ICH3 paper 265

Physics of spontaneous ignition of high-pressure hydrogen release and transition to jet fire

Maxim V. Bragin
Vladimir V. Molkov
HySAFER Centre
University of Ulster
mv.bragin@ulster.ac.uk

Contents

- Motivation
- Spontaneous ignition phenomena following a storage decompression with a downstream confinement
- Transition of ignited mixture into a jet fire
- Conclusions

Motivation

QUANTUM Technologies WorldWide Inc. introduced “all-composite hydrogen storage tank that stores hydrogen at 10,000 psi (700 bar). At 10,000 psi, 80% more hydrogen fuel can be stored in a given space than at 5,000 psi” *

* QUANTUM Technologies WorldWide, Inc
Website: http://www.qtww.com/products/haft/hydrostorage.php

Motivation II

Activation of pressure relief device

↓

High-pressure release of hydrogen

↓

Possible ignition without any apparent reasons

Postulated mechanisms for spontaneous ignition*

- Reverse Joule-Thomson effect
- Electrostatic charge generation
- Diffusion ignition, ignition by shock waves
- Sudden adiabatic compression
- Hot surface ignition

* Astbury G.R., & Hawksworth S.J. Spontaneous ignition of hydrogen leaks: A review of postulated mechanisms. 2005. *Proceedings of The 1st International Conference on Hydrogen Safety*.

Overall aim of the research

Aim of the research:

- To develop understanding of the physical phenomena underlying spontaneous ignition of hydrogen generated by shock waves resulting from sudden storage decompression (or activation of a PRD)
- To construct a model capable of reproducing experimental observations during transition of spontaneously ignited mixture into a jet fire

Planned contribution to knowledge:

<u>Scientific</u>

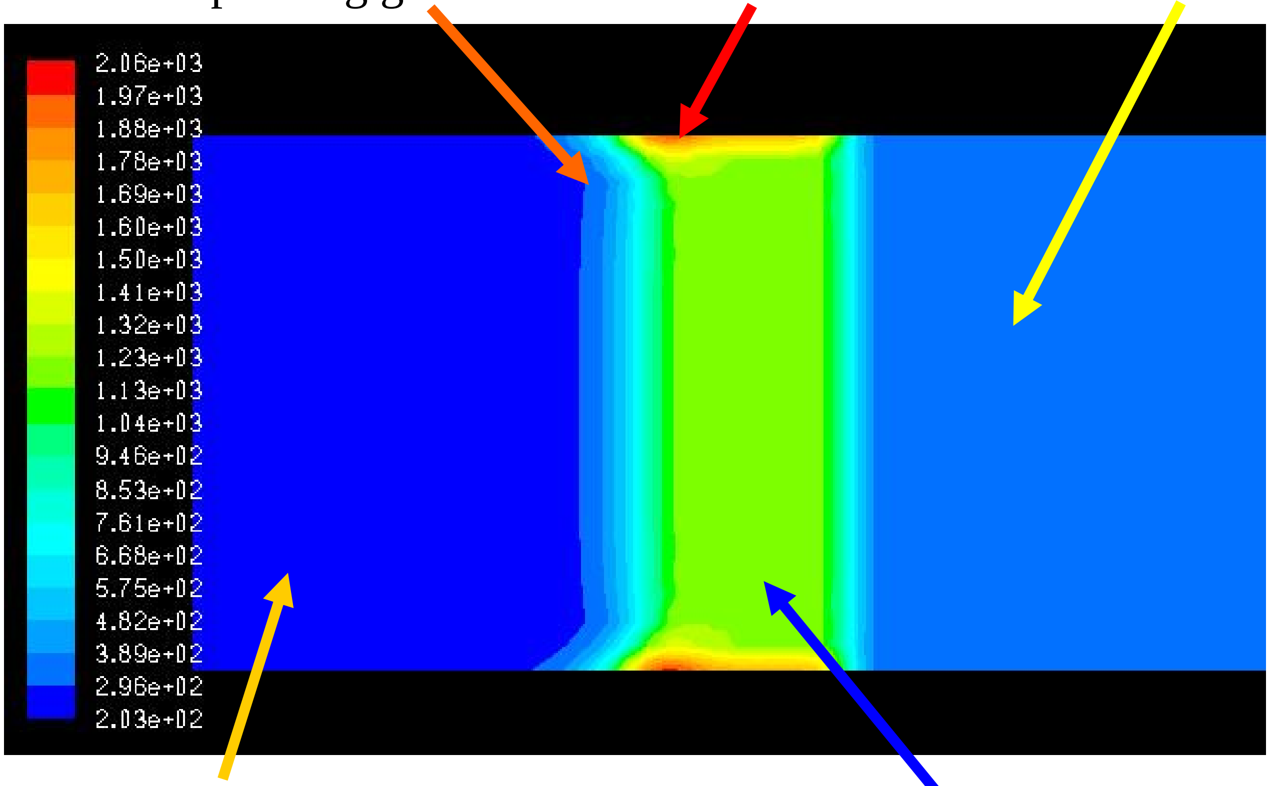
- Determination of critical conditions for ignition during high-pressure releases (i.e. ignited or not) and jet fire onset (sustained or not)

<u>Applied. Recommendations for</u>

- Hazard assessment
- Mitigation techniques
- Risk assessment

Spontaneous ignition of hydrogen following a storage decompression with a downstream confinement

Temperature in flame front



Contact surface separating gases

Regions of ignition onset

Atmospheric air

Cold expanding hydrogen

Shock heated air

Calculation domain

Geometry was taken from experiments by Golub et al.

