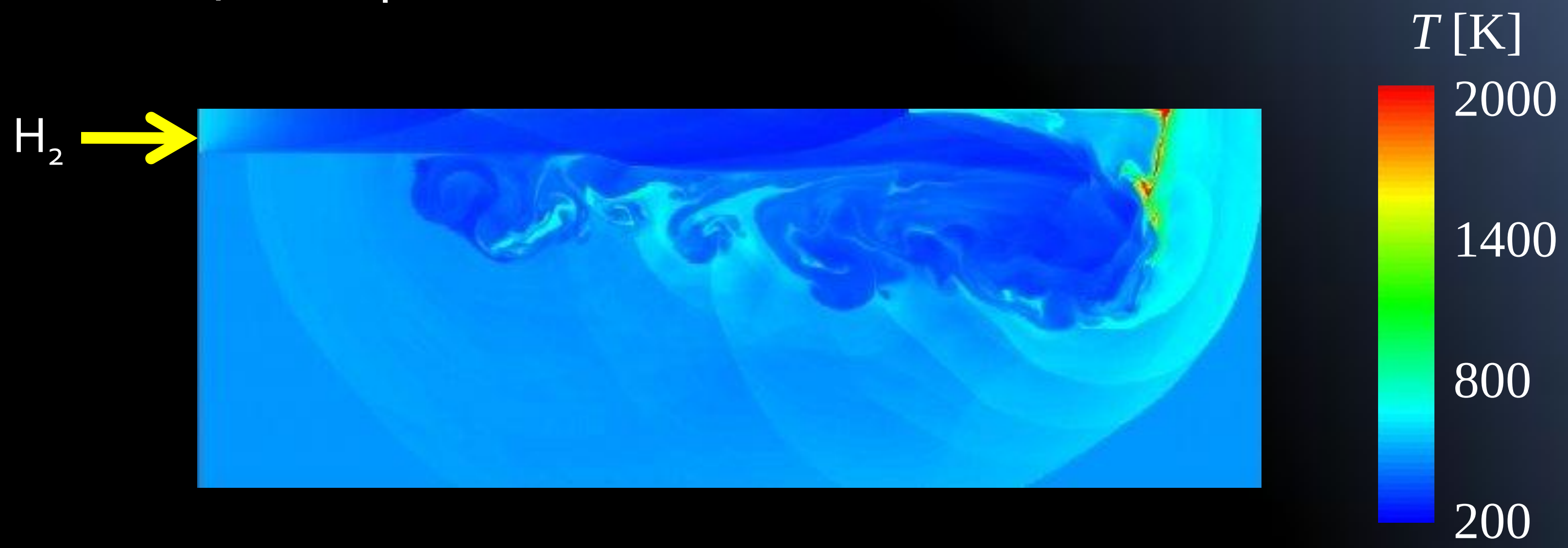
Inside ignition $\Delta r = 5\ \mu m$, $\Delta z = 10\ \mu m$ **Smaller size.**



"L" extends gradually.

