Numerical simulations of under-expanded cryogenic hydrogen jet and flame

Zhaoxin Ren *and Jennifer X Wen*
Warwick FIRE, School of Engineering
University of Warwick

Numerical method

- Compressible reacting flow solver: rhoReactingFoam based on OpenFOAM.

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

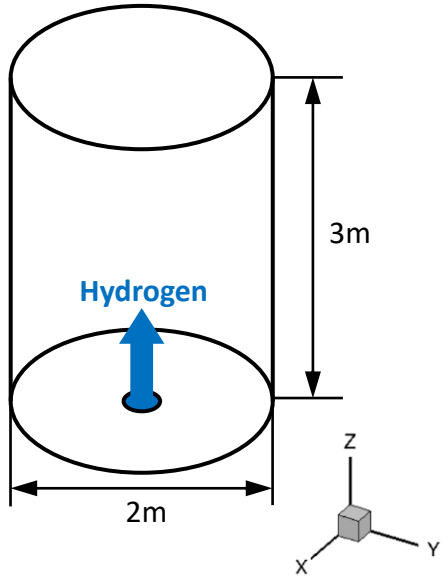
- Eddy Dissipation Concept (EDC) model[2] with H2 detailed chemistry[3] (9 species and 19 steps) for non-premixed flame.

[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.

Computation set-up

Initial parameters[1]

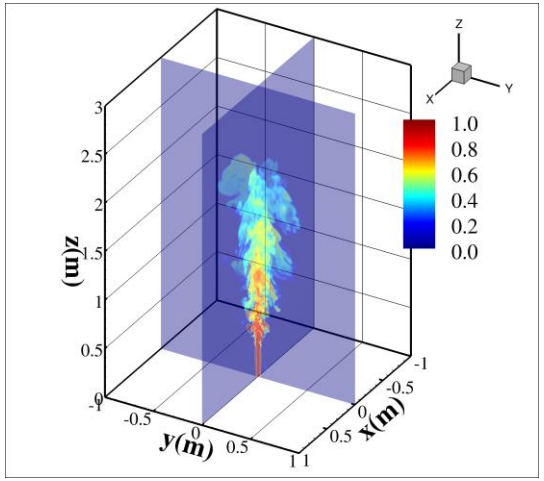
- **Hydrogen**
  - ✓ Total pressure 200bar
  - ✓ Total temperature 80K
  - ✓ Nozzle diameter 4mm
- **Ambient air**
  - ✓ Static pressure 1bar
  - ✓ Static temperature 297K
  - ✓ Velocity 0m/s

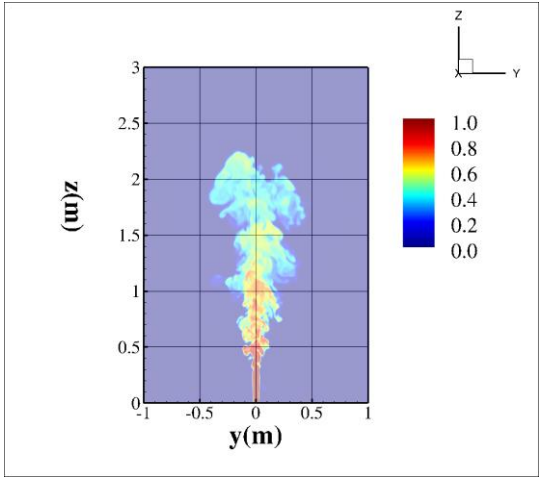


- **Schematics of computation domain.**

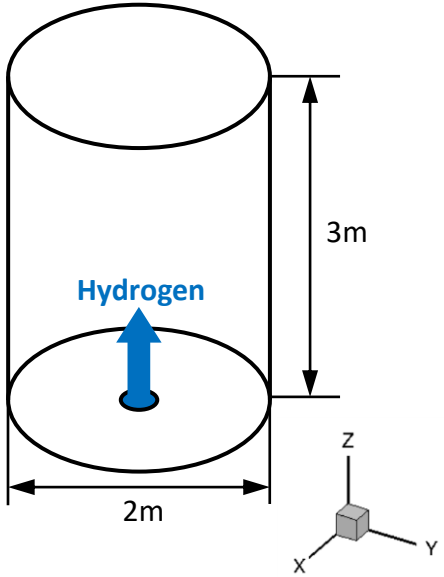
[1] Work Package 5, PRESLHY project, Fuel Cells and Hydrogen 2 Joint Undertaking.