High pressure chamber L = 145mm, d = 20mm

Low pressure chamber (Tube): **L = 140mm, d = 5mm**

Meshed with total number of control volumes 431k in **3D**

Low pressure chamber – uniform mesh with cell size 0.2mm

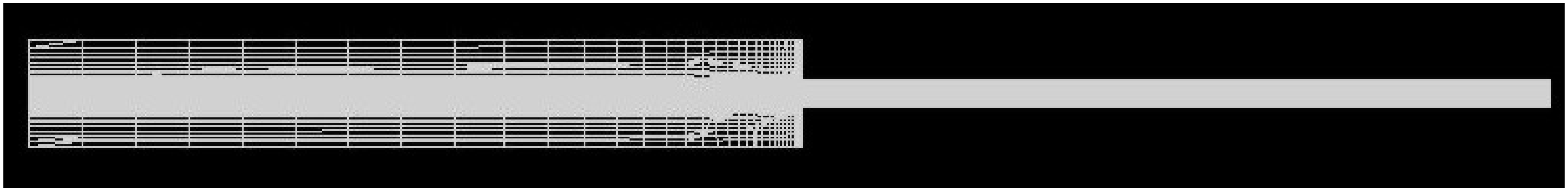
Laminar Finite-Rate model + Dynamic S-L subgrid scale model

The initial conditions:

Low-pressure chamber: air (mass fraction of O2 = 0.23, mass fraction of N2 = 0.77), pressure P = 1 atm, temperature T = 300 K.

High-pressure chamber: hydrogen (mass fraction of H2 = 1), pressure P = **97 bar**, temperature T = 300 K.

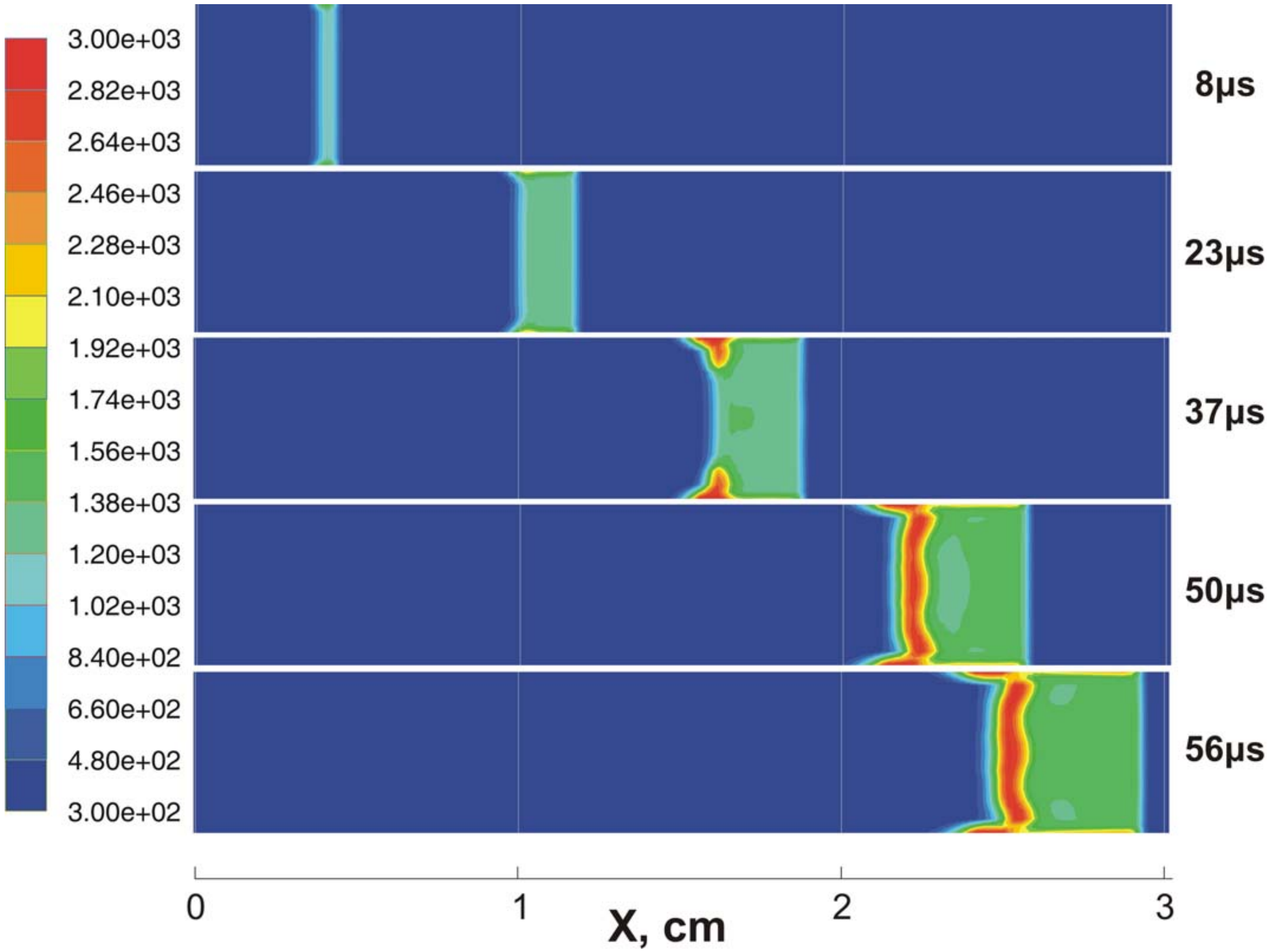
Boundary (burst disk) separating chambers was removed instantly.



