The dynamics and flame characteristics of cryogenic hydrogen jets – a numerical study

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Outline

- Direct Numerical Simulation (DNS) of cryogenic hydrogen jets
- Brief results of the DisCharIgn tests simulation
- LES of cryogenic hydrogen jet flames

DNS of cryogenic hydrogen jets - numerical method and set-up

- In-house compressible/multiphase/reacting flow solver[1].
- Direct numerical simulation (DNS).
- Sixth-order hybrid scheme (WENO-CU6) for the convective fluxes[2].
- Sixth-order compact scheme for the viscous fluxes.
- Third-order Runge-Kutta scheme for the time integrations.
- Thermodynamic properties based on Aly-Lee equation[3].
- Transportation properties based on kinetic gas theory.

[1] Ren Z, Wang B, Xiang G, Zheng L. Proceedings of the Combustion Institute, 2019, 37(3): 3627-3635.
[2] Hu X Y, Wang Q, Adams N A. Journal of Computational Physics, 2010, 229(23): 8952-8965.
[3] Aly F A, Lee L L. Fluid Phase Equilibria, 1981, 6(3-4): 169-179.
[4] Hecht E S, Panda P P. International Journal of Hydrogen Energy, 2019, 44(17): 8960-8970.

DNS of cryogenic hydrogen jet

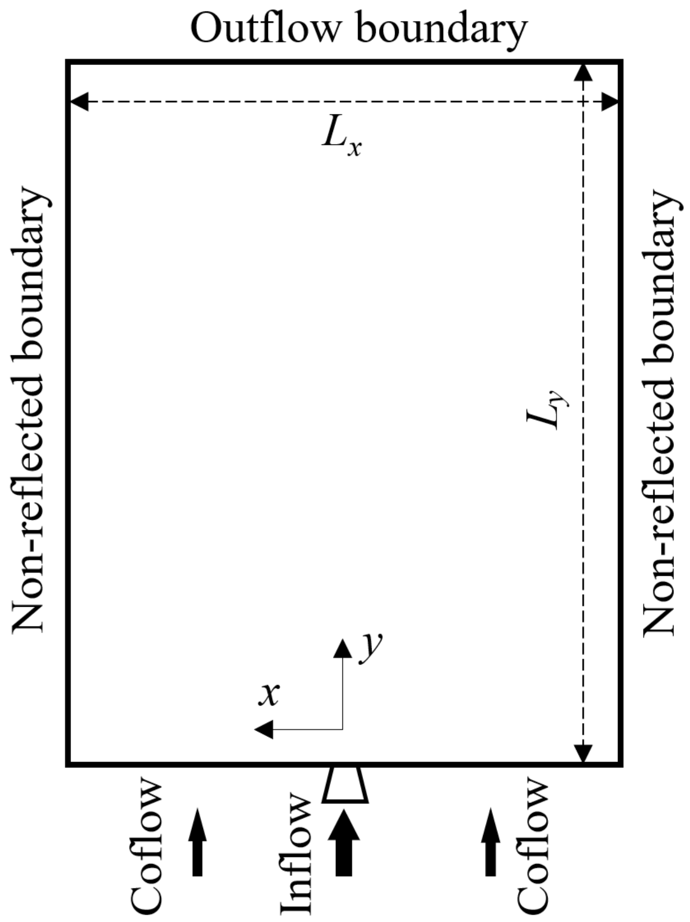


Table 1 Summary of inflow parameters

Case	Nozzle pressure, P_0 (bar)	Nozzle temperature, T_0 (K)	Nozzle diameter, d (mm)
LP	3.0	56	1.0
MP	4.0	53	1.0
HP	5.0	50	1.0
HPD1	5.0	50	0.75
HPD2	5.0	50	1.25
HPD3	5.0	50	1.5

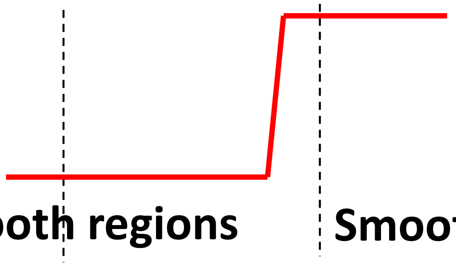
The set up follow the experiments of Hecht et al. (IJHE, 2019), 20μm grids. U_{air} 0.3m/s, 297K

Physical and mathematical model

Sixth-order Hybrid scheme
for the convective fluxes

(Hu, JCP, 2010)

Discontinuity regions → **WENO** captures the shock and eliminate pseudo numerical oscillations



Smooth regions | **Smooth regions** → **Linear scheme** reduces the numerical dissipation and the computation cost

fifth-order compact upwind *fifth-order WENO*

$$\hat{f}_{j+1/2} = \sigma_{j+1/2}\,\hat{f}^{CU}_{j+1/2} + (1-\sigma_{j+1/2})\,\hat{f}^{WENO}_{j+1/2}$$

smoothness indicator $\sigma_{j+1/2} = \min\left(1, \frac{r_{j+1/2}}{r_c}\right)$ r_c is a threshold for identifying the smooth

Sixth-order compact scheme
for the viscous fluxes

$$\frac{1}{3}F'_{v,j-1} + F'_{v,j} + \frac{1}{3}F'_{v,j+1} = \frac{28(f_{v,j+1} - f_{v,j-1}) + (f_{v,j+2} - f_{v,j-2})}{36h}$$

Third-order Runge-Kutta scheme
for the time integrations

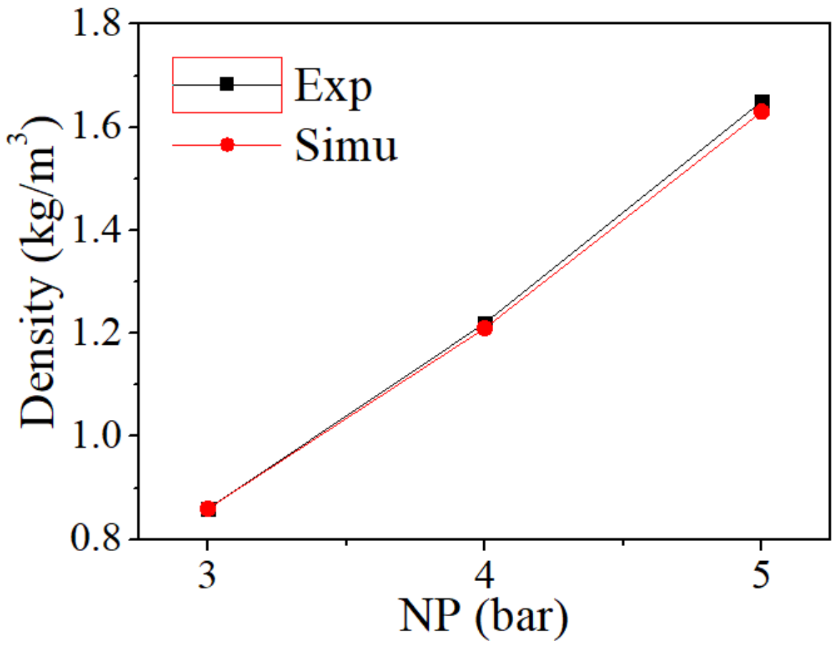
$$U_j^{(1)} = U_j^n + \Delta t L_j(U^n)$$

$$U_j^{(2)} = \frac{3}{4}U_j^n + \frac{1}{4}U_j^{(1)} + \frac{1}{4}\Delta t L_j(U_j^{(1)})$$

