CFD based predictive tools for liquid hydrogen hazards

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Fire and Explosion Modelling Group

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We are a multi-disciplinary research group specialising in the development and validation of consequence modelling tools to address cross cutting safety issues related to energy, transport and environment.

Research areas

- Gaseous hydrogen safety
- Liquid hydrogen safety
- Safety of lithium ion batteries
- Fires in the built and natural environment
- Pipeline safety
- Safety of liquified natural gas

Contents

1. **LH_2 vapour cloud from sudden catastrophic release**
2. Unignited releases of liquid hydrogen
3. Ignited releases of hydrogen jets at cryogenic conditions
4. Vapour cloud explosions from instantaneous large-scale releases of cryogenic liquid hydrogen (LH_2)

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LH$_2$ vapour cloud from sudden catastrophic releasee

Region 1

Wind inlet

Atmospheric Domain

Evaporation

LH$_2$ pool

Region 2

https://technokontrol.com/en/products/bunding.php

Atmospheric conditions according to Pasquill-Gifford stability:

A	unstable
D	neutral
F	stable

Key assumptions:

- LH$_2$ flash evaporation prior to the formation of liquid pool was neglected
- Without retention pit, LH$_2$ spreads instantaneously to the minimum thickness of 5 cm estimated from surface roughness
- A square pool to facilitate meshing and to speed up the simulations.
- With retention pit, LH$_2$ content fills the pit instantaneously.
- Height of retention pit not considered.

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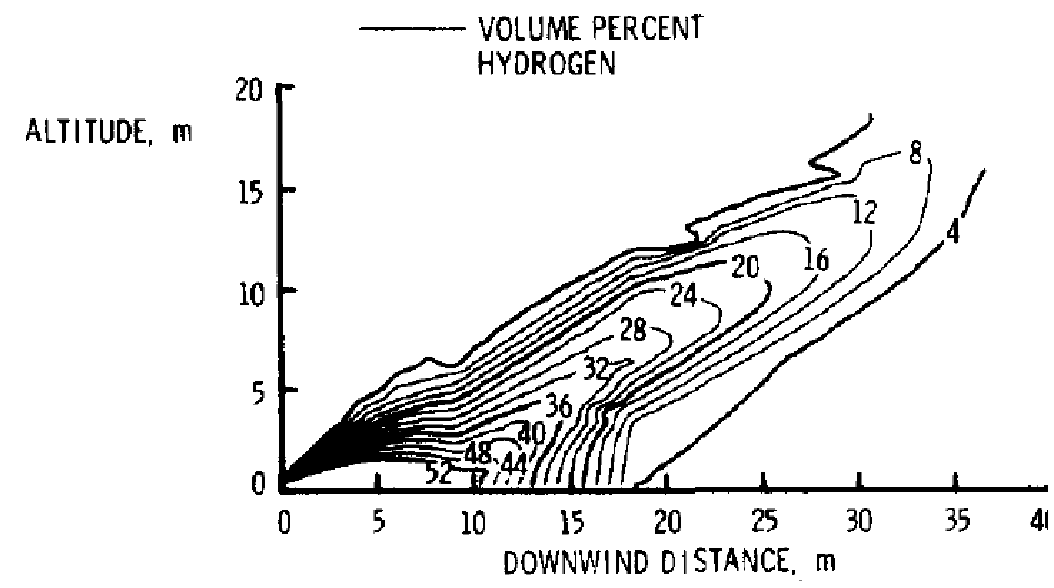
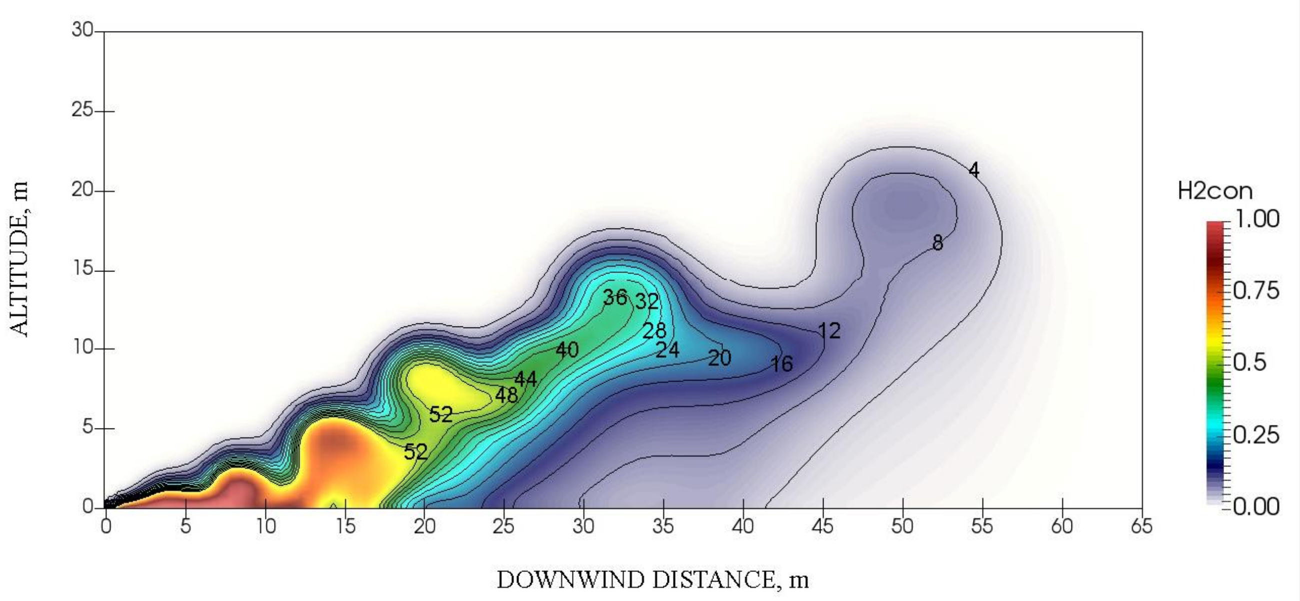
Validation using NASA test 6