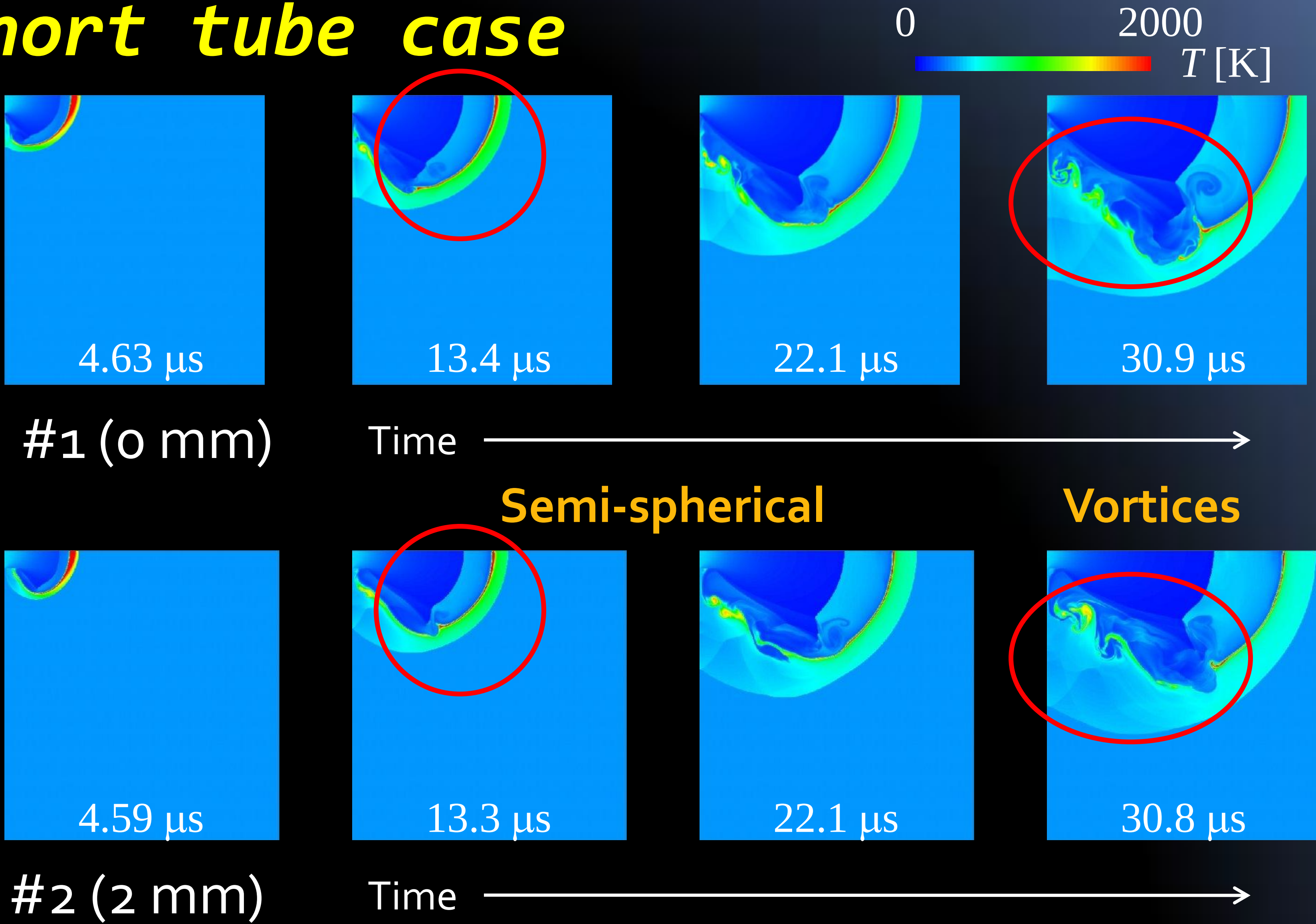
Outside ignition

From the left hand side high pressure hydrogen goes through a thin tube, and spouts into air.