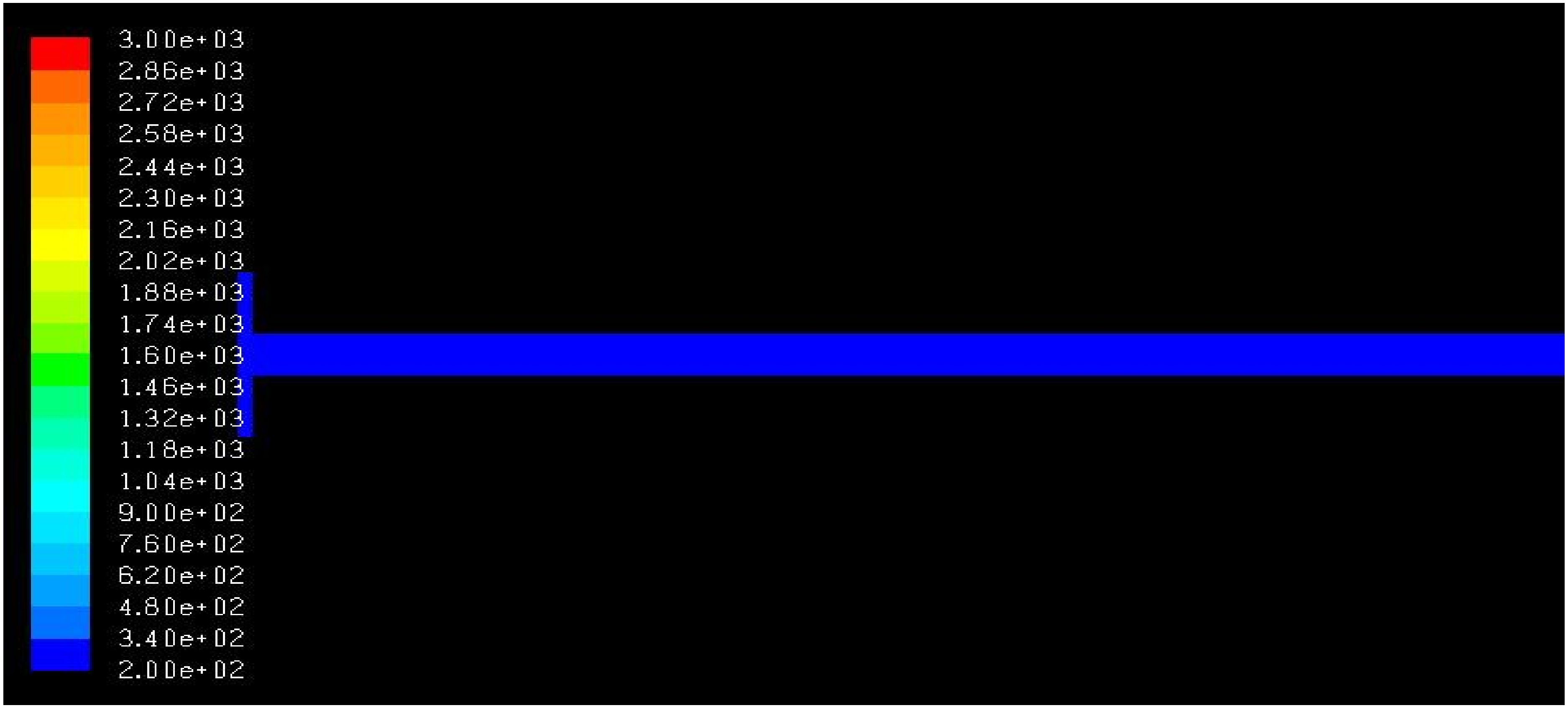
GOLUB, V. V., BAKLANOV, D. I., BAZHENOVA, T. V., BRAGIN, M. V., GOLOVASTOV, S. V., IVANOV, M. F. & VOLODIN, V. V. (2007) Hydrogen auto-ignition during accidental or technical opening of high pressure tank. *Journal of Loss Prevention in the Process Industries,* 20**,** 439-446.