Witcofski RD, Chirivella JE. Experimental and analytical analyses of the mechanisms governing the dispersion of flammable clouds formed by liquid hydrogen spills. Int J Hydrogen Energy 1984; 9(5): 425-35.

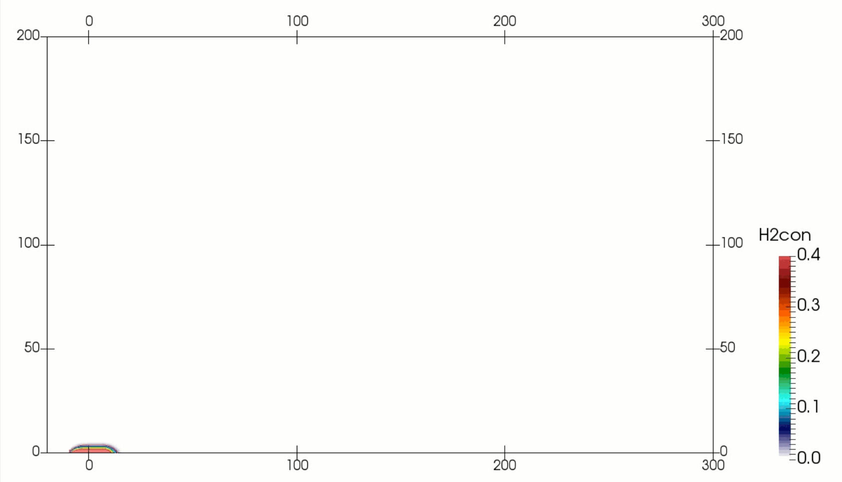


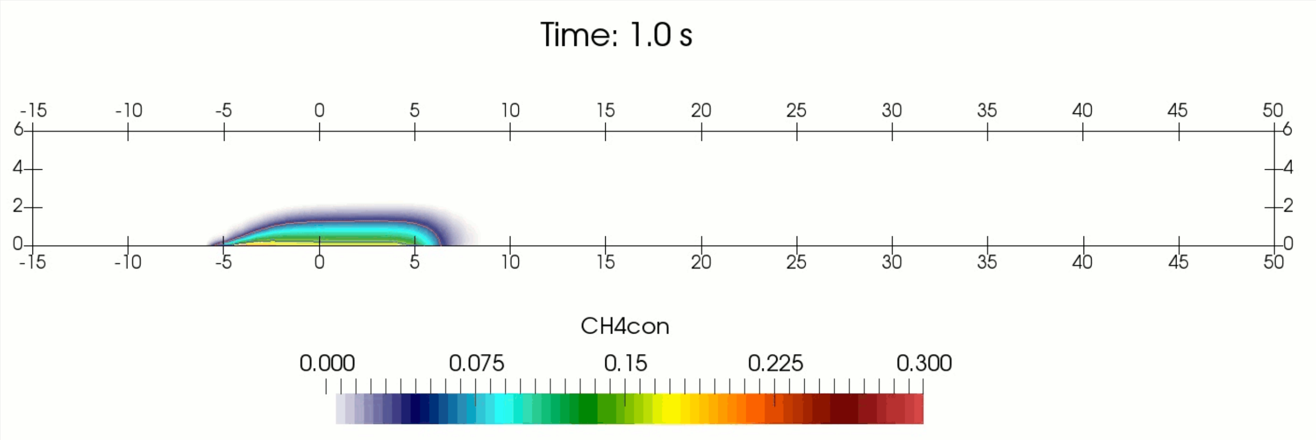
Predicted H_2 molar concentration at = 20.0 s

	Experiment	Prediction
Horizontal extent of visible cloud	160	173
Vertical extent of visible cloud	65	69
Duration of visible cloud	90	88

Vapour cloud from 1 ton release of LH_2 and LNG

Ambient temperature: 293K
3 m/s stable condition





LH_2

Without retention pit (**3F**) 0 – 100 s

Red line: 4% H_2 molar concentration

LNG

Without retention pit (**3F**) 0 – 150 s

Red line: 5% CH_4 molar concentration.