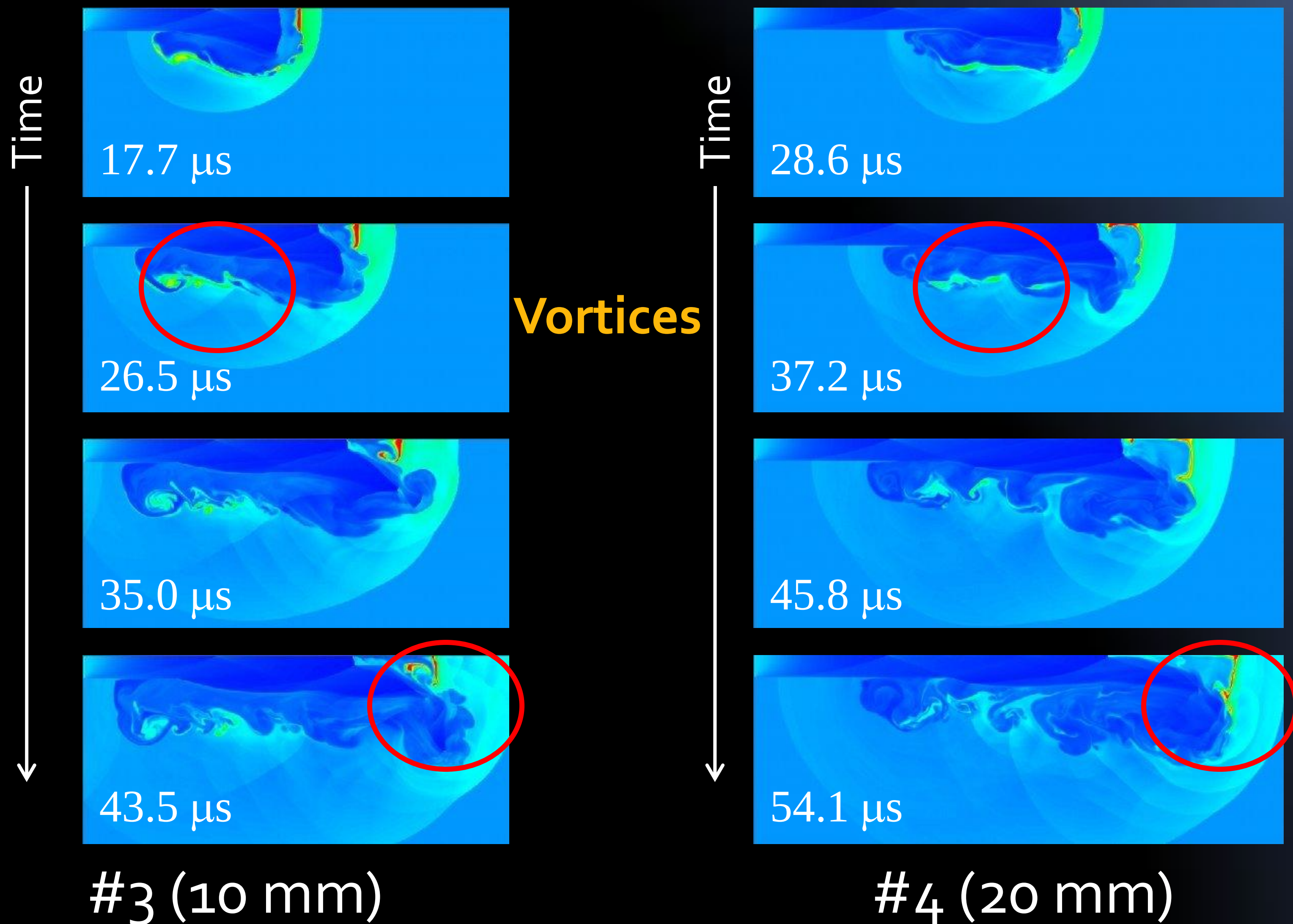
The shock wave heats air to a high temperature over 2000 K which is enough energy to induce an auto-ignition of hydrogen. Mixing of hydrogen and air is promoted by vortices generated around the side area. This mixture layer might lead to a strong chemical reaction.

