



Modelling LH₂ jet fires and their interaction with insulation materials

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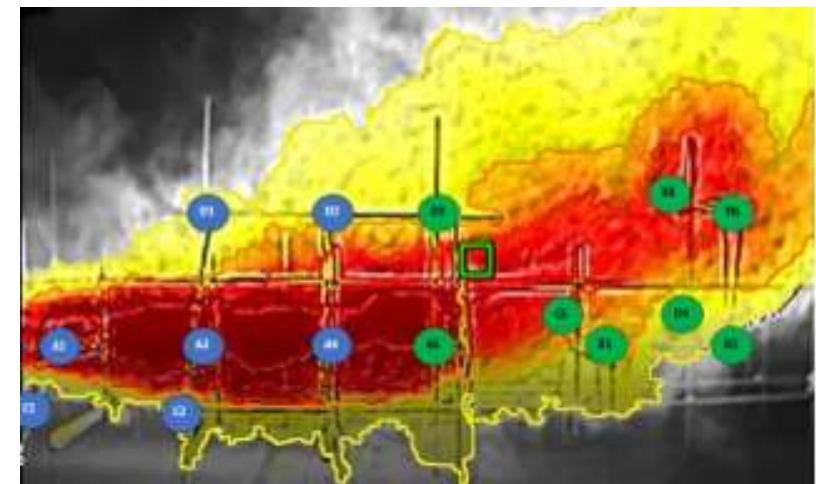
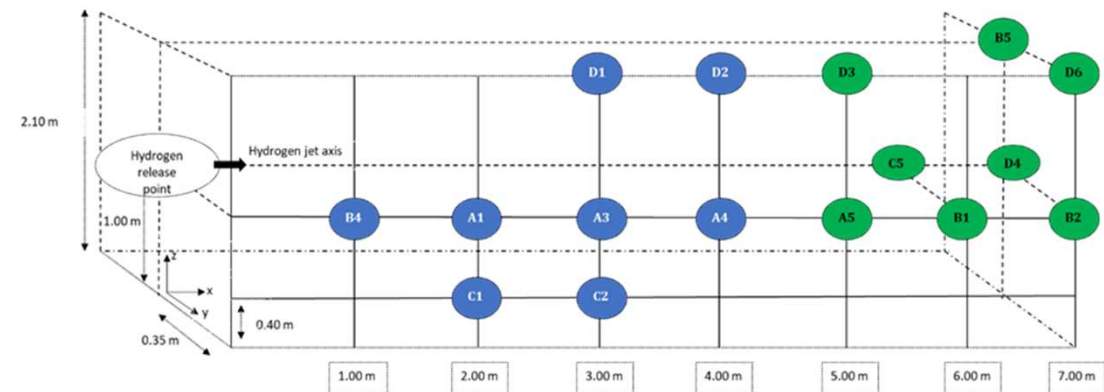
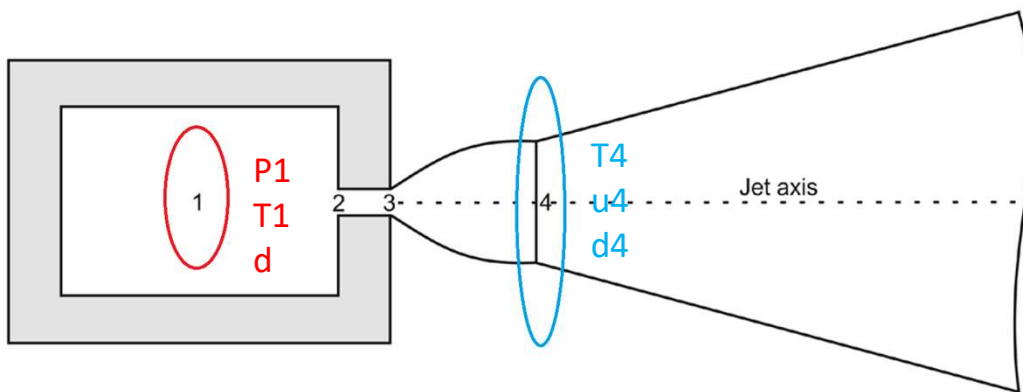


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Introduction – Hydrogen storage

The jetfires deriving from the accidental release of compressed hydrogen has been intensively investigated.