Unignited cryogenic jet





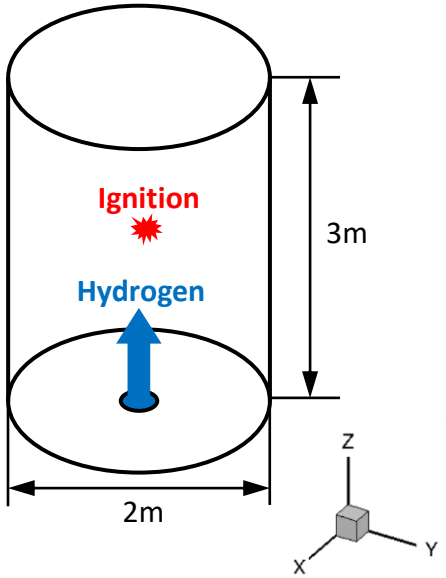
- **Instantaneous distributions of H2 mole fraction.**



- **Schematics of computation domain.**

Ignited cryogenic jet

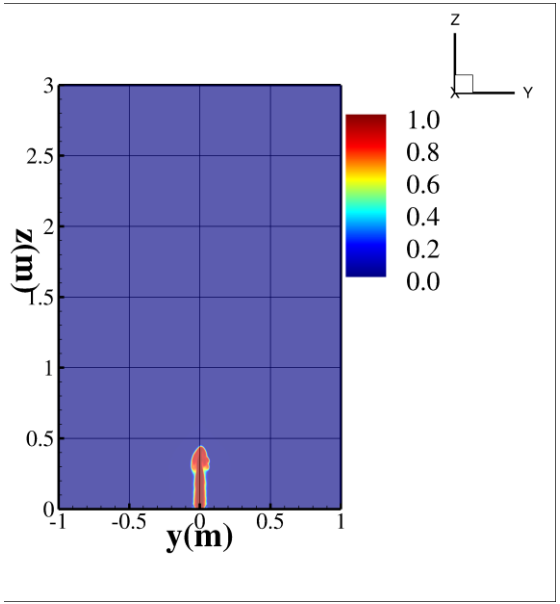
Case	Ignition position, z (m)	Ignition temperature (K)
0.5IG	0.5	2000
2.0IG	2.0	2000