Short tube case



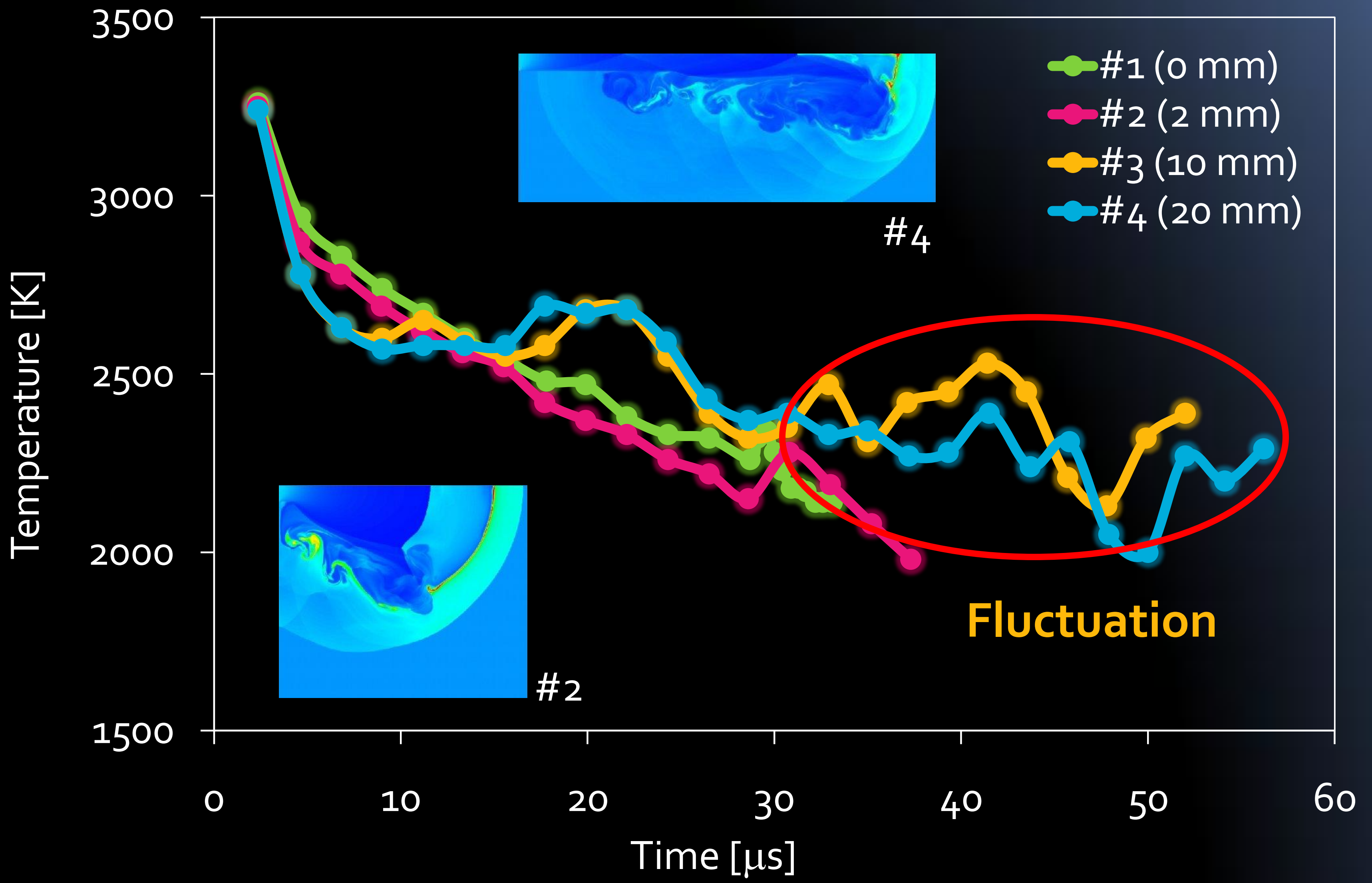
Vortices are important factor for the outside ignition.