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DNS of the near-field features of cryogenic jets (1)

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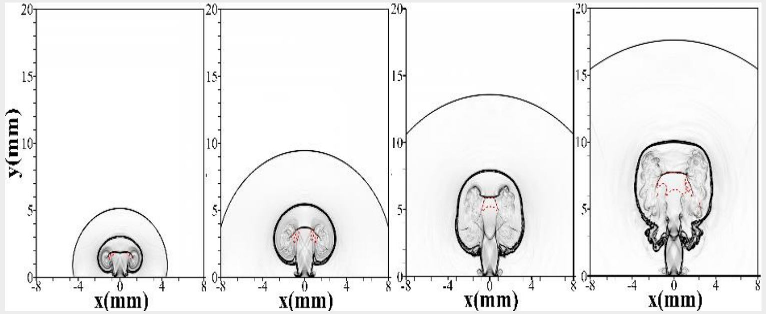
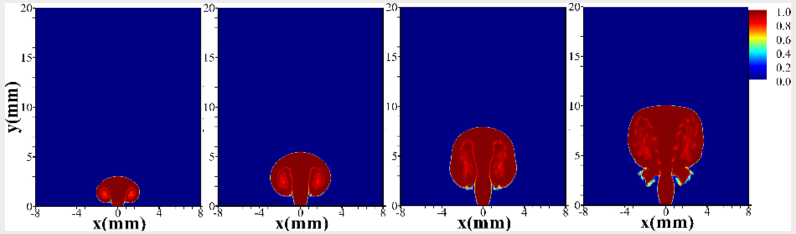
Subtopic 1

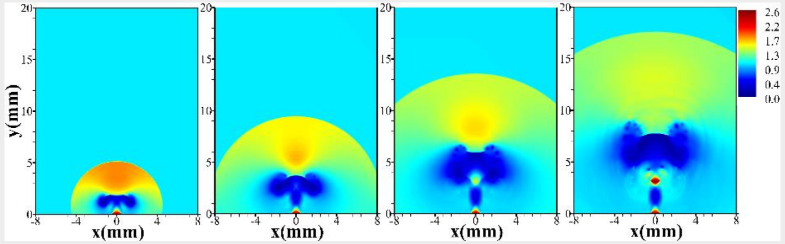
Density gradient



H2 mass fraction



Pressure

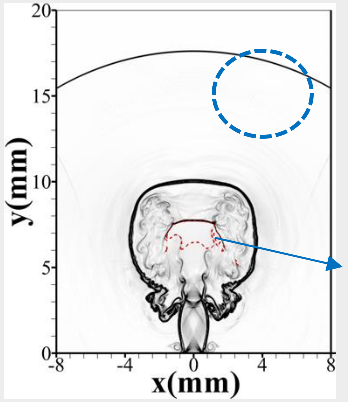


5 bar

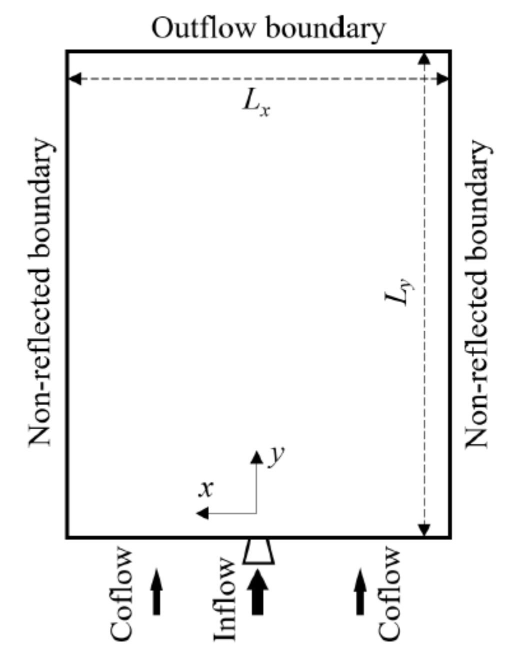
- Transient development of the near-nozzle flow structure from t = 10 to 40μs shown in time interval of 10 μs.
- The red dashed lines denote the regions with **HLP > 0**.

The hydrogen liquefaction potentiality (**HLP**)

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



liquefaction



Ren, Zhaoxin and Wen, Jennifer X. (2020) AIP Advances, 10 (9). 095303.

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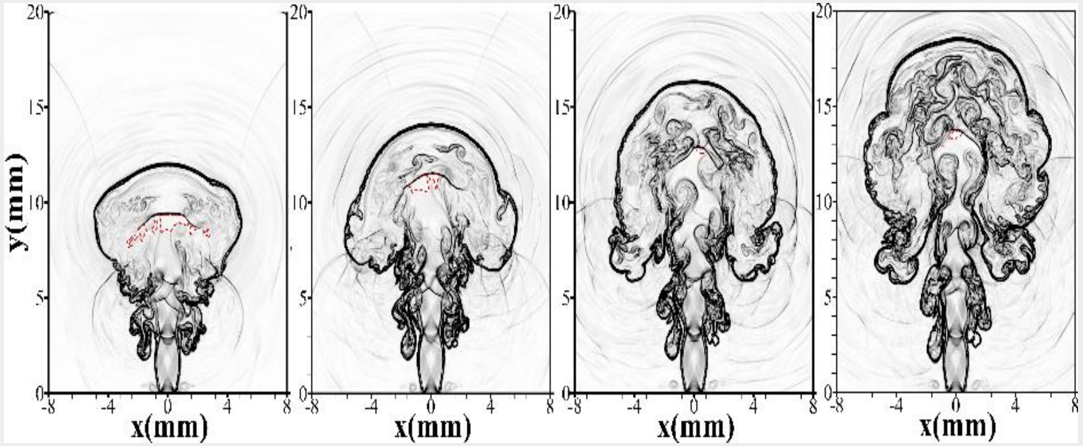
DNS of the near-field features of cryogenic jets (2)