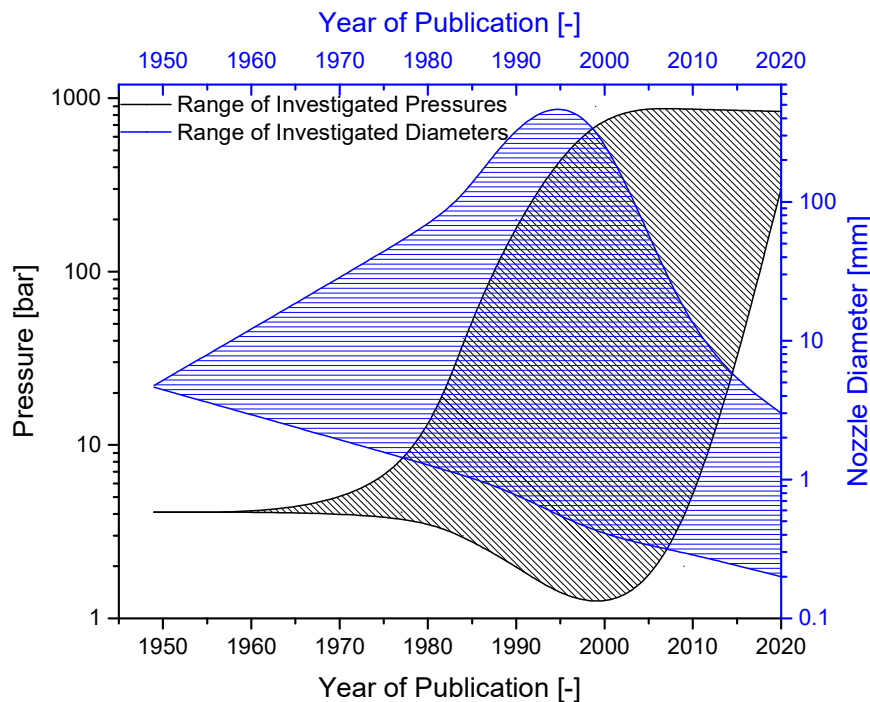
A dearth of data for the case of cryogenic release can be observed in the current literature.



State of the art: Releasing conditions of Hydrogen Jet fires

Commonly analysed conditions (pressure and nozzle diameter) can be identified.

Under these conditions, flame length can be preliminary assessed and employed for the **definition of the numerical domain**.



Carboni M. et al. (2020). 10.1016/j.ijhydene.2022.05.010

Reference	Pressure [bar]	Nozzle diameter (D_N)	Flame length [m]
Hawthorn (1949)	< 41	~4.7	[0.6 - 0.7]
Kalghatgi et al. (1984)	< 41	[1.1 - 10.1]	[0.2 - 1.7]
Mogi et al. (2005)	[3 - 1100]	[0.4 - 4.0]	[0.6 - 6.0]
Schefer et al. (2006)	[41 - 112]	[1.9 - 7.9]	[0.3 - 4.3]
Schefer et al (2007)	[7 - 262]	5.1	[2.4 - 10.0]
Imamura et al. (2008)	[2 - 30]	[1.0 - 4.0]	[0.3; 1.8]
Proust et al. (2009)	[12 - 869]	[1.0 - 3.0]	[1.3 - 5.8]
Studer et al. (2009)	[2 - 83]	[4.0 - 10.0]	[1.7 - 6.9]

Aim of the work: Evaluate the existing open-source tools (OpenFOAM) for the advanced characterization of LH2 jet fires

- 1) Analysis on the suitability of the existing OpenFOAM solvers against the accidental release of compressed hydrogen (larger availability of experimental data for model validation);
- 2) Optimization of the computational domain by identifying the most critical regions in terms of expected fluid dynamic regimes as well as the intensity of physical and chemical phenomena, starting from expected flame length (from empirical correlations).
- 3) Evaluation of the expected outcomes and possible integration for the consequence analysis.