Long tube case



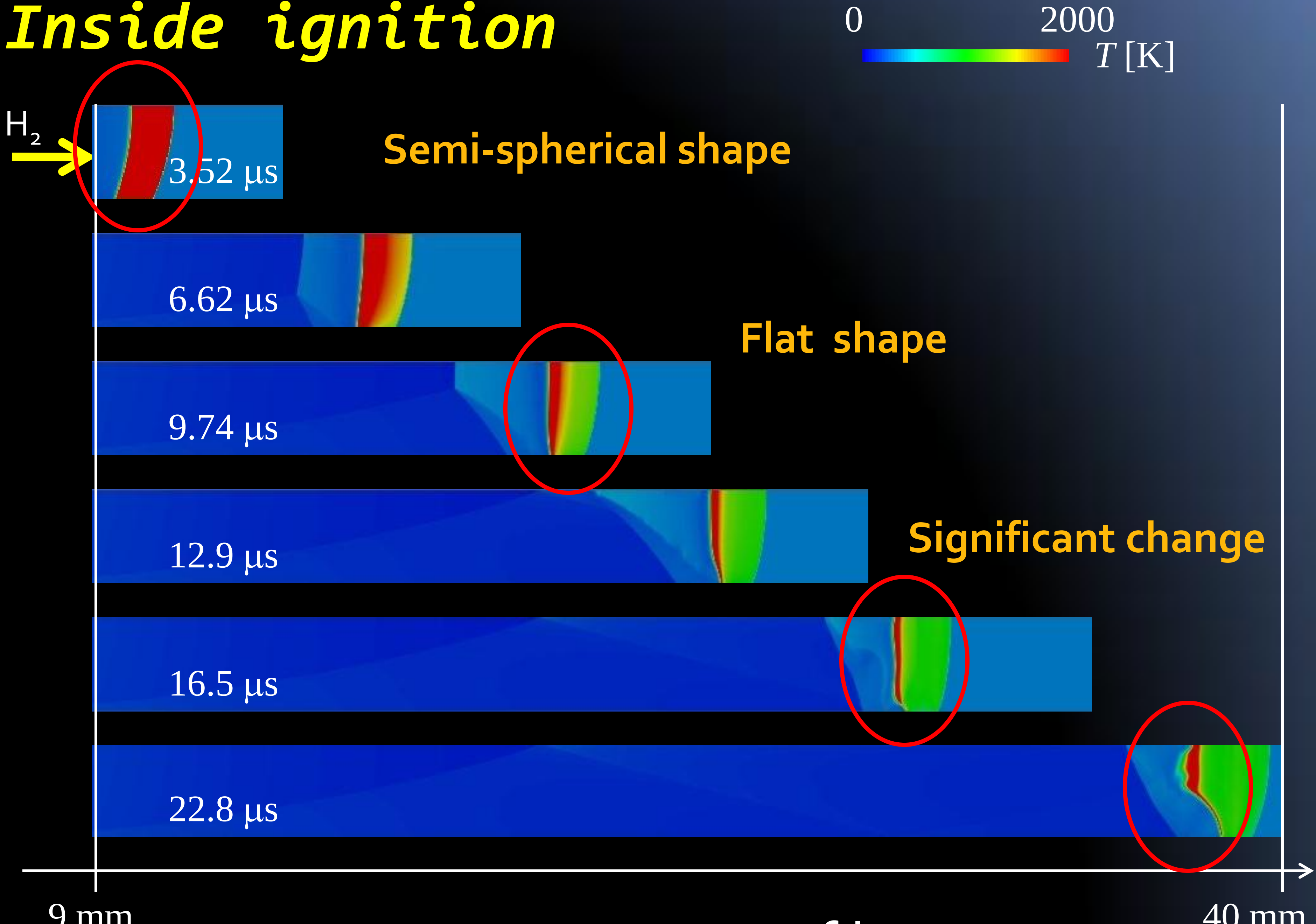
The shock wave decays and many vortices are generated.