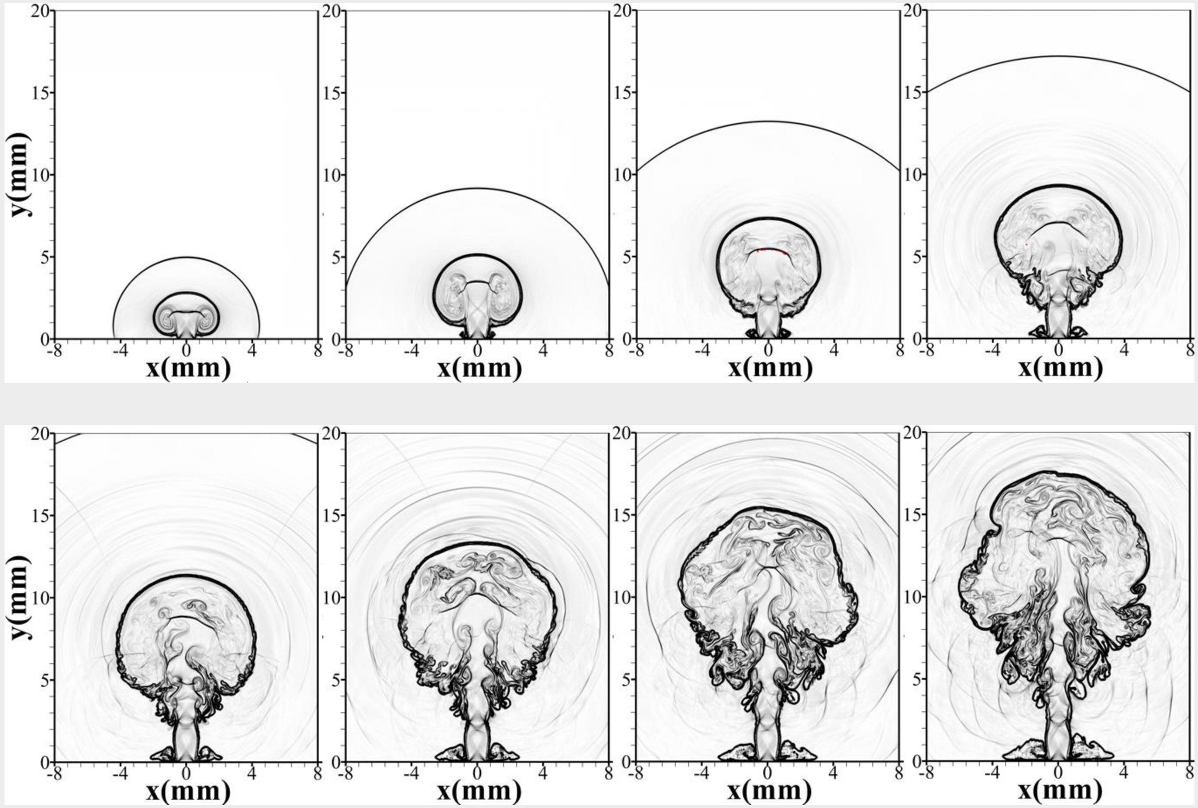
Subtopic 1

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**.

3 bar



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

Ren, Zhaoxin and Wen, Jennifer X. (2020) AIP Advances, 10 (9). 095303.
E. S. Hecht and P. P. Panda, Int. J. Hydrogen Energy 44(17), 8960–8970 (2019).

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LES of ignited releases of hydrogen jets at cryogenic conditions (1)