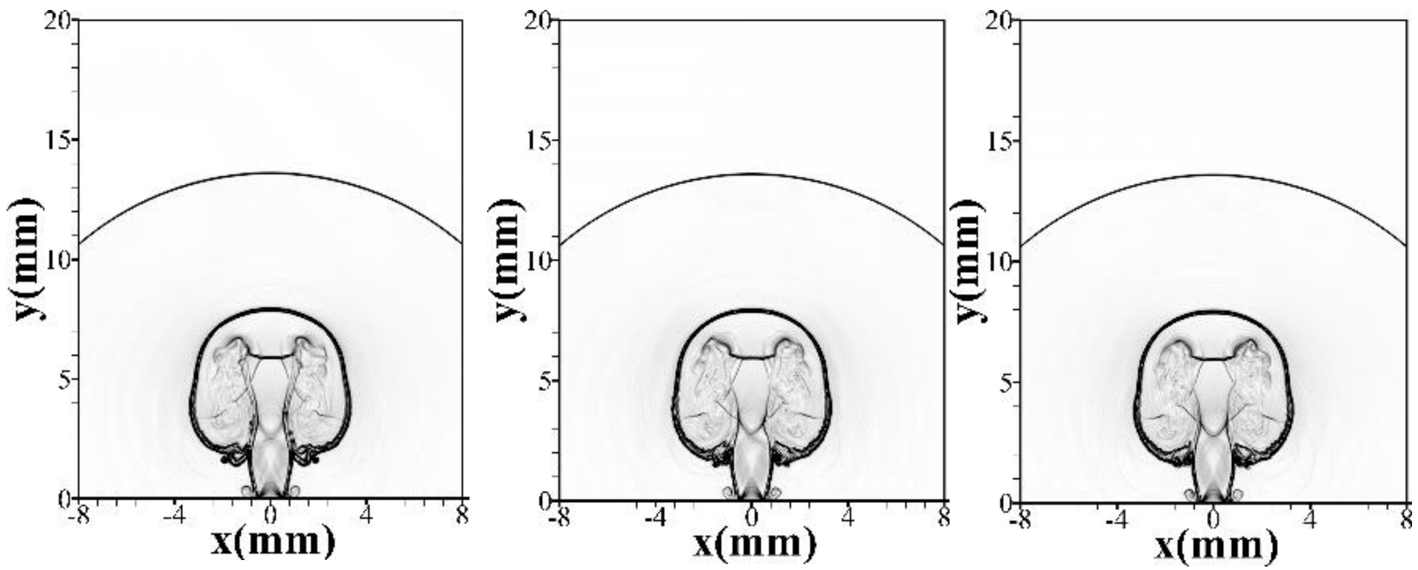
$$U_j^{n+1} = \frac{1}{3}U_j^n + \frac{2}{3}U_j^{(2)} + \frac{2}{3}\Delta t L_j(U_j^{(2)})$$

Numerical method and set-up

Code verification and grid sensitivity study



Comparison between the predicted and measured cryogenic hydrogen density.



- 30μm
- 20μm
- 10μm

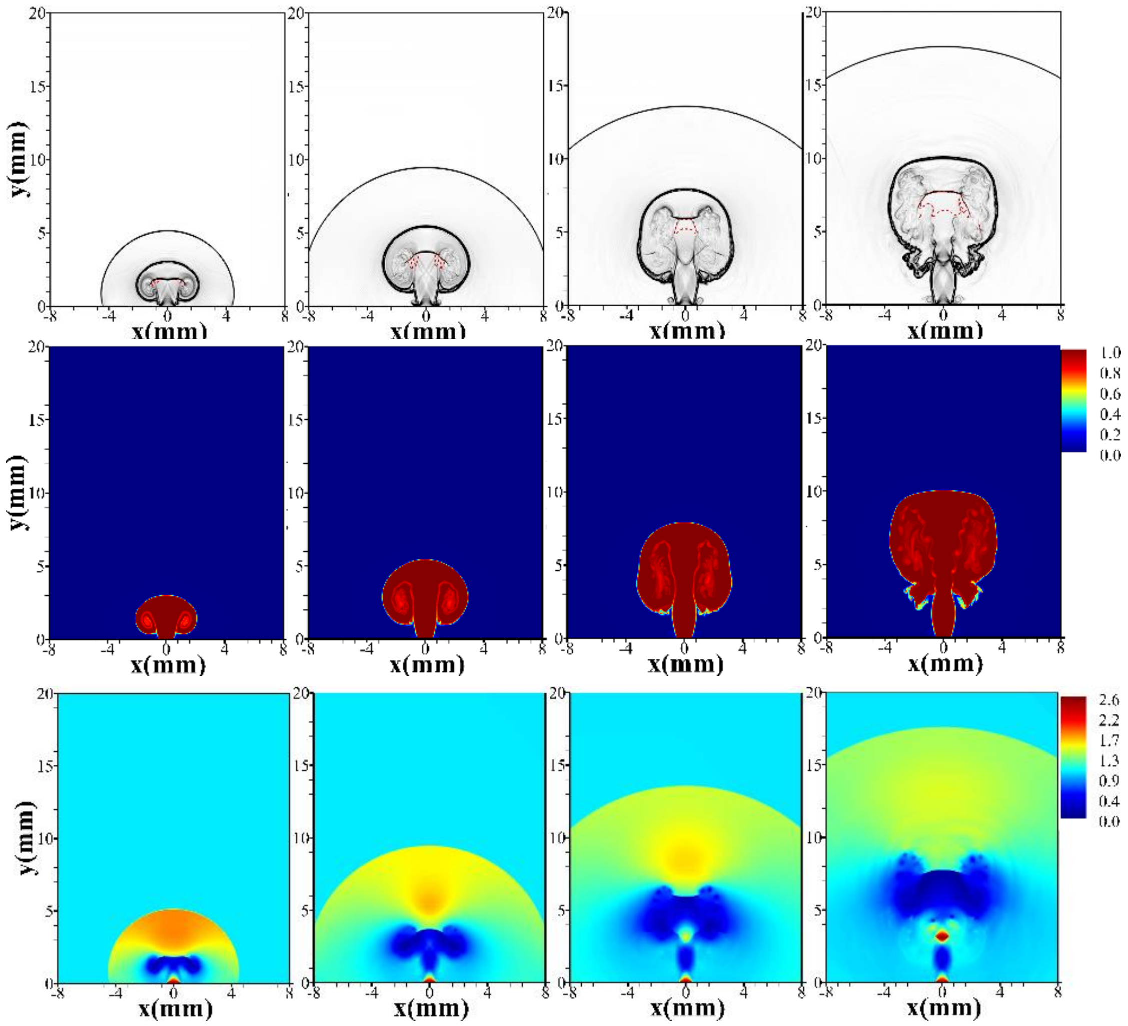
Distributions of density gradients predicted with different mesh resolutions.