Methodology (1): Implemented solver and sub-models

Numerical simulations were carried out considering the following OpenFOAM submodels and solvers:

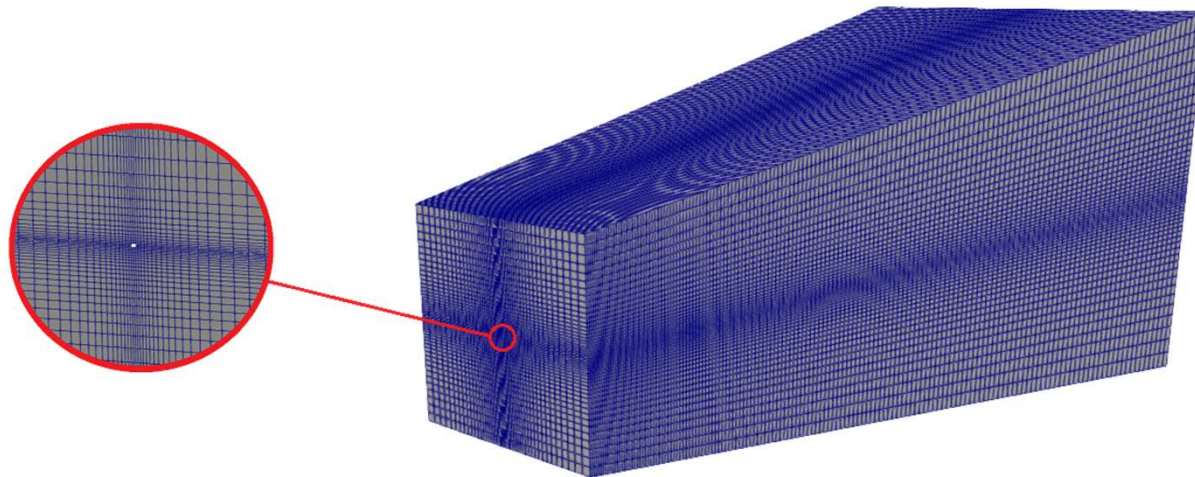
- 1) Solver based on reactingFOAM to account for transient, turbulent, and reactive systems;
- 2) Large Eddy Simulation (LES) to optimize computational requirements and accuracy
- 3) Eddy dissipation concept (EDC) to locally evaluate the reaction rates;
- 4) Single-step reaction having the overall kinetic from the literature $k = A \cdot T^n \cdot e^{-\frac{E_a}{R \cdot T}} = 1.734 \cdot 10^5 \cdot T^{1.51} \cdot e^{-\frac{1726}{T}}$

Source (Year)	Software	Turbulence model	Combustion model
Wang et al. (2014)	OpenFOAM	LES	EDC
Keenan et al. (2017)	OpenFOAM	RANS k-ε	
Cirrone et al. (2019)	Fluent	RANS k-ε	EDC
Cirrone et al. (2019)	Fluent	RANS k-ε	EDC
Carboni et al. (2022)	Fluent	RANS SST k-ω	EDM
Ren et al. (2022)	OpenFOAM	LES	EDC
Ba et al. (2022)	Fluent	RANS k-ε	EDM

Methodology (2): Implemented Domain and Boundary Conditions

The numerical domain was defined under the following assumptions:

- 1) No slip and adiabatic conditions for bottom surface (ground), “open surface” for the lateral and top sides.
- 2) Adaptive mesh size refinement (maximum Courant number of 0.7), having overall sizes 3 m x 3 m x 6 m.
- 3) Atmosphere: Absent and Delayed ignition (@ 2s), stagnant air at atmospheric pressure and initial temperature of 290 K.