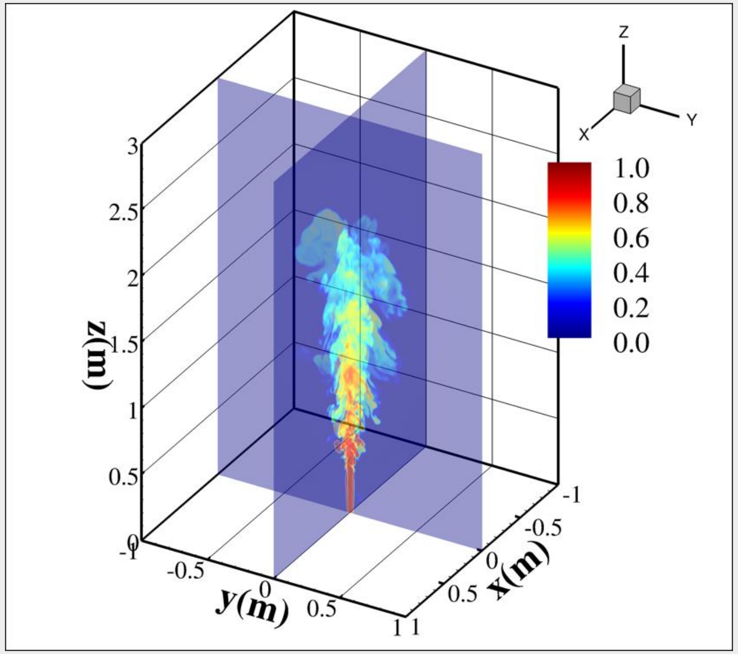
Subtopic 1

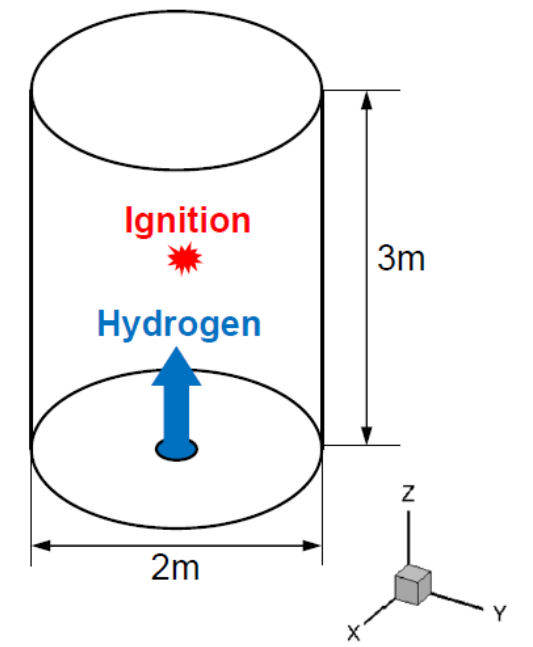
One equation eddy-viscosity SGS model[1] for compressible flow

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

None-unity Lewis number effect: The molecular transport model of Burali N, et al. (2016)

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





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

Yoshizawa A. Physical Review E, 1993, 48(1): 273.
Parente A, Malik M R, Contino F, Cuoci A, Dally B B. Fuel, 2016, 163: 98-111.
Ó Conaire M, Curran H J, Simmie J M, Simmie J M, Pitz W J, Westbrook C K. Int J of Chemical Kinetics, 2004, 36(11): 603-622.
N. Burali, S. Lapointe, B. Bobbitt, G. Blanquart, Y. Xuan,, Combustion Theory and Modelling, 2016, 20(4).

LES of ignited releases of hydrogen jets at cryogenic conditions (2)

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Subtopic 1

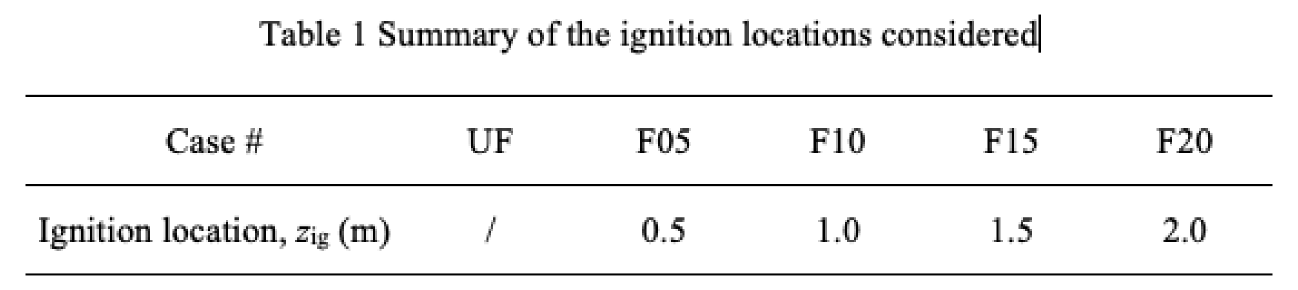
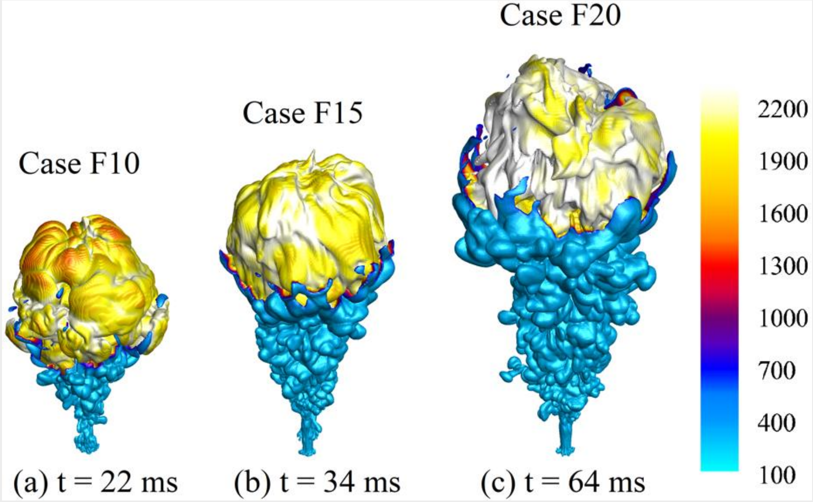


Table 1 Summary of the ignition locations considered

Case #	UF	F05	F10	F15	F20
Ignition location, z_{ig} (m)	/	0.5	1.0	1.5	2.0



(a) t = 22 ms (b) t = 34 ms (c) t = 64 ms

Flame structure of ignited jet for Case F10, Case F15, and Case F20 marked using X_{H2} = 0.04 iso-surface colored by temperature (K).