Near-field features

Density gradient

H2 mass fraction

Pressure



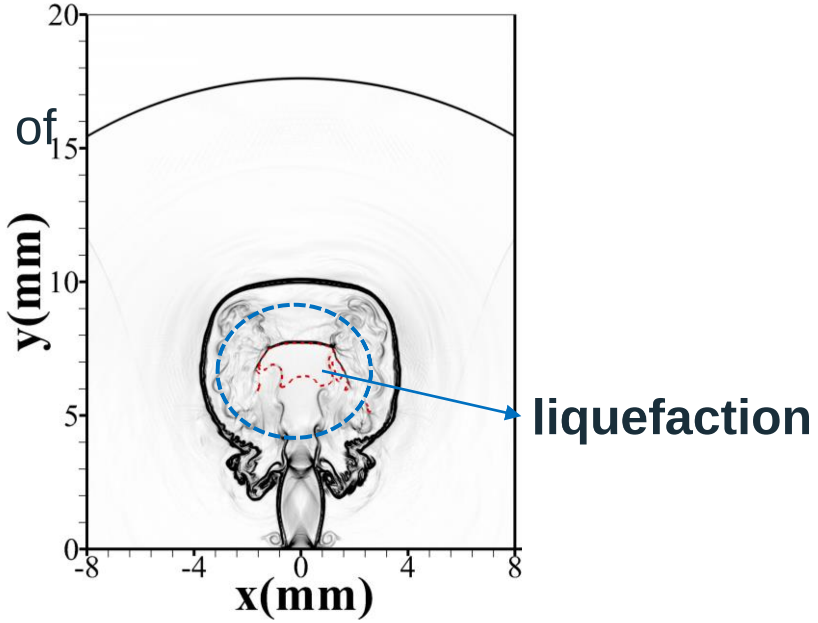
NP = 5 bar

- Transient development of the near-nozzle flow structure from t = 10 to 40μs shown in time interval of 10 μs.
- The red dashed lines denote the regions with **HLP > 0**.

The hydrogen liquefaction potentiality (**HLP**)

$$\mathrm{HLP} = P_{\mathrm{H2}} - P_{\mathrm{vap}}$$

HLP > 0 means the appearance of local liquefaction.