Methodology (3): Releasing Conditions Analysed

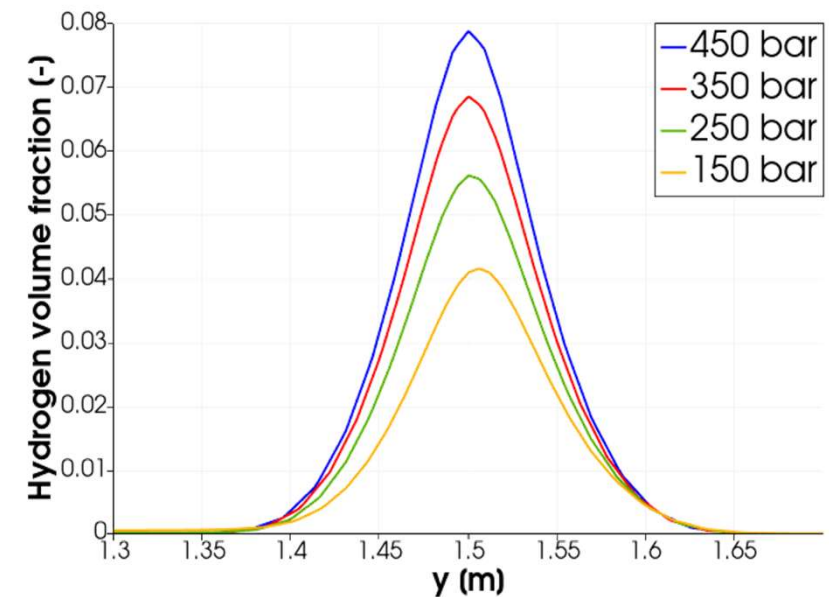
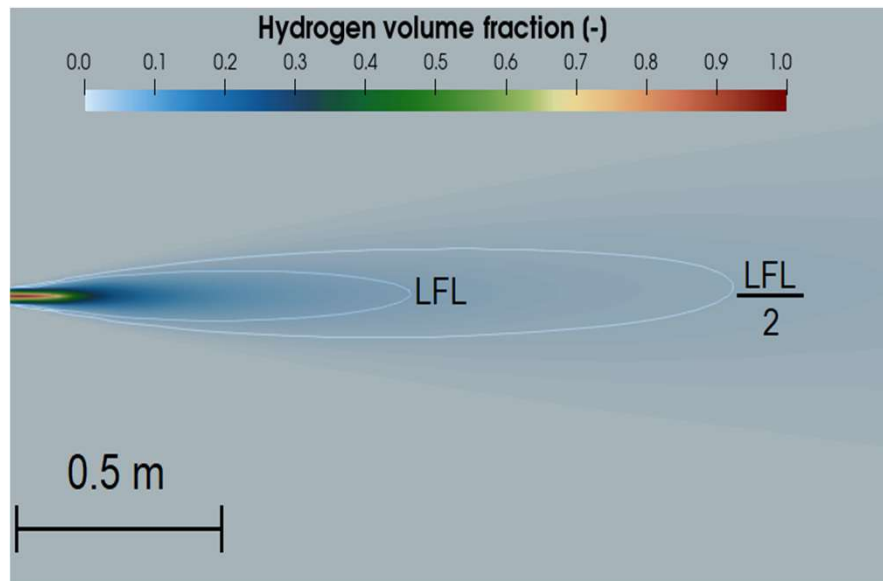
Numerical simulations were carried out under the following conditions

- 1) Under expanded jet of pure hydrogen at $H = 1.5$ m,
- 2) Notional Nozzle model implemented for the determination of numerical conditions (e.g., nozzle size);
- 3) Gas Phase Release: Storage pressure 150 – 450 bar at ambient temperature, nozzle diameter 5 mm;
Liquid Phase Release: Case ID # 1 – 5.

Case ID #	Pressure [bar]	Temperature [K]	Nozzle diameter [mm]
1	2	22	50
2	5	27	50
3	10	31	5
4	10	31	11.2
5	10	31	50