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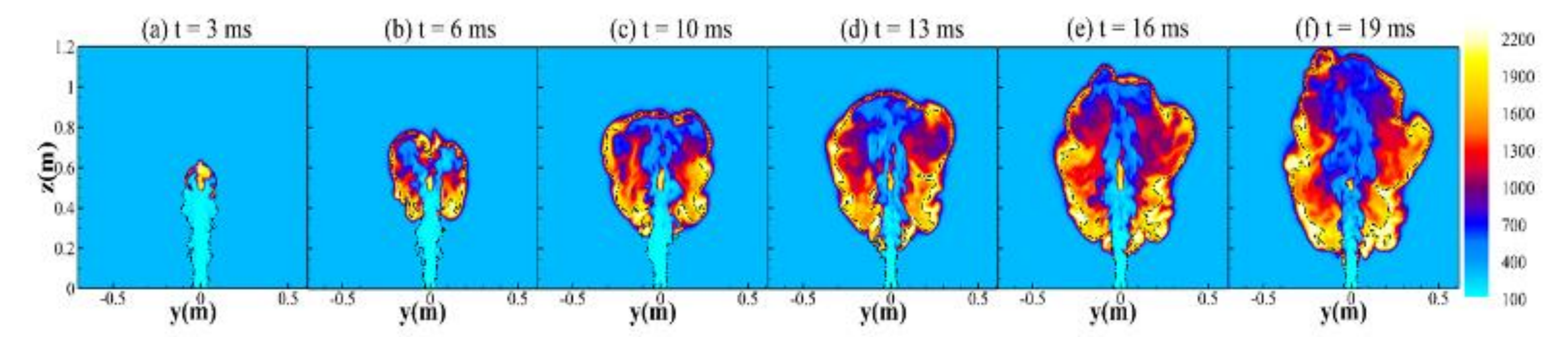
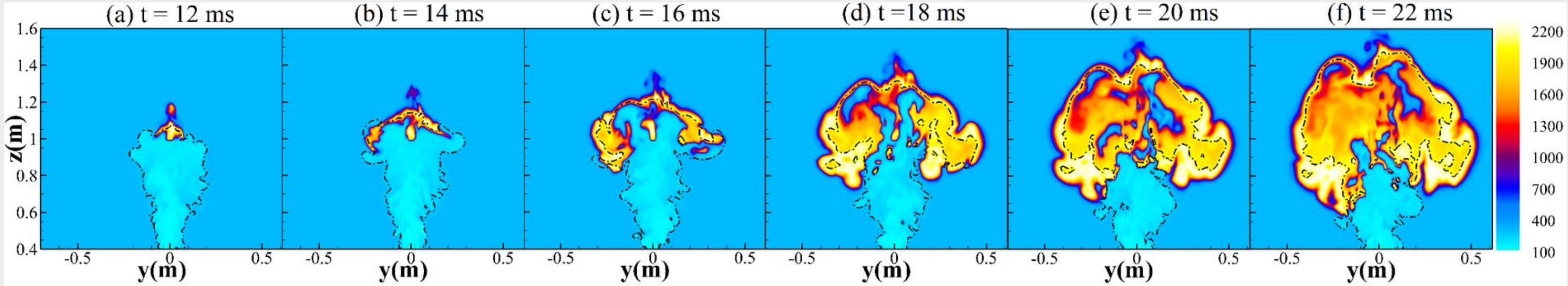
LES of ignited releases of hydrogen jets at cryogenic conditions (4)

Subtopic 1



Evolution of combustion field at the *y*-*z* middle-plane for Case F05.

Here, the contours are temperature (K), and the black dashed isolines refer to hydrogen mass fraction Y_{H2} = 0.02.



Evolution of combustion field at the *y*-*z* middle-plane for Case F10.

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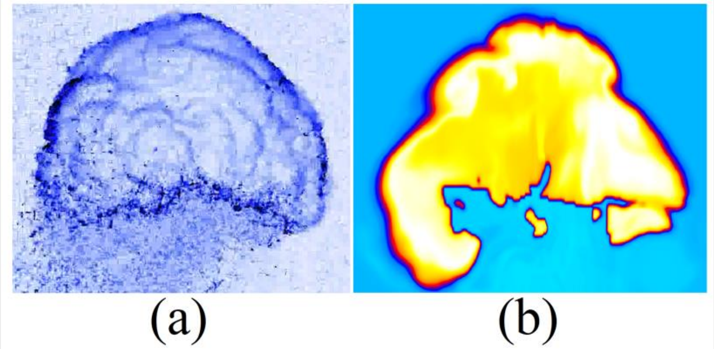
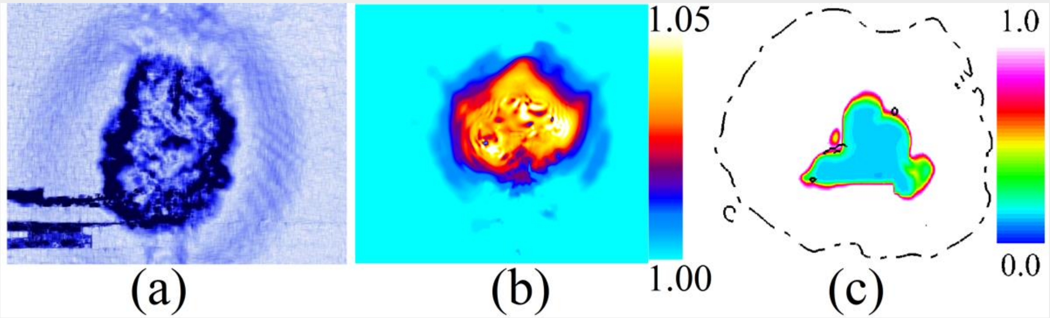
LES of ignited releases of hydrogen jets at cryogenic conditions (5)

Subtopic 1



Snapshots of the flame shapes: (a) experiment (reproduced from Friedrich et al. (2021) and (b) Case F20.