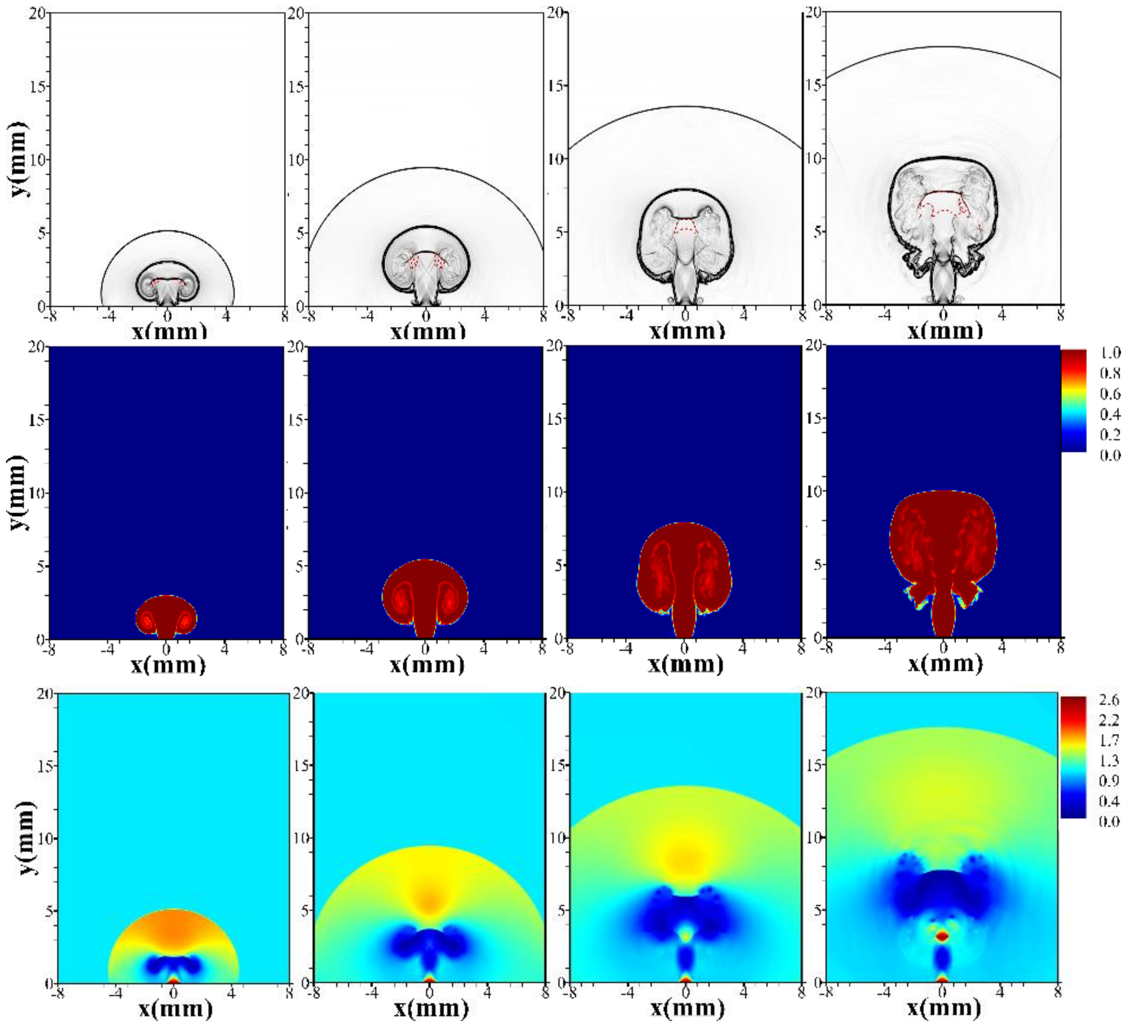


Near-field features

Density gradient

H2 mass fraction

Pressure



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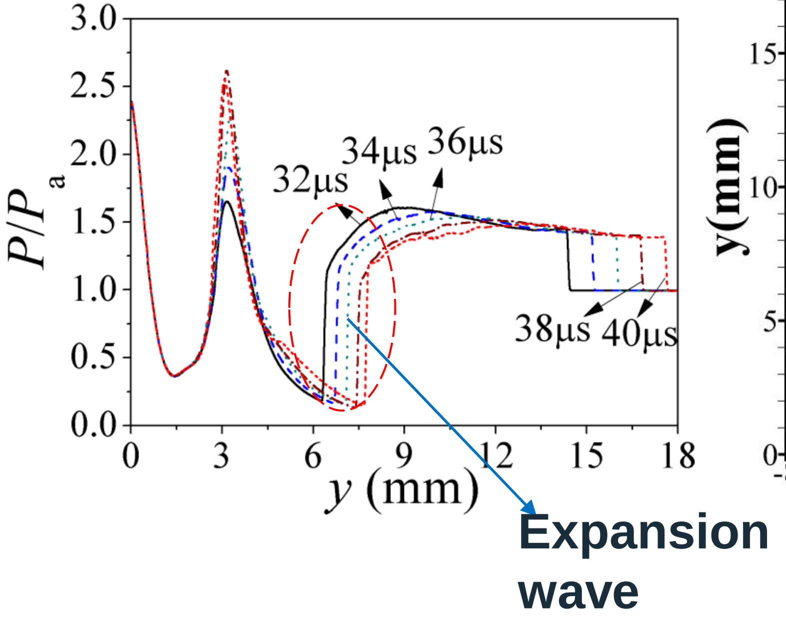
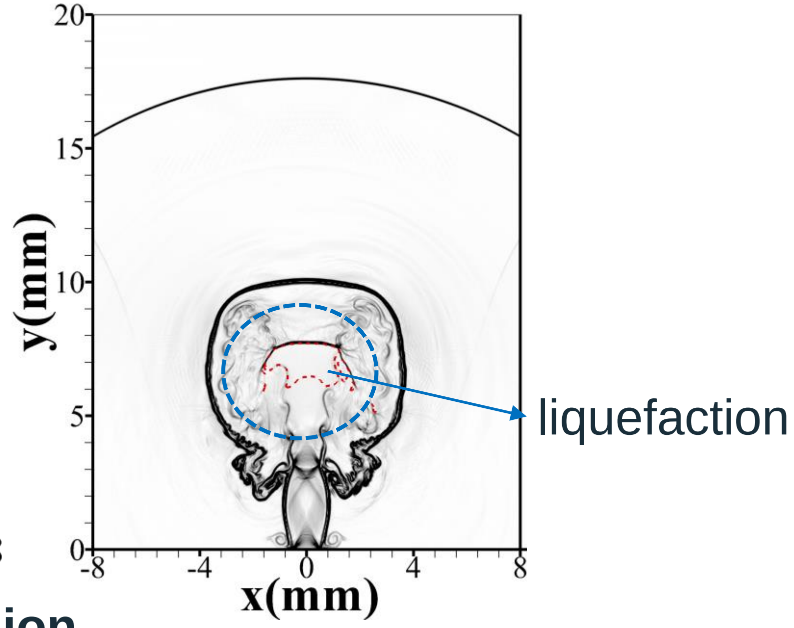
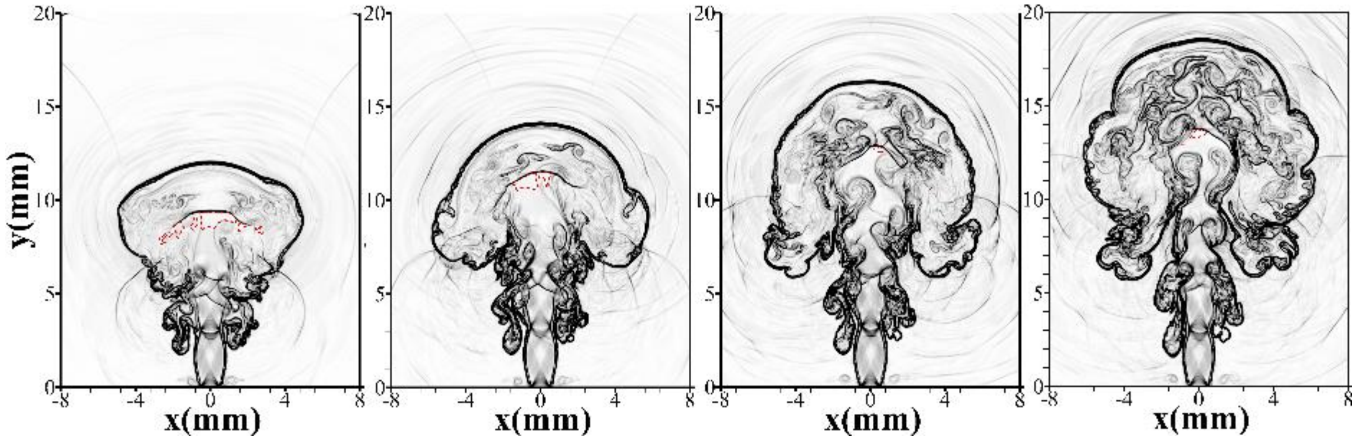




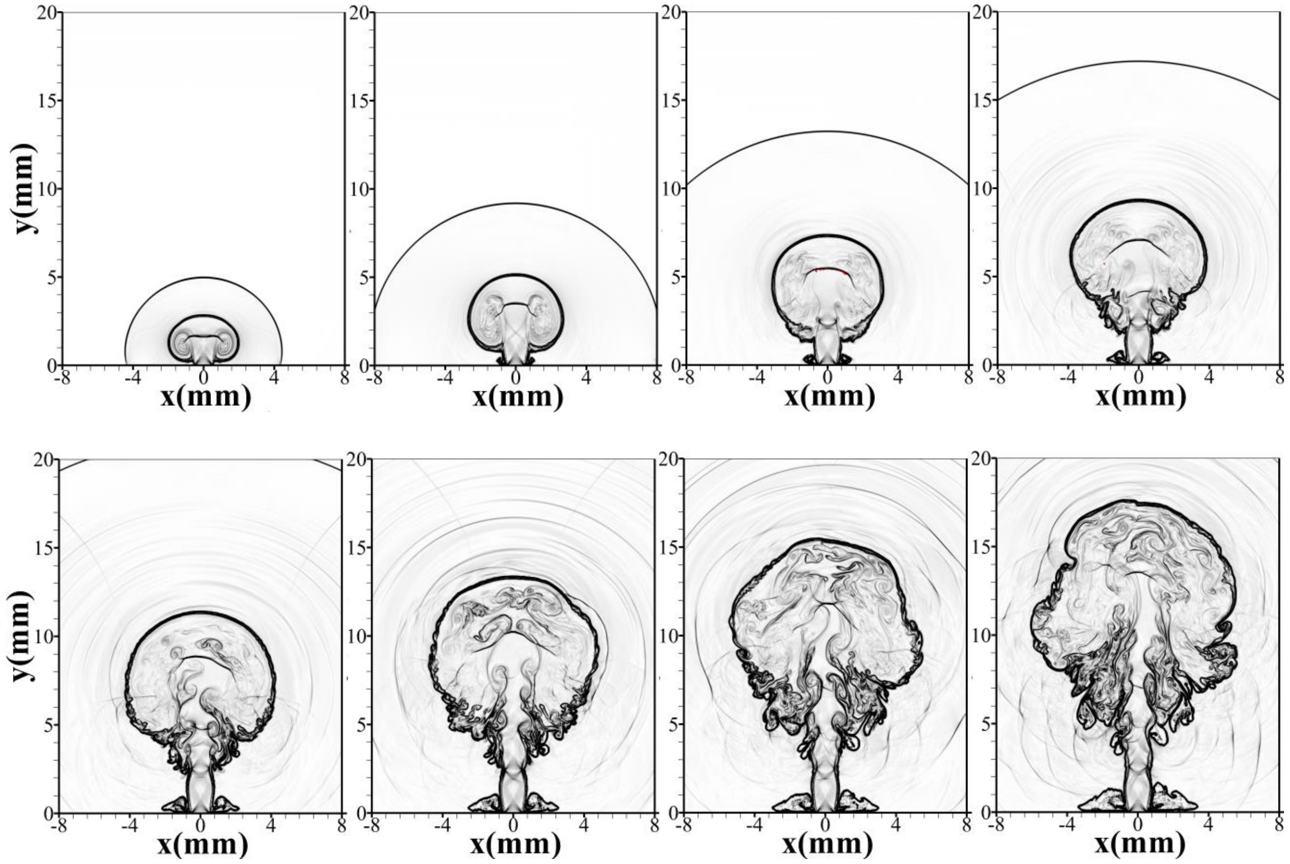
Near-field features

NP = 5 bar



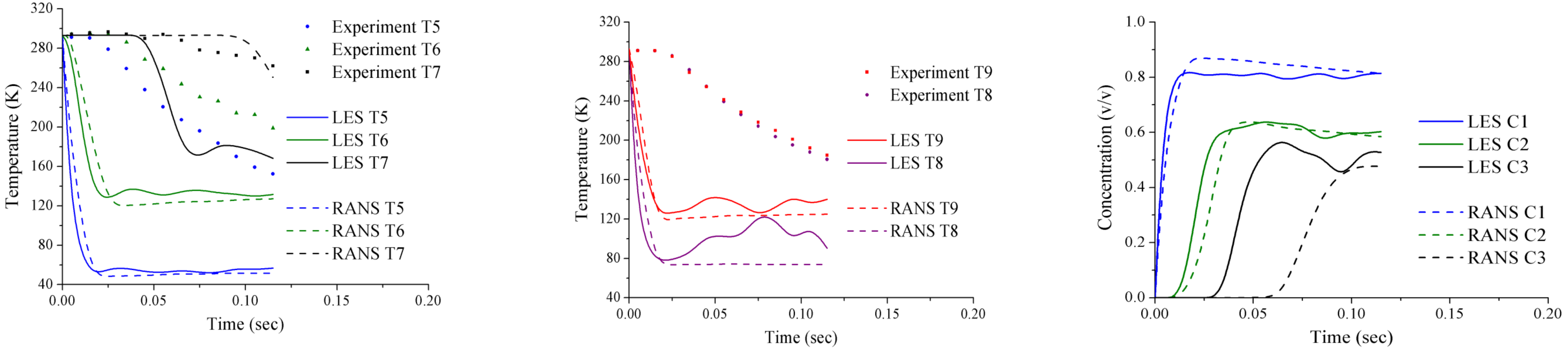
- Instantaneous distributions of density gradient for Case HP from *t* = 50 to 80μs shown in time interval of 10 μs.
- The red dashed lines denote the region of **HLP > 0**.