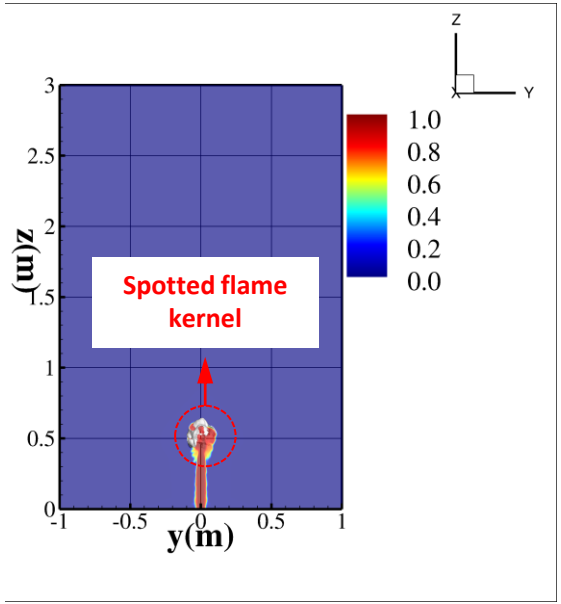


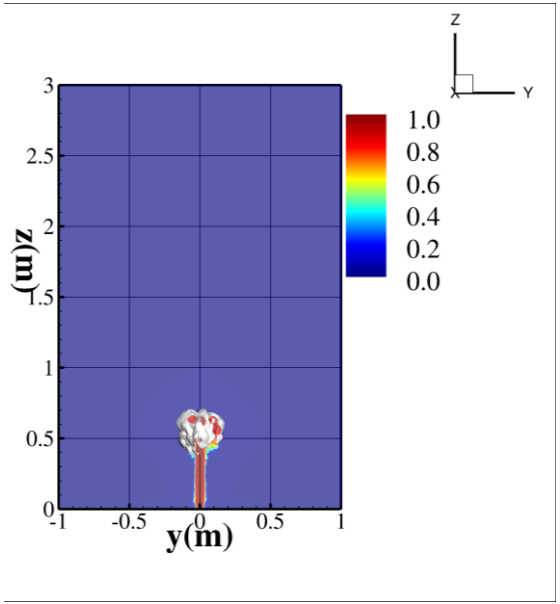
- **Schematics of computation domain.**

Results

Case 0.5IG (ignition at z = 0.5 m)





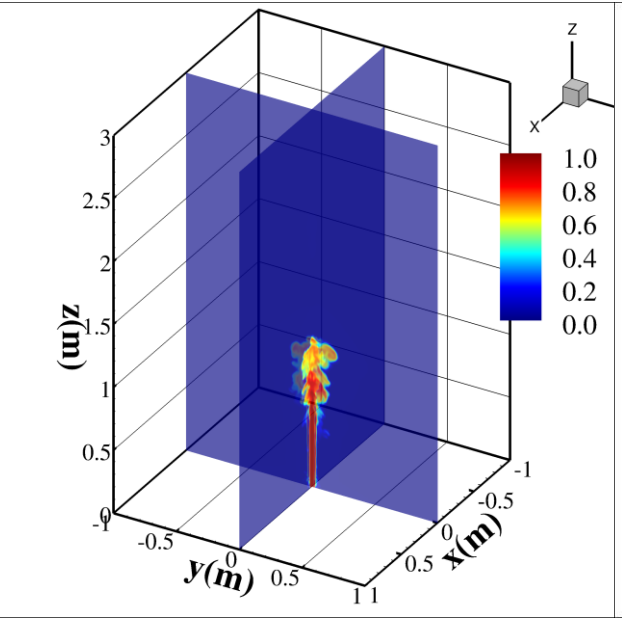


- Distributions of H2 mole fraction, from left to right: time = 0.002s, 0.003s, 0.004s.
- Iso-surface (white color) of OH mass fraction (0.003) to indicate the flame front.

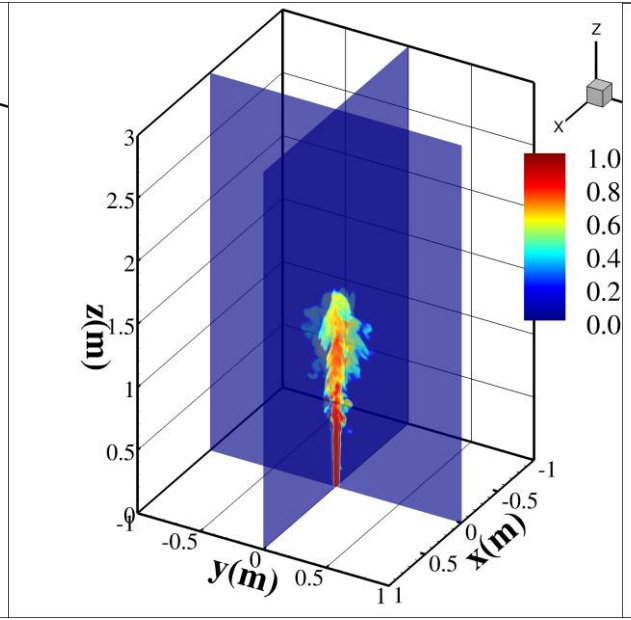
Results

Case 2.0IG (ignition at z = 2.0 m)