Snapshot of the deflagration waves: (a) experimentally observed (reproduced from [20]), (b) predicted pressure contour for Case F15, (c) predicted density contour (kg/m^3) with static pressure iso-line of 1.03 atm.

A. Friedrich, A. Veser, G. Necker, J. Gerstner, N. Kotchourko, M. Kuznetsov, T. Jordan, Characterization of high-pressure cryogenic hydrogen jet fires (ignited DISCHA), *PRESLHY Dissemination Conference*, 5-6 May, 2021.

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Vapour cloud explosions from instantaneous large-scale releases of cryogenic liquid hydrogen (1)

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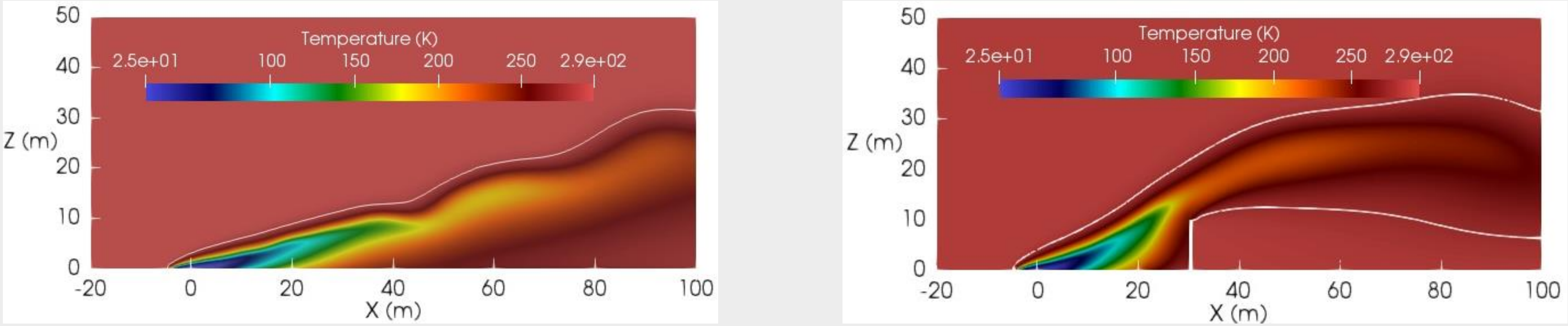
Subtopic 3

Pool size	$5 \times 5\ m^2$
Mass	600 kg LH_2
Wind	3 m/s
Temperature	20.4 K
Barrier walls	5 or 10 m at 30 or 40 m from pool centre.
Ignition	40 s for a duration of 0.5 s.

Predicted temperature for the cases with and without a barrier just prior to the ignition



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Vapour cloud explosions from instantaneous large-scale releases of cryogenic liquid hydrogen (2)

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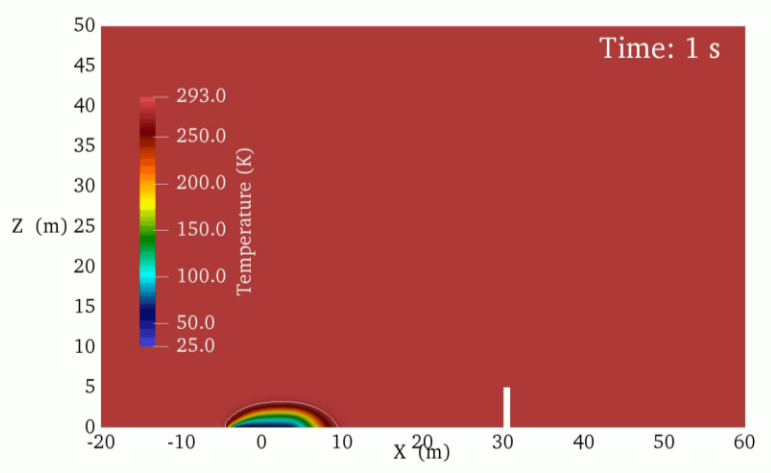
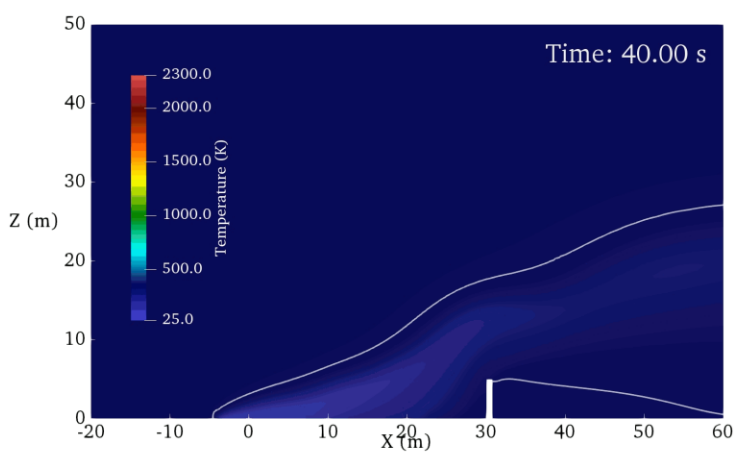
Subtopic 3