NP = 3 bar



- Low-pressure jet: **no liquefaction** occurs.

Brief results of the DisCharIgn simulation with LES and RANS



Comparison of the results between LES and RANS: (a) temperature of sensors T5, T6 and T7, (b) temperature of sensors T8 and T9, (c) hydrogen concentration of sensors C1, C2 and C3.

Outline

- Direct Numerical Simulation (DNS) of cryogenic hydrogen jets
- Brief results of the DisCharIgn tests simulation
- **LES of cryogenic hydrogen jet flames**

Numerical method

- Compressible reacting flow solver: rhoReactingFoam based on OpenFOAM

- 3D Large Eddy Simulation (LES) with one-equation eddy-viscosity SGS model[1] for compressible flow

- Eddy Dissipation Concept (EDC) model[2] with detailed hydrogen chemistry[3] (9 species and 19 steps) for non-premixed flame

[1] Yoshizawa A. Physical Review E, 1993, 48(1): 273.
[2] Parente A, Malik M R, Contino F, Cuoci A, Dally B B. Fuel, 2016, 163: 98-111.
[3] Ó Conaire M, Curran H J, Simmie J M, Simmie J M, Pitz W J, Westbrook C K. International Journal of Chemical Kinetics, 2004, 36(11): 603-622.

Computational set-up

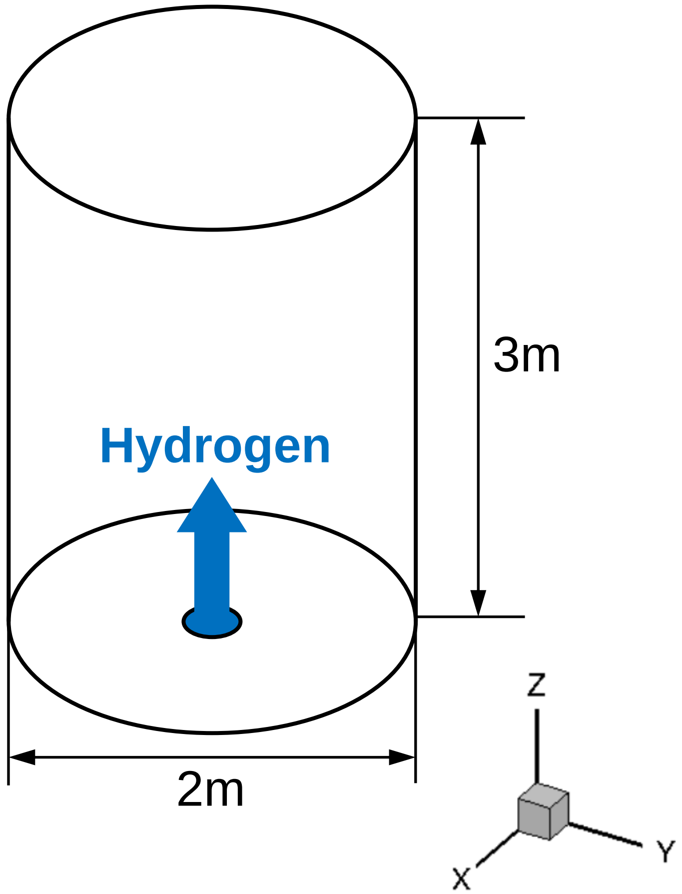
Initial parameters[1]

Hydrogen

Total pressure	200bar
Total temperature	80K
Nozzle diameter	4mm

Ambient air

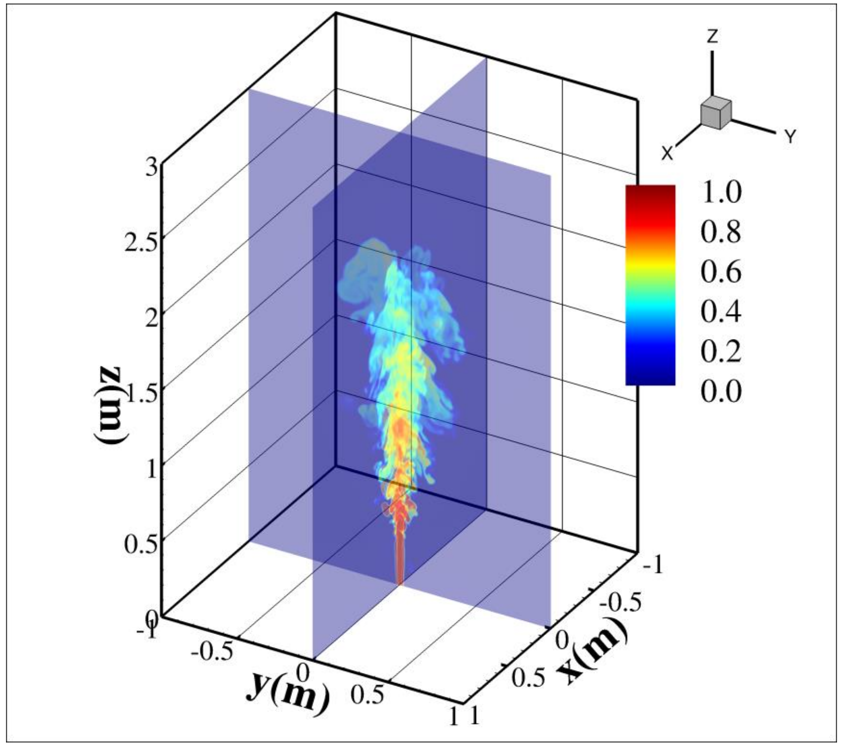
Static pressure	1bar
Static temperature	297K
Velocity	0m/s