Maximum temperature history



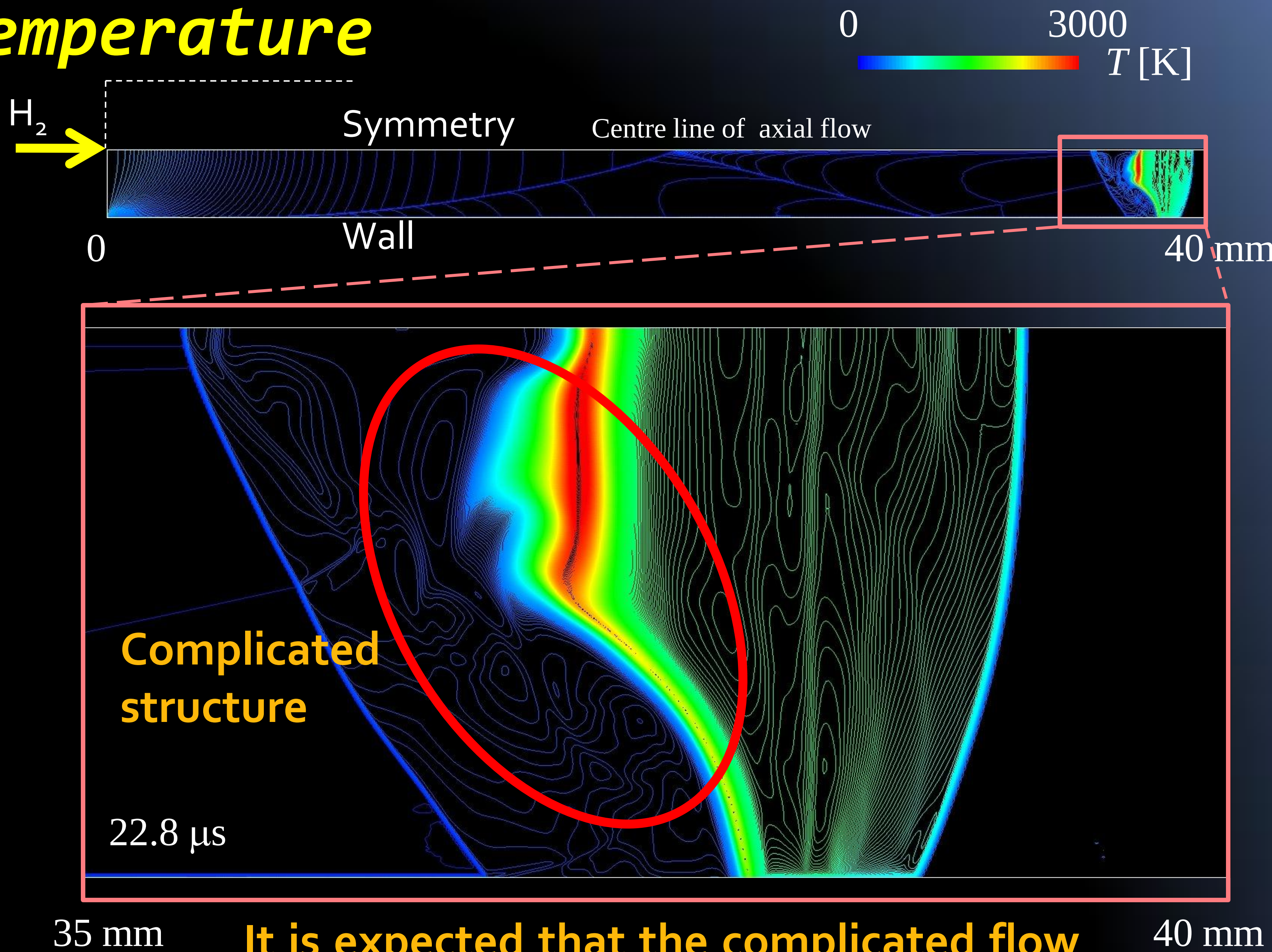
It seems that a chemical reaction is maintained for a while.