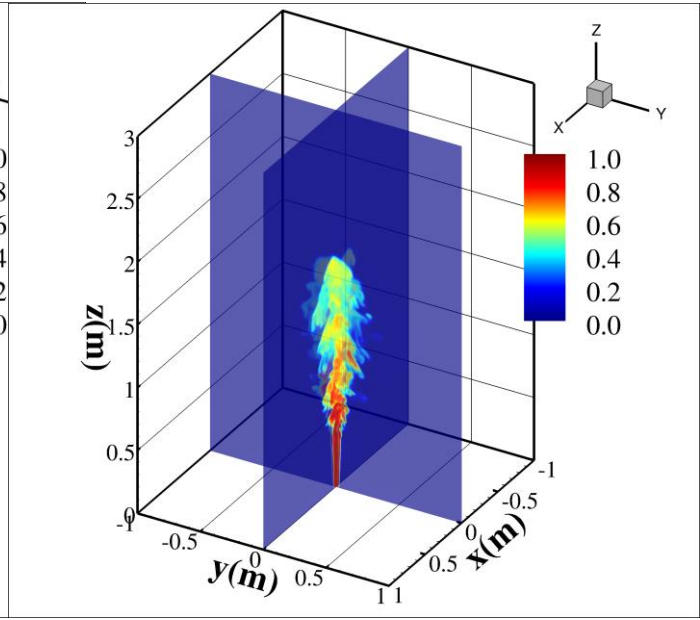
- Development of jet flow **before the hot spot**.



H2 mole fraction, time = 0.01s



H2 mole fraction, time = 0.02s



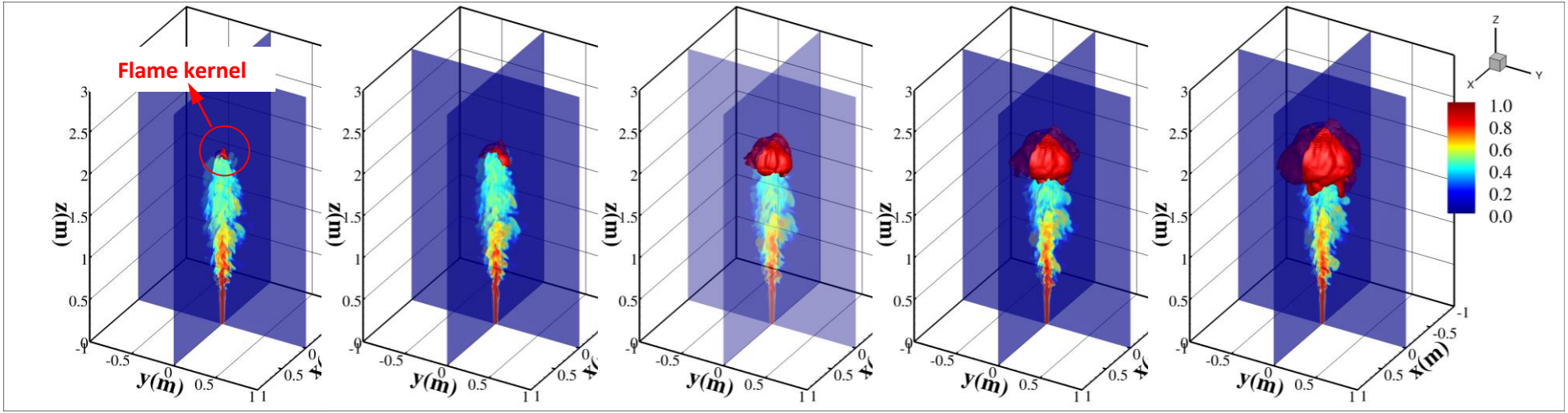
H2 mole fraction, time = 0.03s

Results

Case 2.0IG (ignition at z = 2.0 m)

WARWICK
THE UNIVERSITY OF WARWICK

- Development of jet flow **after the hot spot**.