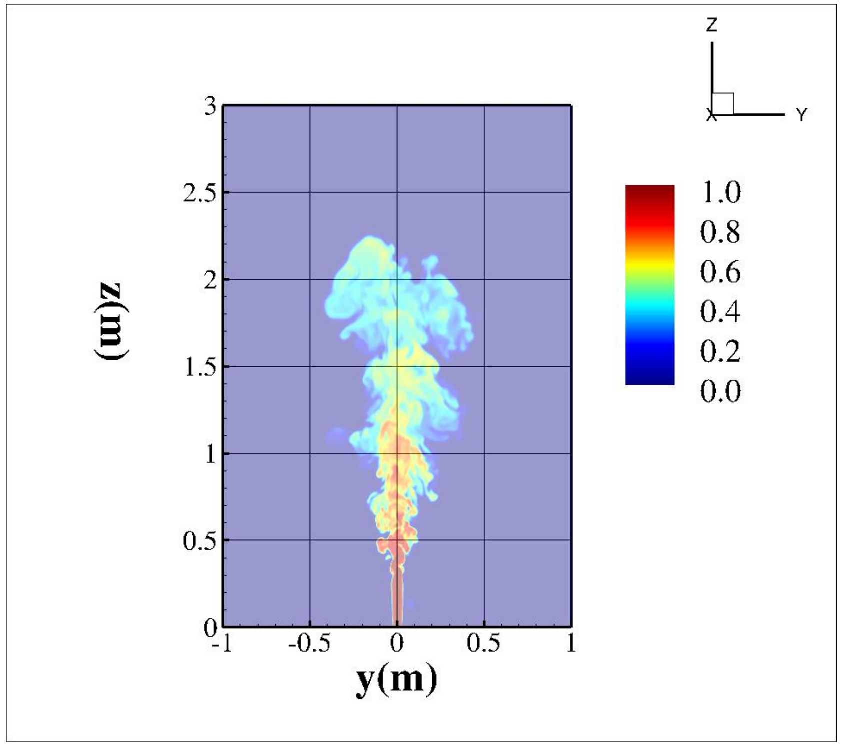


- **Schematics of computation domain.**

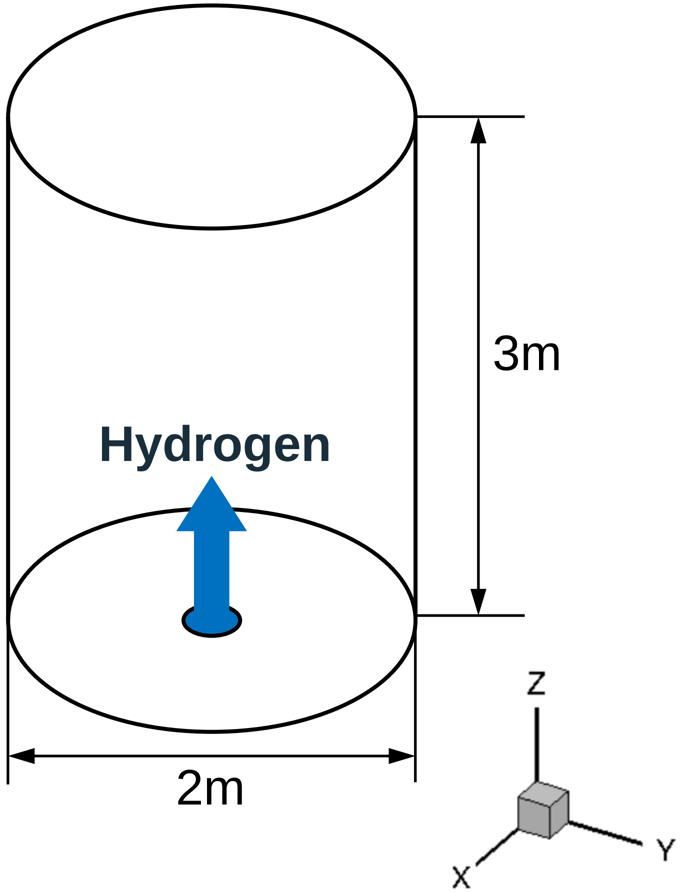
[1] Work Package 5, PRESLHY project, Fuel Cells and Hydrogen 2 Joint Undertaking.

Unignited cryogenic jet





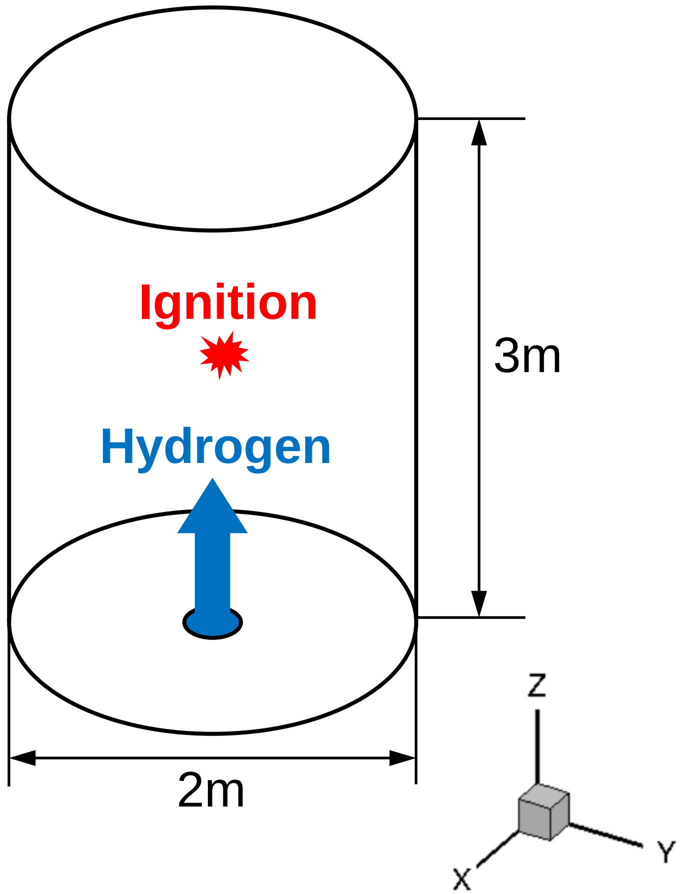
Instantaneous distributions of H2 mole fraction.



Schematics of computation domain.

Ignited cryogenic jet

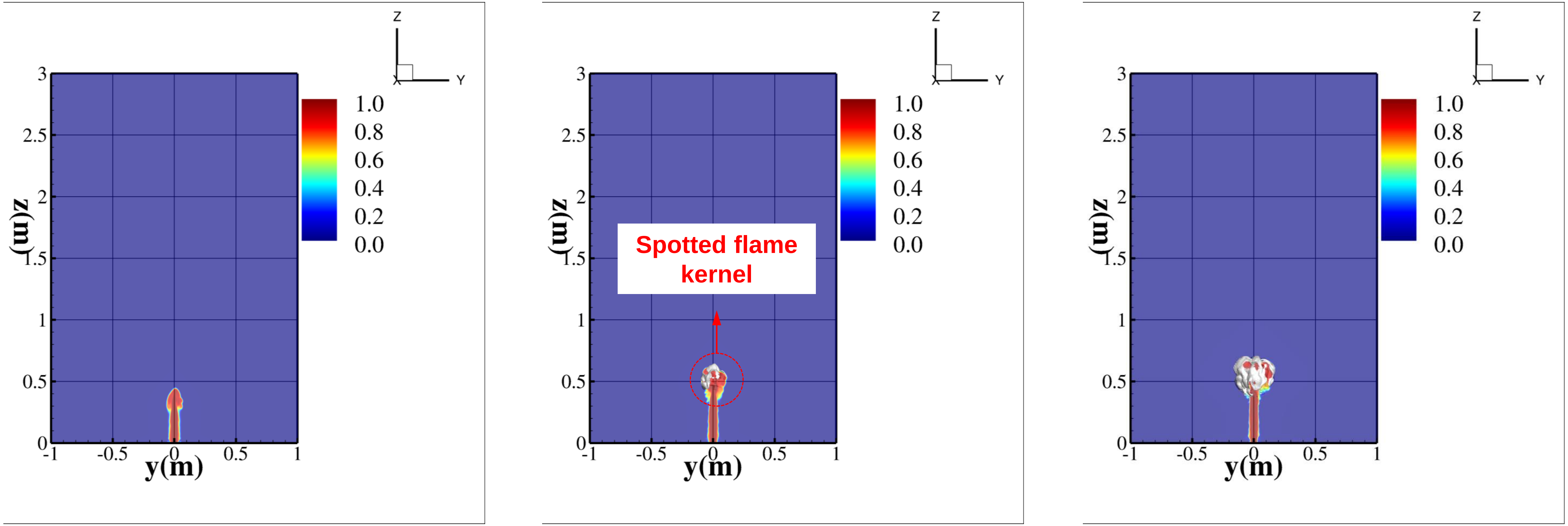
Case	Ignition position, z (m)	Ignition temperature (K)
0.5IG	0.5	2000
1.0IG	1.0	2000
2.0IG	2.0	2000



Schematics of computation domain.