University of ULSTER

Dynamics of temperature

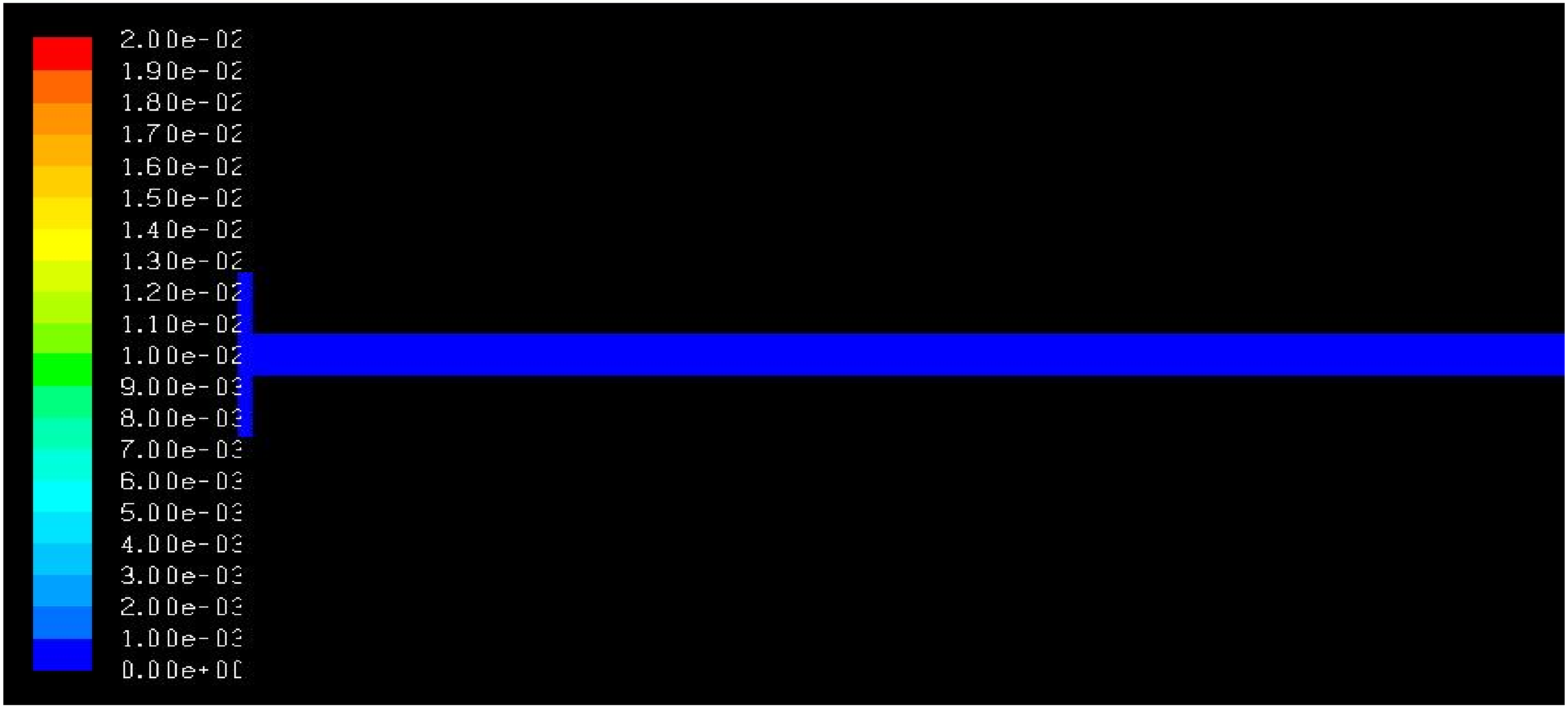


Temperature movie



Shown tube length corresponds to 13cm

Hydroxyl mole fraction



Shown tube length corresponds to 13cm

Transition of spontaneous ignition into a jet fire

Calculation domain

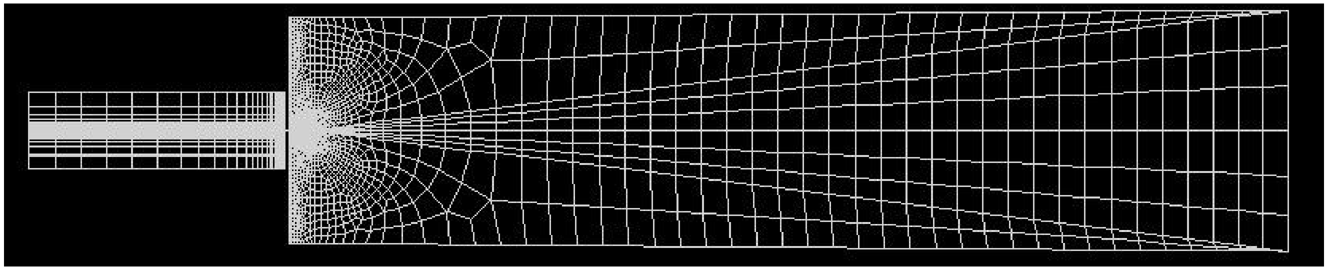
Geometry was taken from experiments by Mogi et al.
Tube: **L = 185mm, d = 5mm** was uniform mesh with cell size 0.4mm
Outside mesh was adapted as the process evolved
Maximum number of control volumes was 479k,
but only the first 0.05s of the process were simulated
Eddy-Dissipation Concept model + RNG subgrid scale model

The initial conditions:

Low-pressure chamber: air (mass fraction of O_2 = 0.23, mass fraction of N_2 = 0.77), pressure P = 1 atm, temperature T = 300 K.