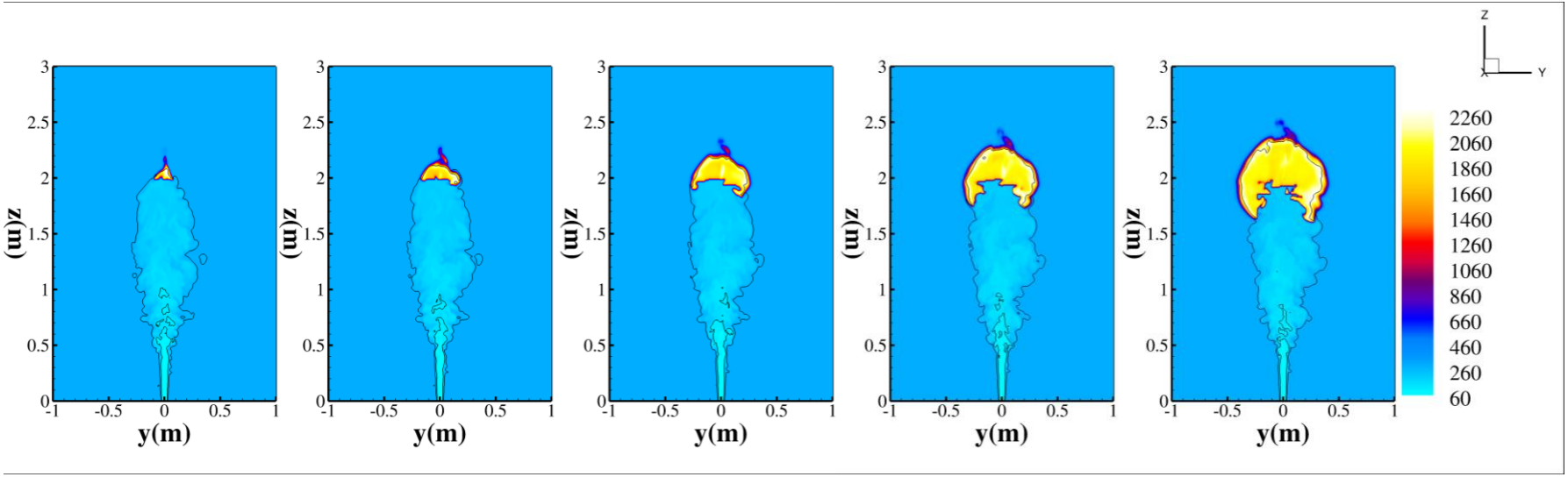
- Distributions of H2 mole fraction, from left to right: time = 0.037s, 0.039s, 0.041s, 0.043s, 0.045s.
- Iso-surface (red color) of OH mass fraction (0.005) to indicate the flame front.

Results

Case 2.0IG (ignition at z = 2.0 m)

WARWICK
THE UNIVERSITY OF WARWICK

- **Development of jet flow after the hot spot.**



- Distributions of temperature (K) at *y-z* plane, from left to right: time = 0.037s, 0.039s, 0.041s, 0.043s, 0.045s.
- Black iso-lines refer to the hydrogen explosion limit, MolH2 = (0.04, 0.756).