RESULTS

Case 0.5IG (ignition at z = 0.5 m)

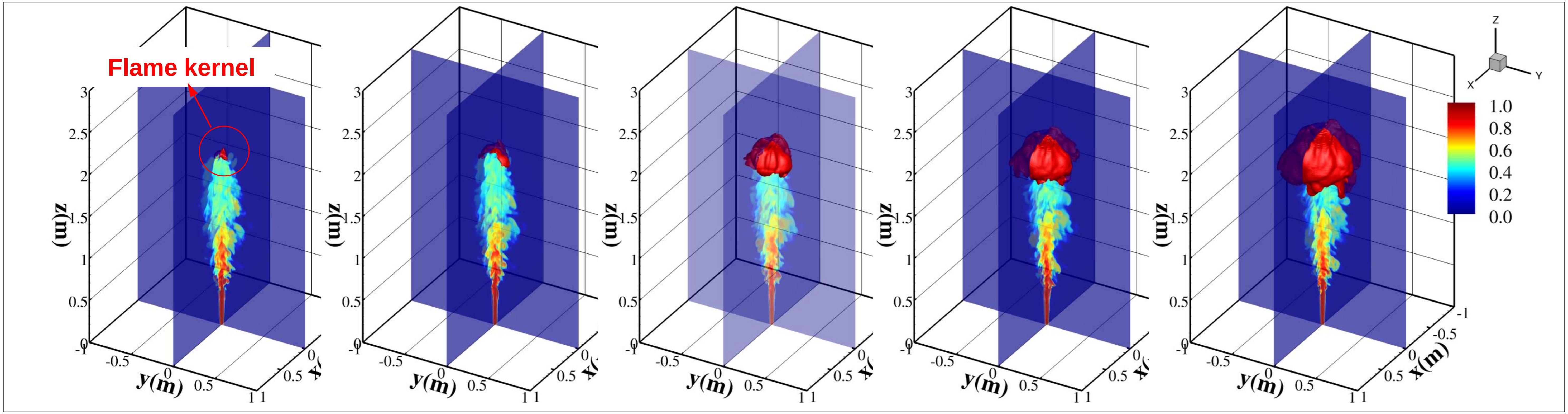


Distributions of H2 mole fraction, from left to right: time = 0.002s, 0.003s, 0.004s.
Iso-surface (white color) of OH mass fraction (0.003) to indicate the flame front.

RESULTS

Case 2.0IG (ignition at z = 2.0 m)

Development of jet flow after the hot spot.

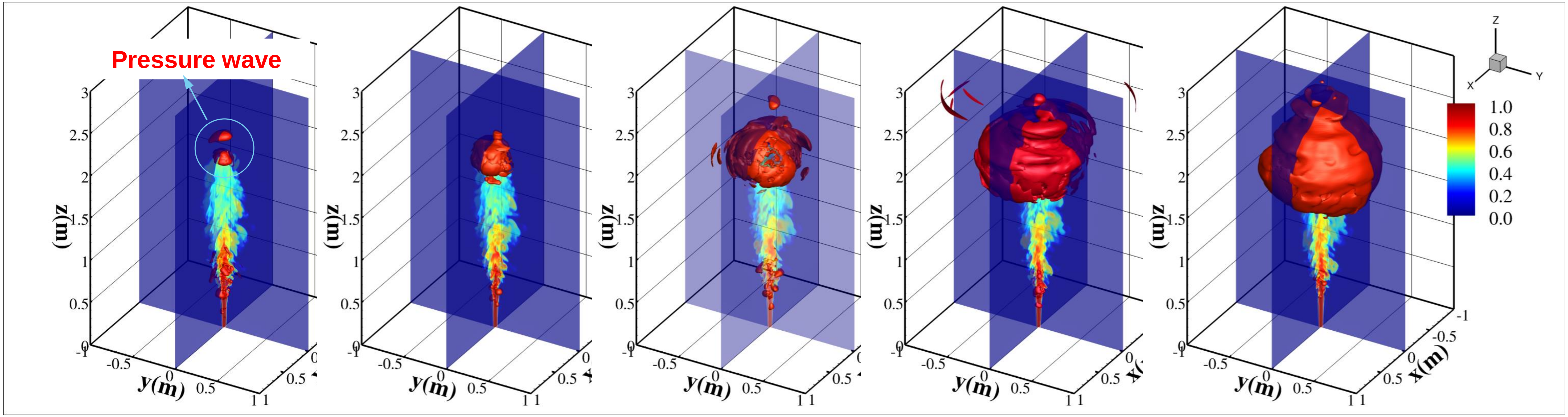


Distributions of H2 mole fraction, from left to right: time = 0.037s, 0.039s, 0.041s, 0.043s, 0.045s.
Iso-surface (red color) of OH mass fraction (0.005) to indicate the flame front.

RESULTS

Case 2.0IG (ignition at z = 2.0 m)

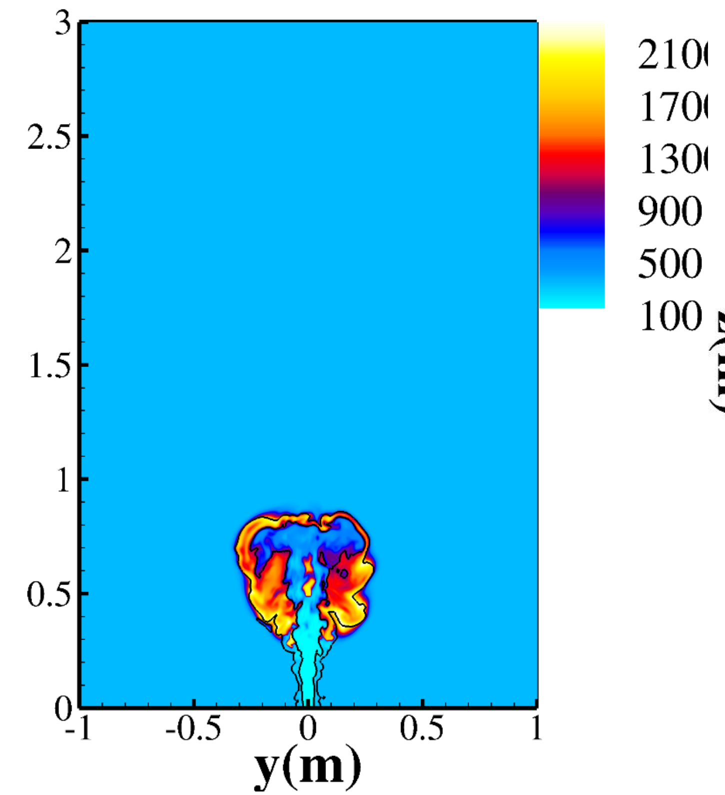
Development of jet flow after the hot spot.