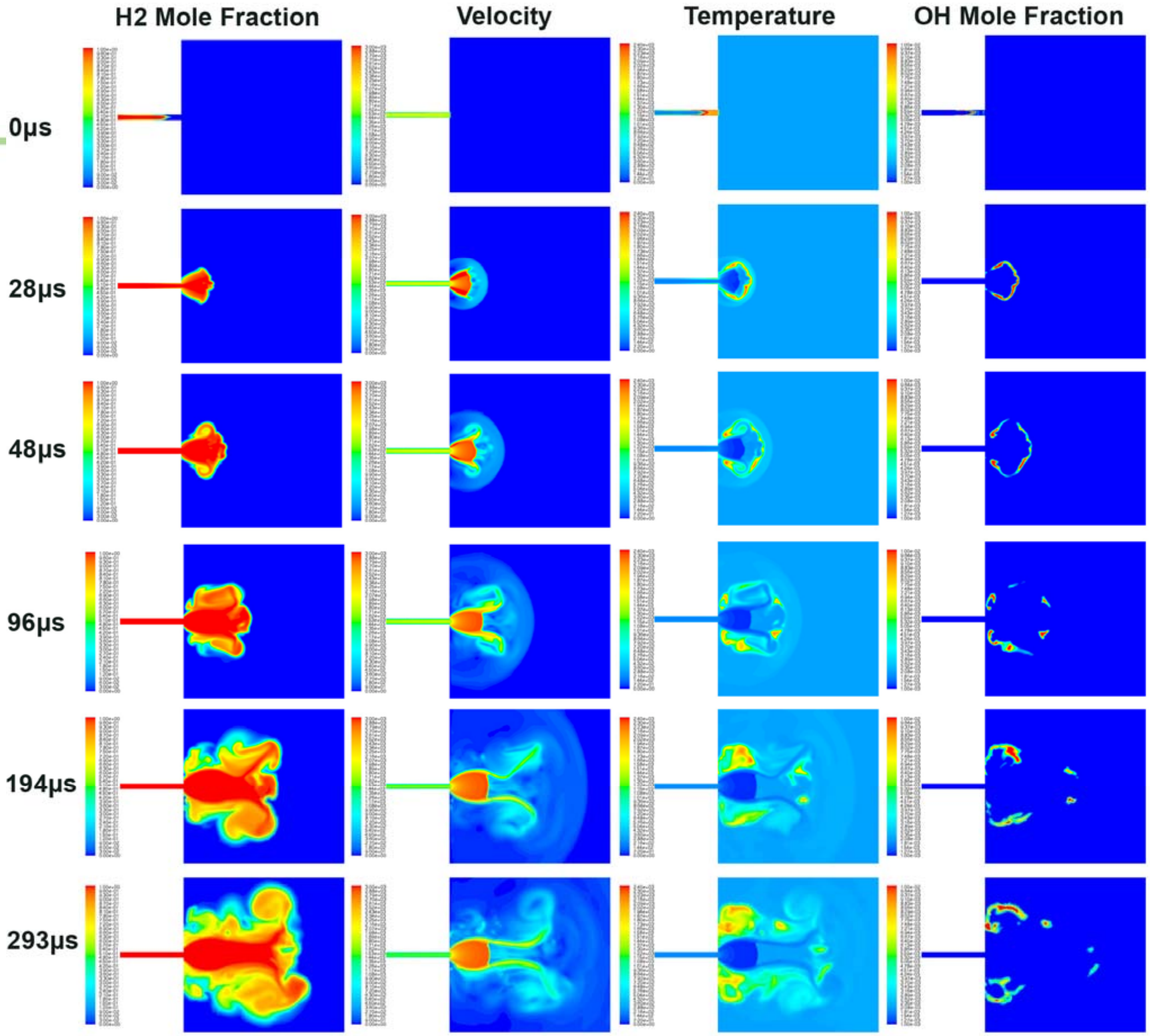
High-pressure chamber: hydrogen (mass fraction of H_2 = 1), pressure **P = 145 bar**, temperature T = 300 K.

Boundary (burst disk) separating chambers was removed instantly.

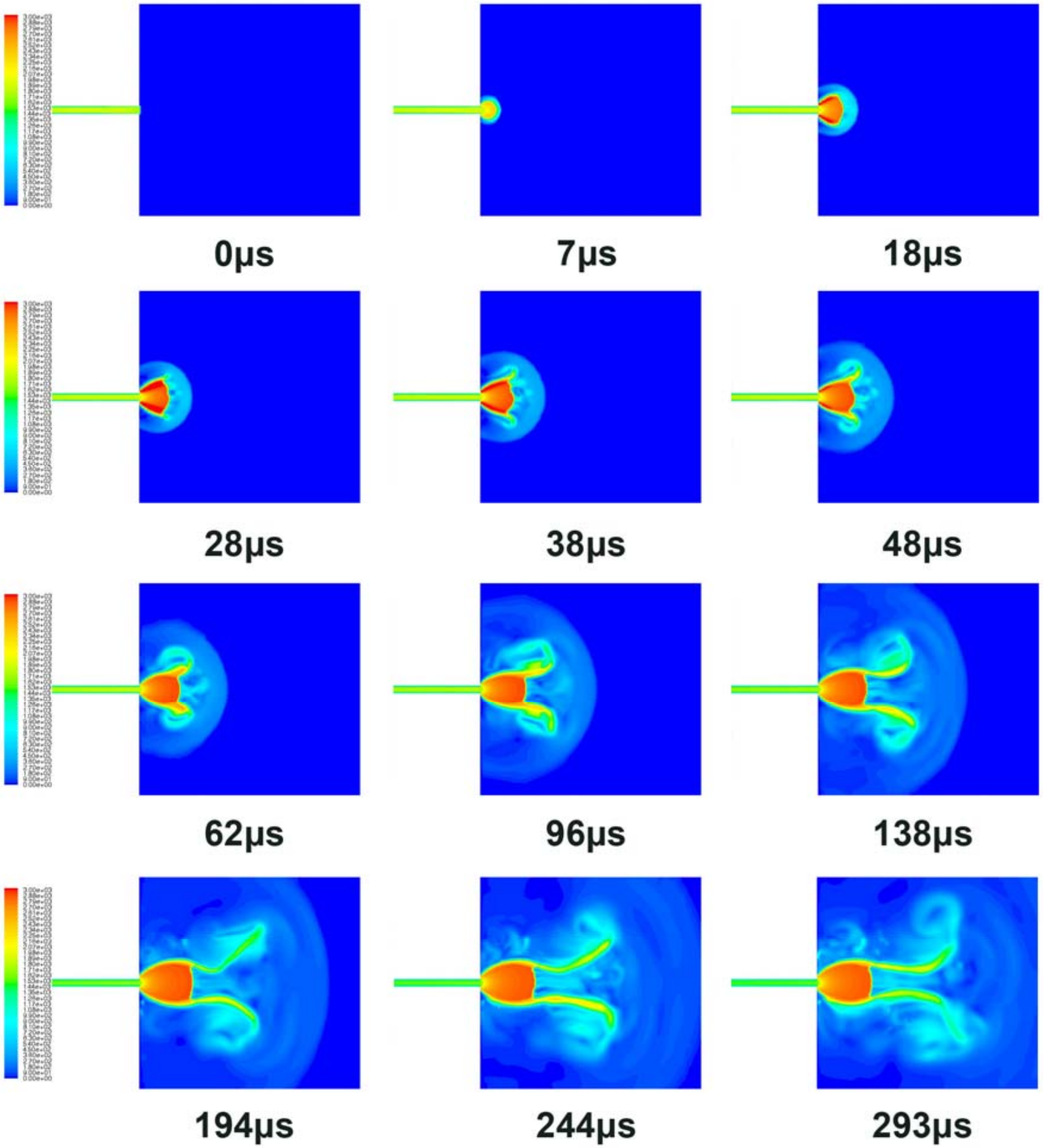


MOGI, T., KIM, D., SHIINA, H. & HORIGUCHI, S. (2008) Self-ignition and explosion during discharge of high-pressure hydrogen. *Journal of Loss Prevention in the Process Industries*, 21**,** 199-204.