Cloud before ignition

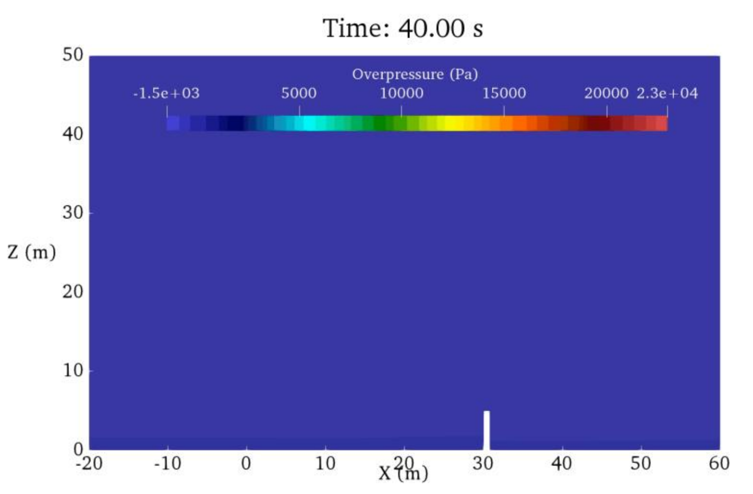


Post ignition

Temperature



Overpressure



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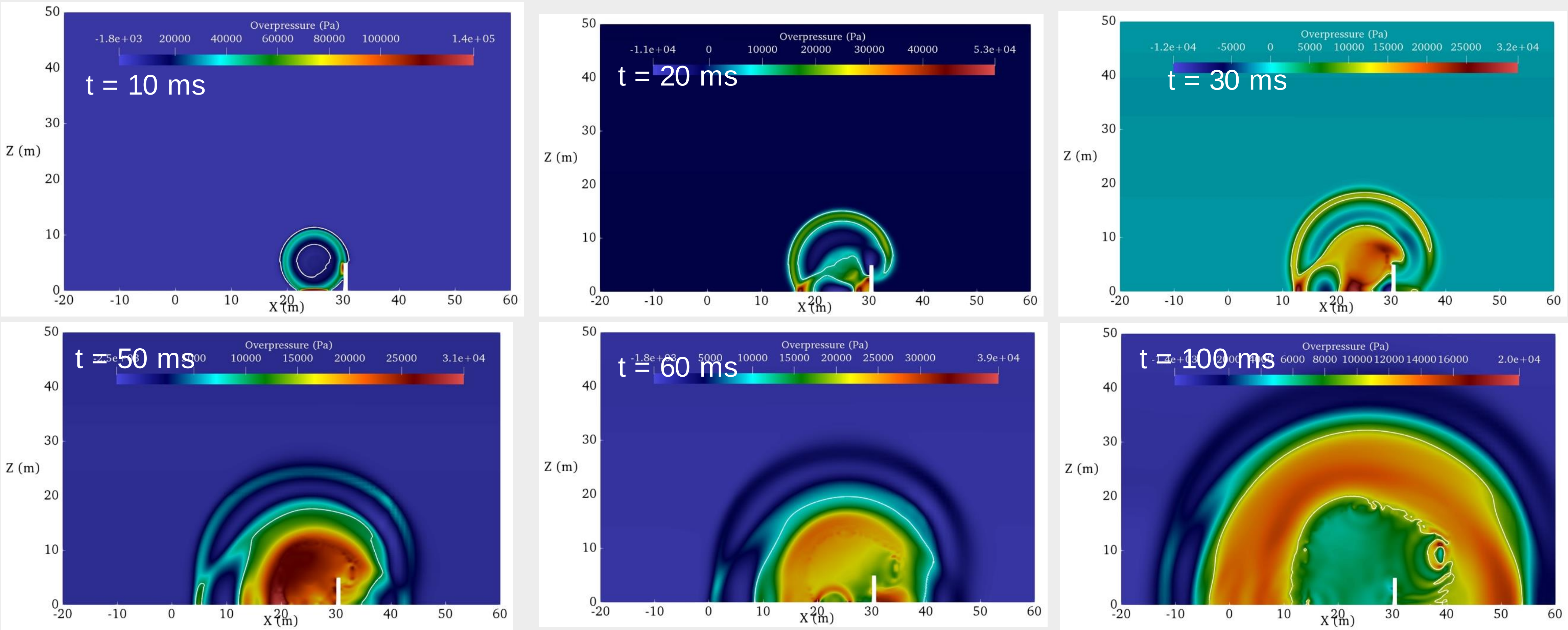
Vapour cloud explosions from instantaneous large-scale releases of cryogenic liquid hydrogen (3)

Subtopic 3



Pressure contours in the middle plane at 10 ms, 20 ms, 30 ms, 50 ms, 60 ms, 100 ms after the ignition.

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Concluding remarks

- The use of hydrogen as aviation fuels brings new challenges associated it with accidental releases and ignition.

- Further knowledge gaps also exist the hydrogen is most likely to be stored onboard in its liquid form.

- If potential releases (*united/ignited*) exit the aircraft, knowledge gaps also exist about how they affect the aerodynamics of the aircraft and its contrails.