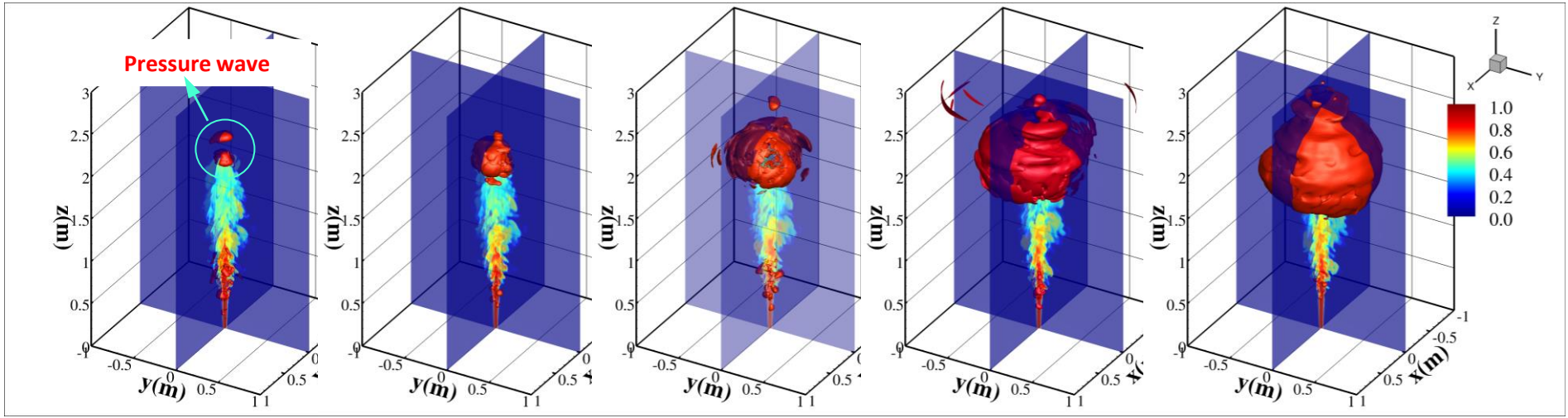
Warwick FIRE
THE UNIVERSITY OF WARWICK

Results

Case 2.0IG (ignition at z = 2.0 m)

WARWICK
THE UNIVERSITY OF WARWICK

- Development of jet flow **after the hot spot**.



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

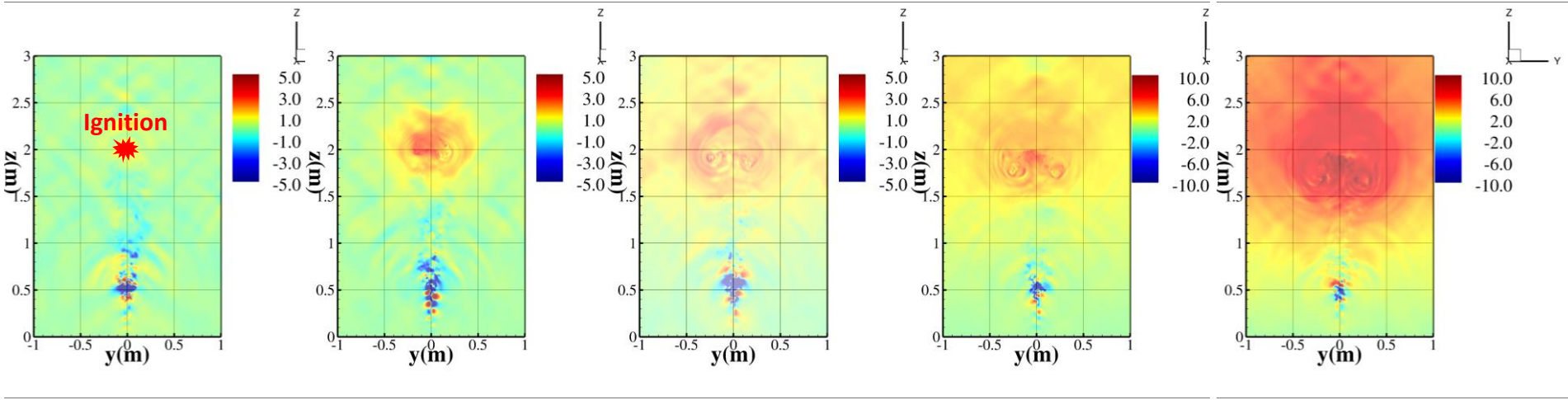
- Distributions of H2 mole fraction, from left to right: time = 0.037s, 0.039s, 0.041s, 0.043s, 0.045s.
- Iso-surface (red color) of pressure to indicate the pressure wave and the values, $\Delta P = P - P_a$, increase from left to right.

Results

Case 2.0IG (ignition at z = 2.0 m)

WARWICK
THE UNIVERSITY OF WARWICK

- Development of jet flow **after the hot spot**.



- Distributions of ΔP (kPa) at *y-z* plane, from left to right: time = 0.037s, 0.039s, 0.041s, 0.043s, 0.045s.

Knowledge gaps

- Lack of measurements with fine details in the near field for both unignited and ignited jets from cryogenic releases?

- Small-scale laboratory scale experiments may be useful to gain insight of some fine details.

- Large-scale experiments need more details measurement of the flame dynamics.

Acknowledgement

- The work presented here is funded by the Fuel Cells and Hydrogen Joint Undertaking through the PRESLHY project.

- The computational support of ARCHER/ARCHER2 are gratefully acknowledged.