Dynamics of the velocity, temperature and mole fractions of hydrogen and hydroxyl in 2D slice along the tube axis.



Velocity distribution in the underexpanded jet during development stage

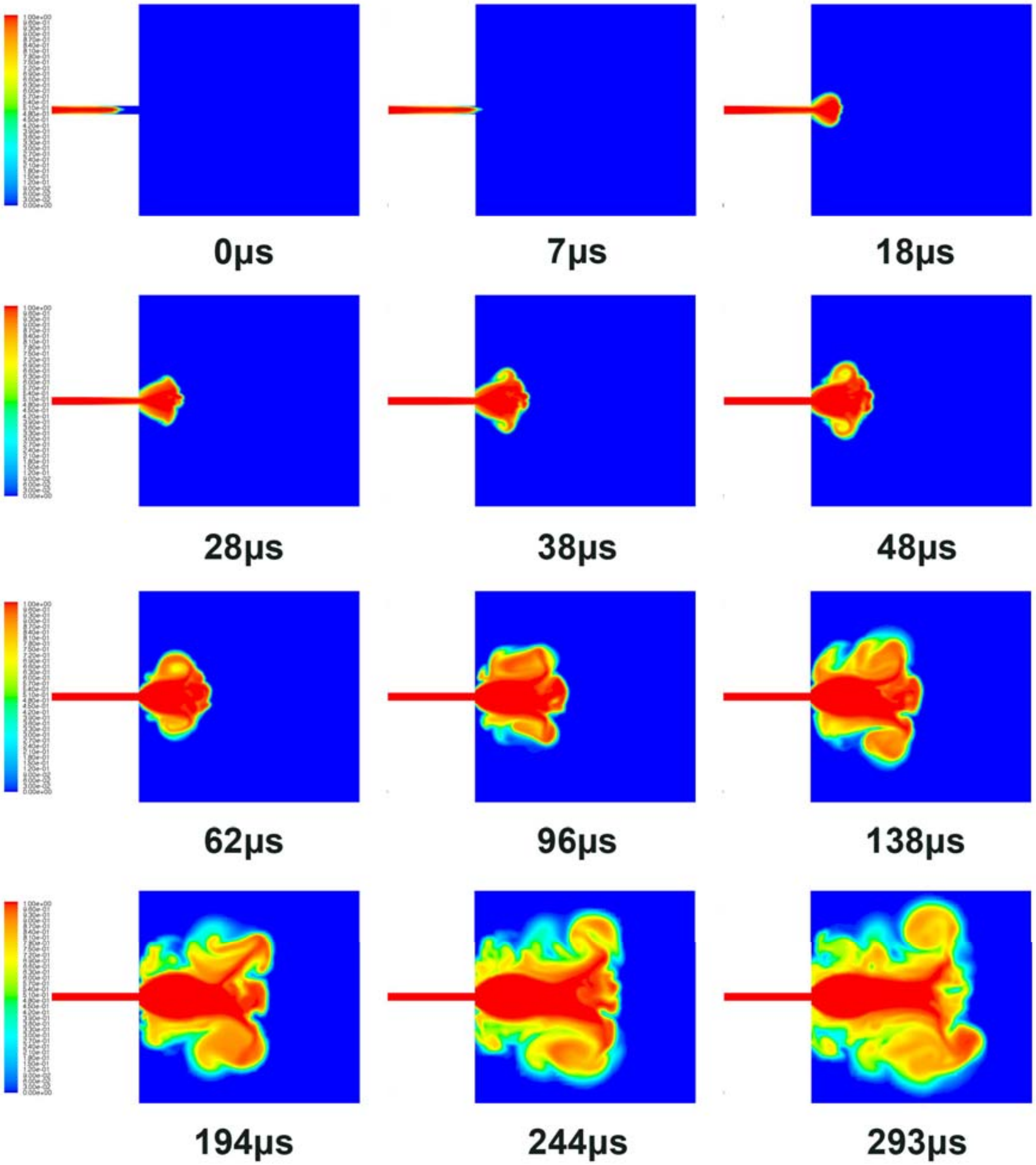


Formation of barrel-like shock structure is followed by the formation of annular vortex, which moves downstream