Inside ignition



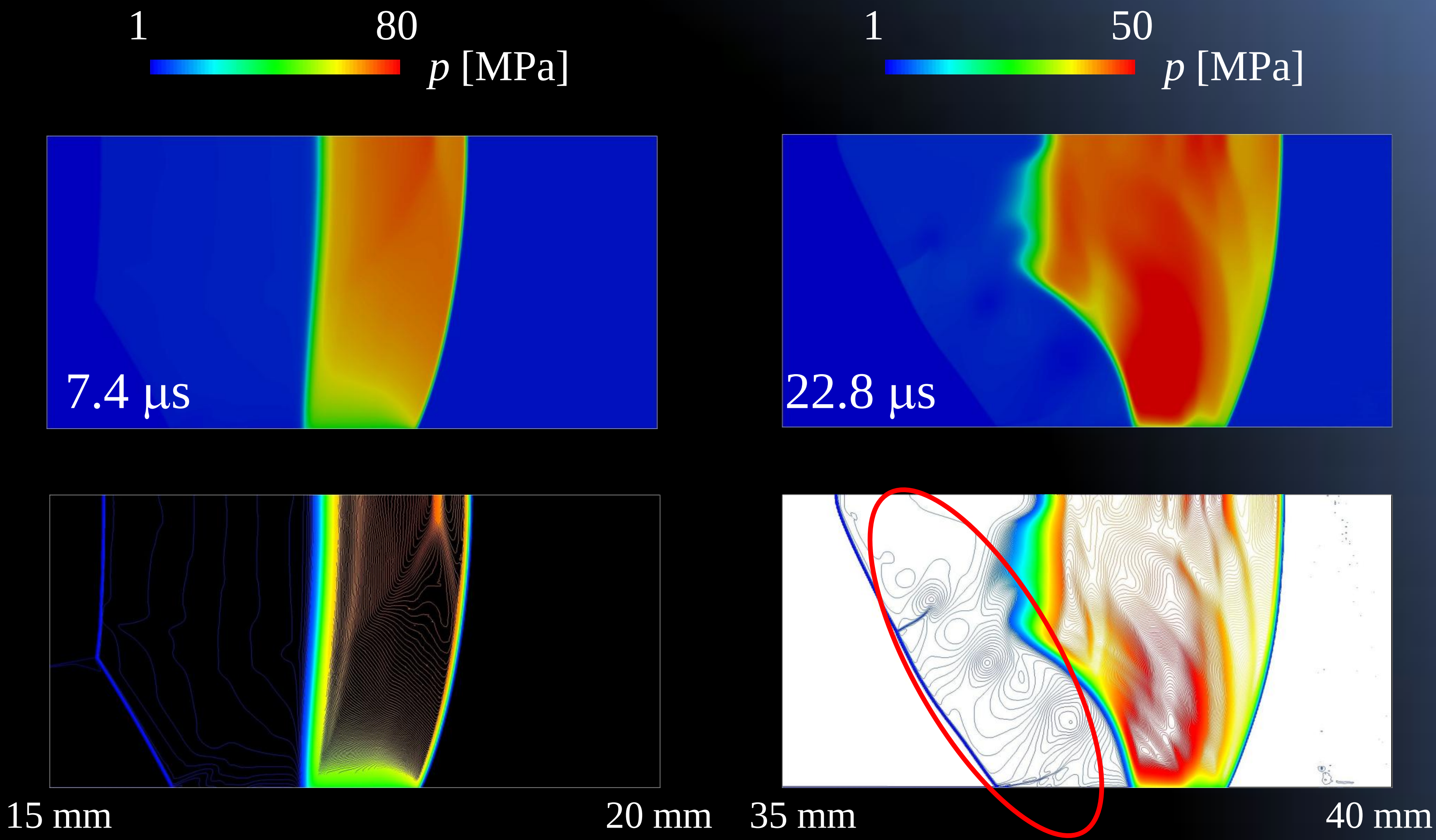
Temperature profiles

Temperature



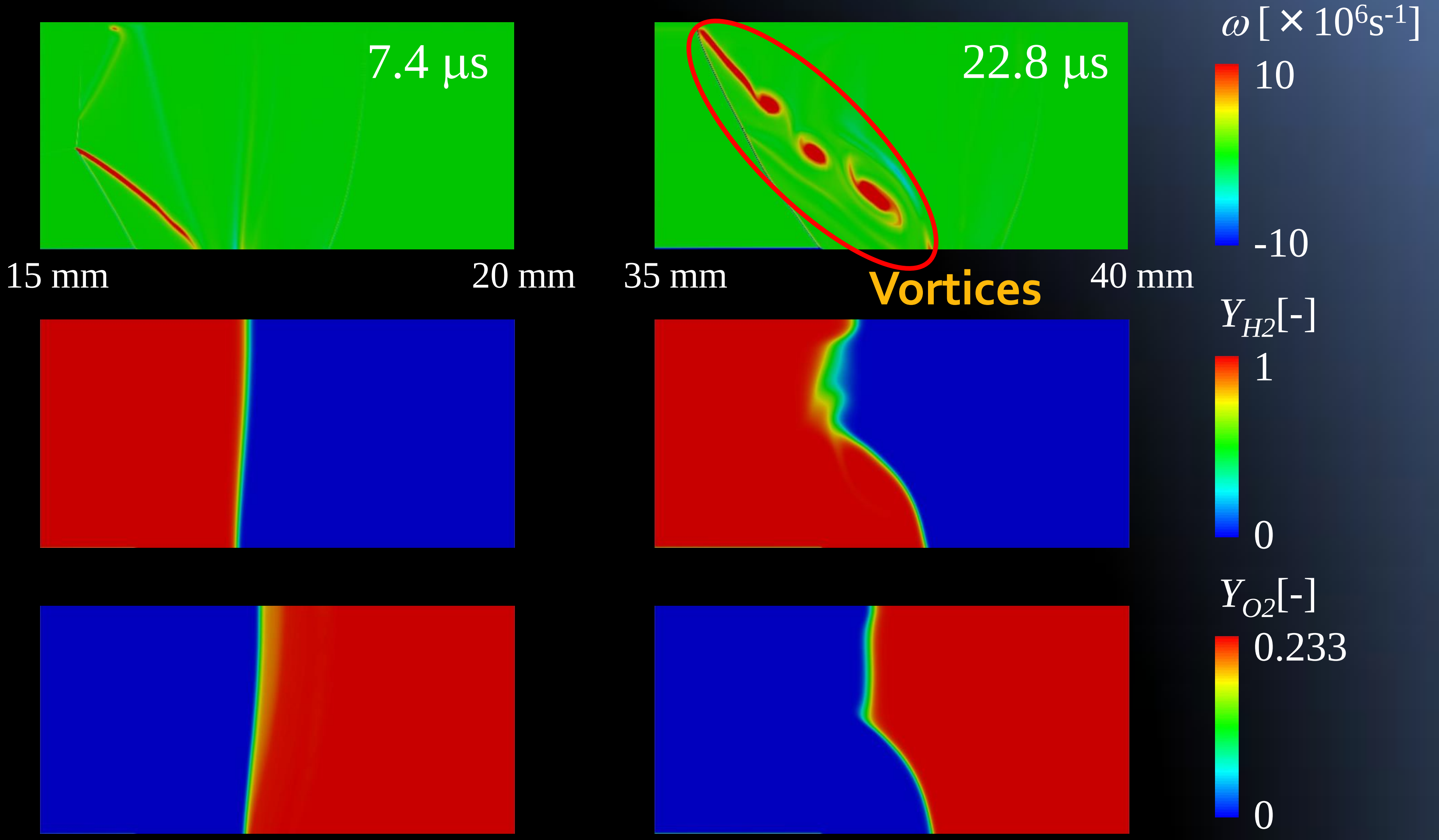
It is expected that the complicated flow structure mixes hydrogen with air.

Pressure



Vortices and whiskers

Vorticity & Mass fractions



When these vortices grow more, an effective mixing of H2 and O2 might be caused.

Conclusions

Outside ignition:

Many vortices are generated when the shock wave exit the tube. It seems that the vortices are important factor for the outside ignition. The longer tube, which has enough space to mix hydrogen with air, tends to make more complicated flow structure. Therefore, to reduce the outside ignition, **it is necessary to reduce the space near the exit.**

Inside ignition:

The shape of the contact surface is changed significantly. The complicated flow structure with some vortices and whiskers is formed behind the contact surface. This can cause an effective mixing, and then an inside ignition may occur. To reduce the inside ignition, **we need to understand this phenomenon better.**