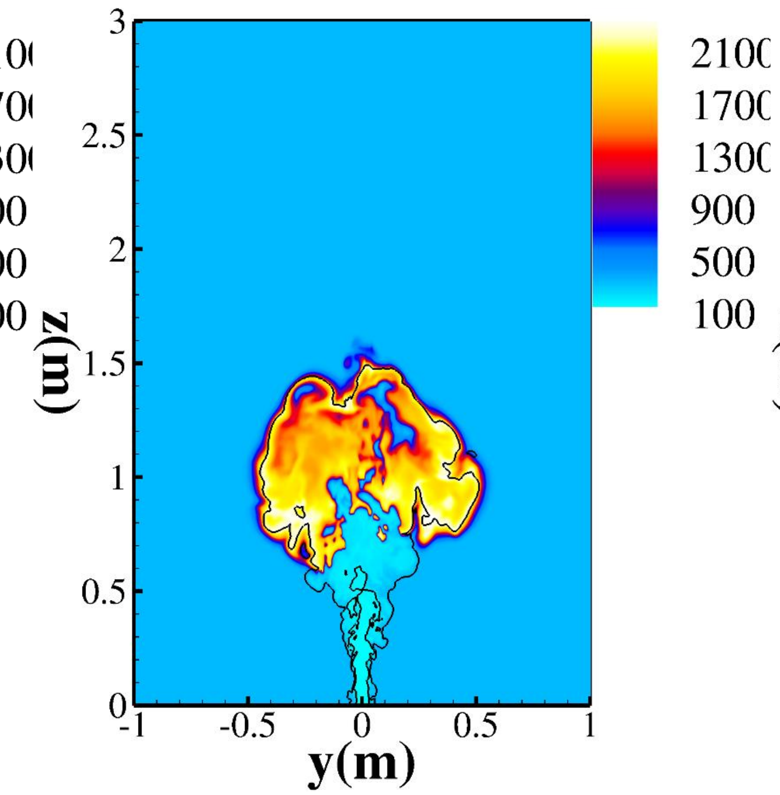
ΔP = 1 kPa ΔP = 2 kPa ΔP = 2 kPa ΔP = 3 kPa ΔP = 6 kPa

Distributions of H2 mole fraction, from left to right: time = 0.037s, 0.039s, 0.041s, 0.043s, 0.045s.
Iso-surface (red color) of pressure to indicate the pressure wave and the values, $\Delta P = P - P_a$, increase from left to right.

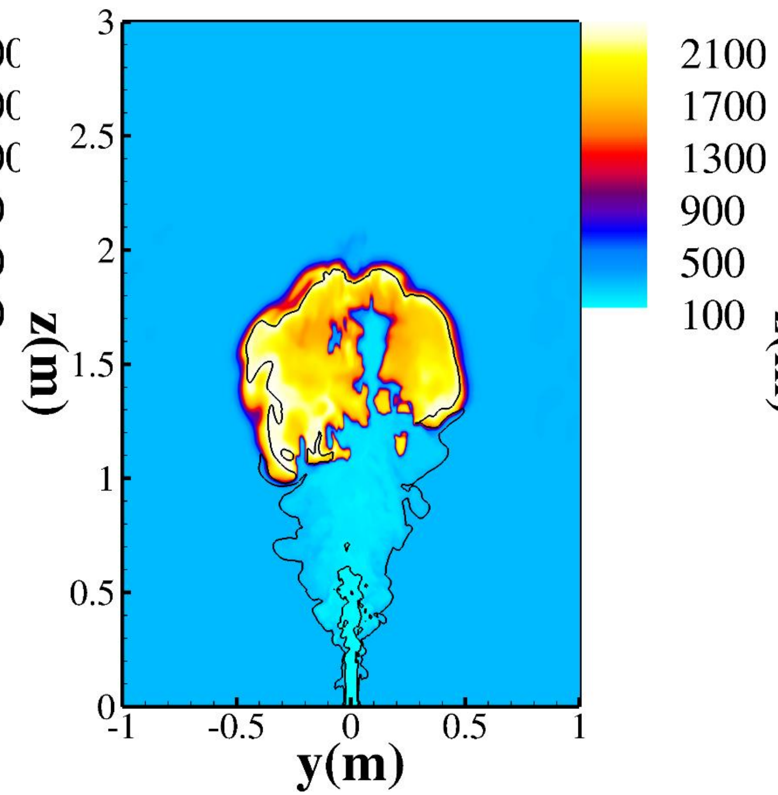
Overall flame structures



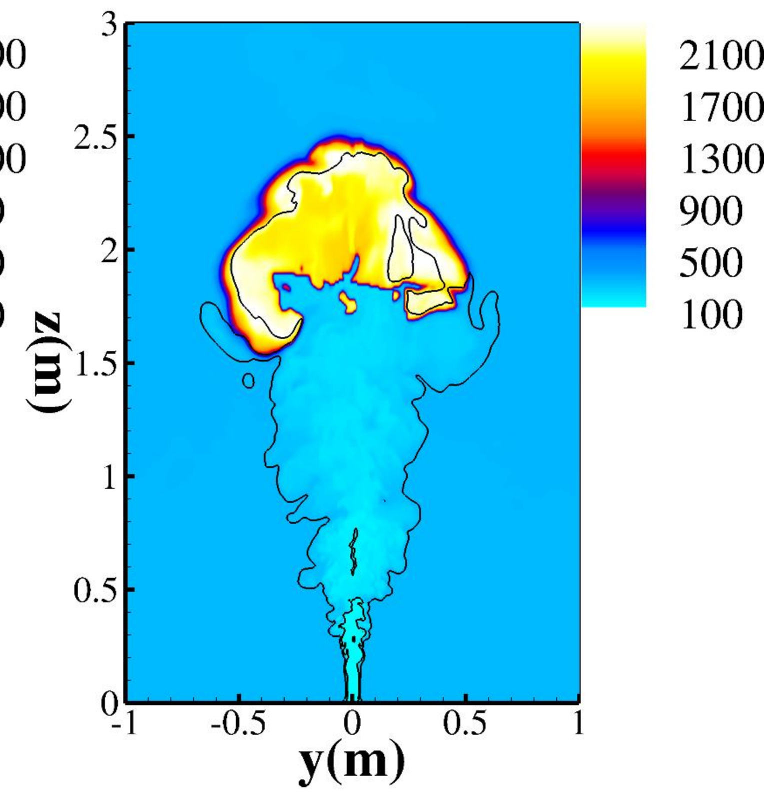
0.5 m ignition, t = 9 ms



1.0 m ignition, t = 21.6 ms



1.5 m ignition, t = 34.7 ms



2.0 m ignition, t = 64.2 ms

The contours are temperature (K) at the *y*-*z* plane and the black iso-lines denote concentrations within the flammability limit, Mol_{H2} = (0.040, 0.756).

Concluding remarks

Unignited cryogenic jets:

- The early evolution consists of initial penetration, near-nozzle expansion, downstream compression and wave propagation.
- Strong expansion in the jet head can lead to localized liquefaction.
- CFD simulations of Dischlarlg tests will be presented at ICHS 2021 as part of joint paper at ICHS2021

Ignited cryogenic hydrogen jets:

- If the spark is too close to the exit, the flame cannot propagate inside the cold jet and a side flame is formed.
- For the medium- and far-range ignitions, an envelope flame around the jet is formed.
- The unsteady flame dynamics are determined by the complex interactions between turbulence, fuel-air mixing and chemical reactions.
- CFD simulations of Dischlarlg tests are currently in progress with assistance from NCSRD to provide the transient nozzle condition.

Acknowledgement

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