Mole fraction of hydrogen distribution

Annular vortex induces mixing

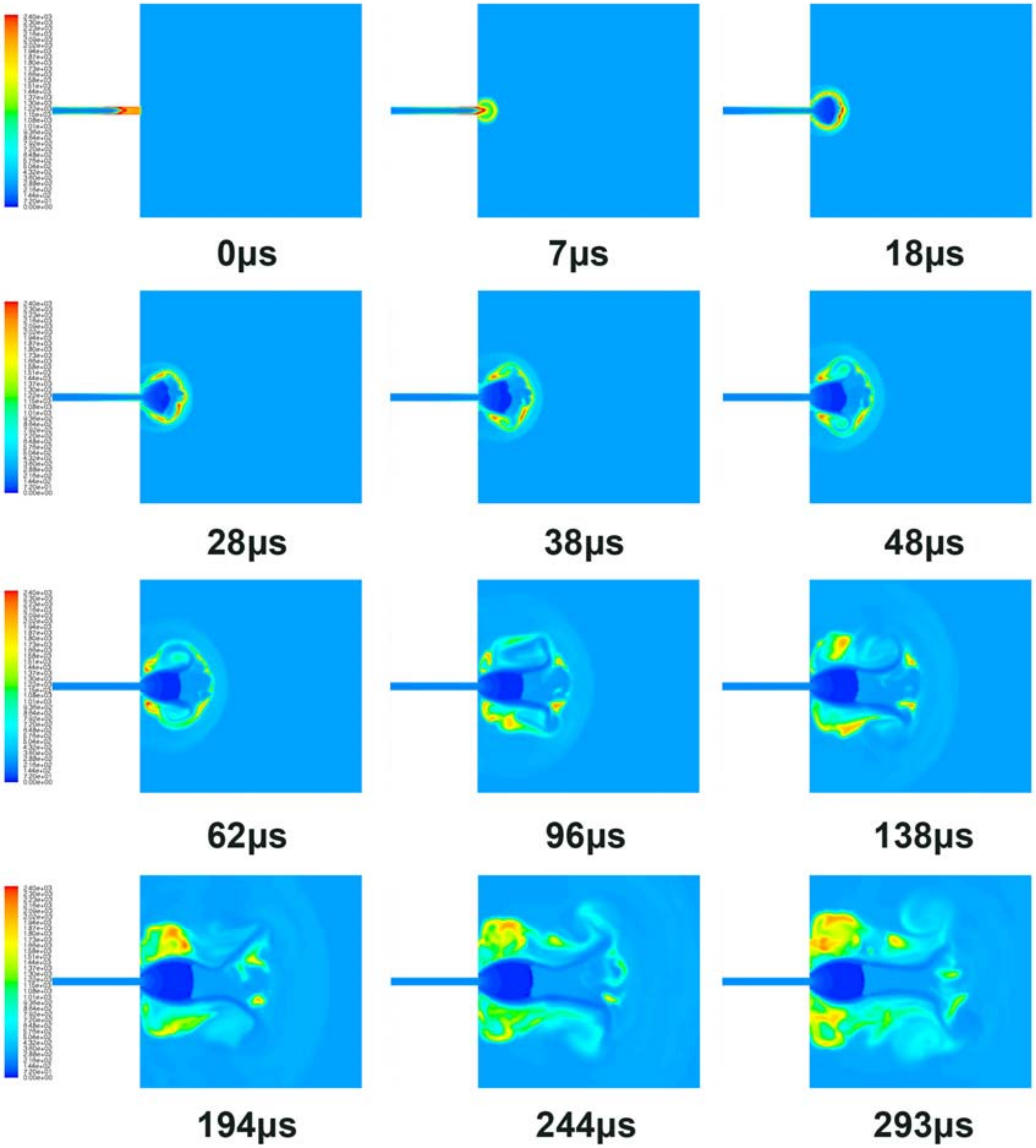
Combustible mixture is formed as the vortex propagate downstream



Temperature distribution

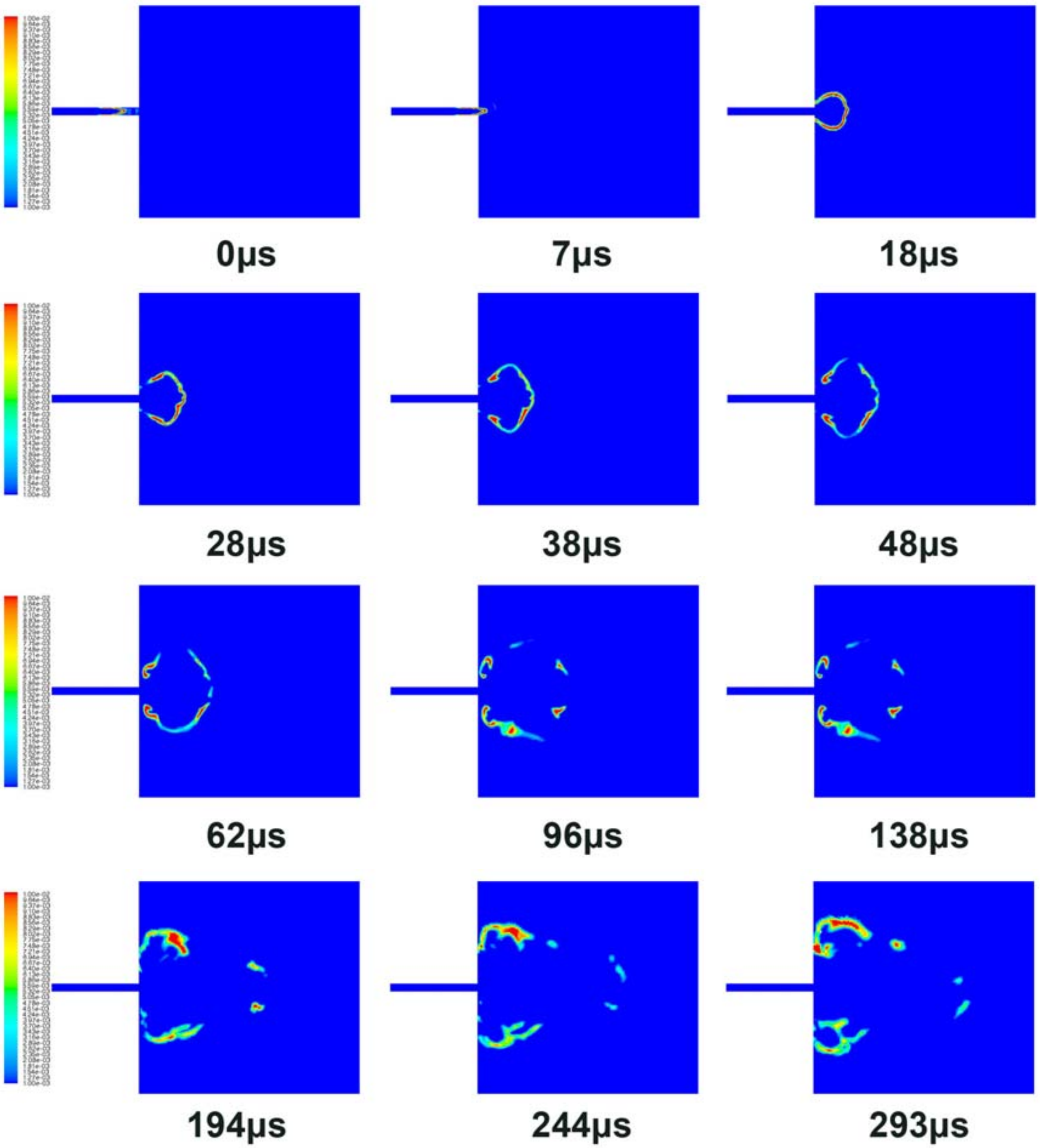
Cocoon of combusting mixture is broken by developing vortex

Upstream part is pushed back to the tube exit



Hydroxyl mole fraction distribution

Downstream combustion regions are extinguished, while in the upstream region flame is stabilized



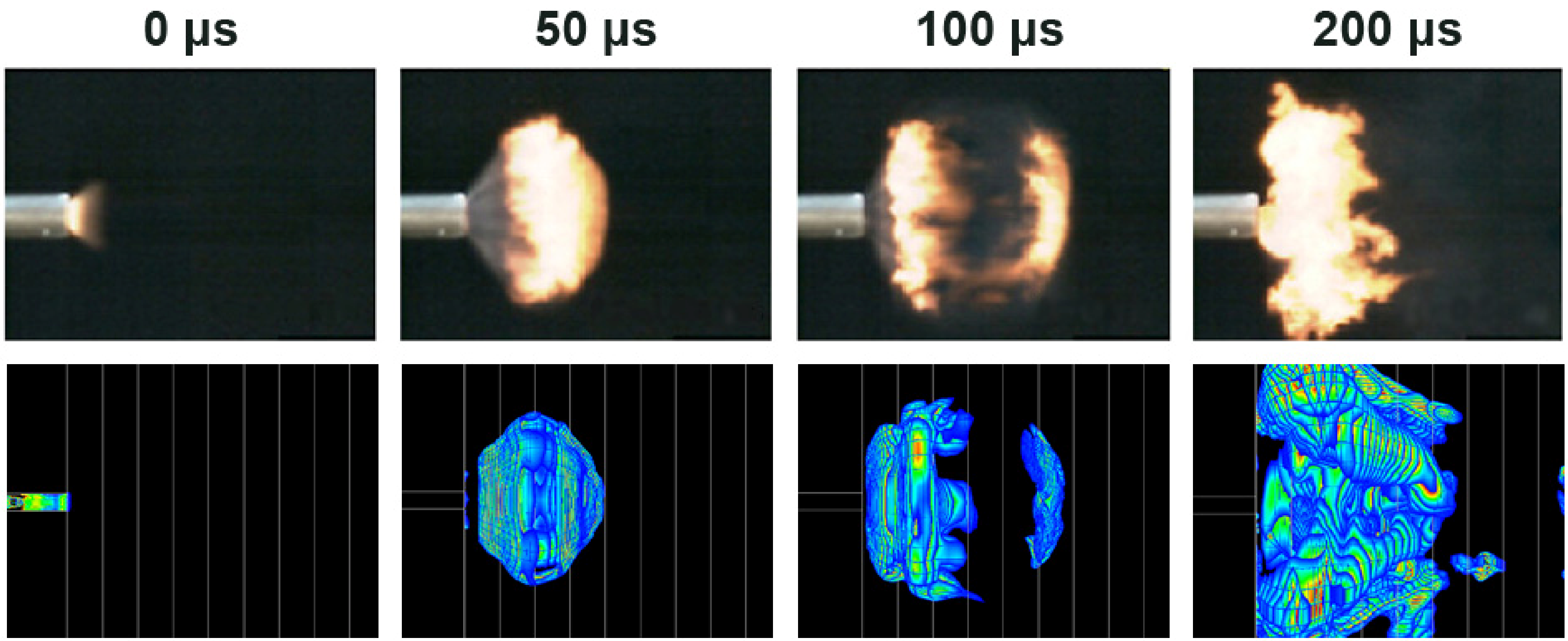
0μs 7μs 18μs

28μs 38μs 48μs

62μs 96μs 138μs

194μs 244μs 293μs

Comparison



Comparison of simulation results against experimental photographs from experiments by Mogi et al

Conclusions

- Mechanism of spontaneous ignition of high-pressure hydrogen discharges into downstream confinement (tube) was investigated
- It was demonstrated that ignition occurs in the boundary layer
- Dynamics of the spontaneous ignition process was demonstrated
- Mechanism of initial stage of transition of combusting mixture into a jet fire was investigated
- The transition largely depends on initial jet formation stage, where vortices push combusting mixture in recirculation zone. Once the flame is stabilized near the tube exit, it acts as a pilot flame and ignites jet fire later on (according to experimental observations by Mogi et al, 2008)

Thank you for your attention!
Questions?

Contact information:

Maxim Bragin
Hydrogen Safety Engineering and Research
University of Ulster
Shore Road, Newtownabbey, BT37 0QB. UK
Tel: +44(0)2890366073
mv.bragin@ulster.ac.uk