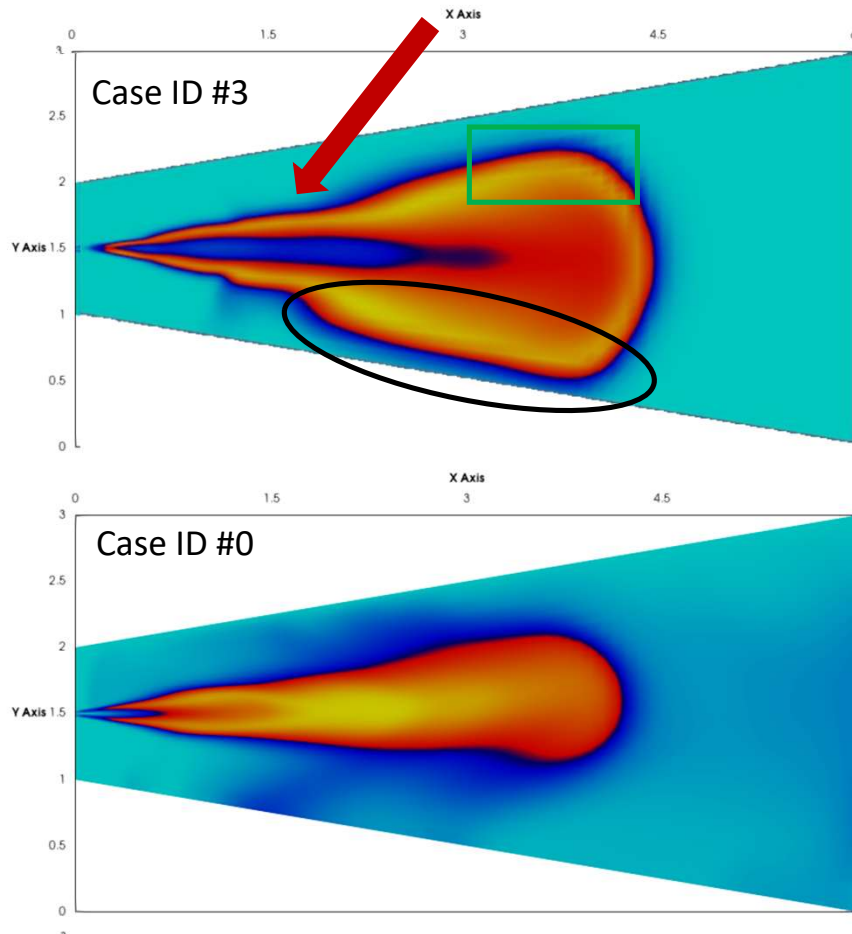
Results (1): Characterisation of Compressed Hydrogen Release before Ignition

Hydrogen distribution before ignition at $y = 1$ m as obtained for the case of 450 bar as initial pressure (left) and at $x = 1$ m as a function of initial pressure (right).



Results (2): Comparison of ignited jets

Temperature distribution 0.5 s after ignition (ignition was at $t = 2$ s)



Although similar lift-off distances can be observed between Case ID #3 and the release of compressed hydrogen at 450 bar (Case ID #0), a different flame structure is obtained:

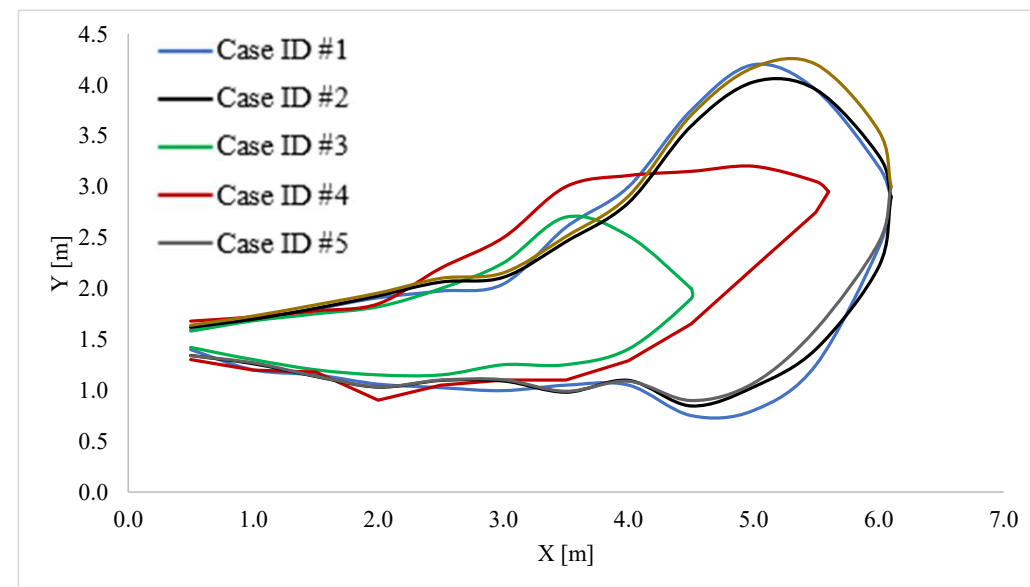
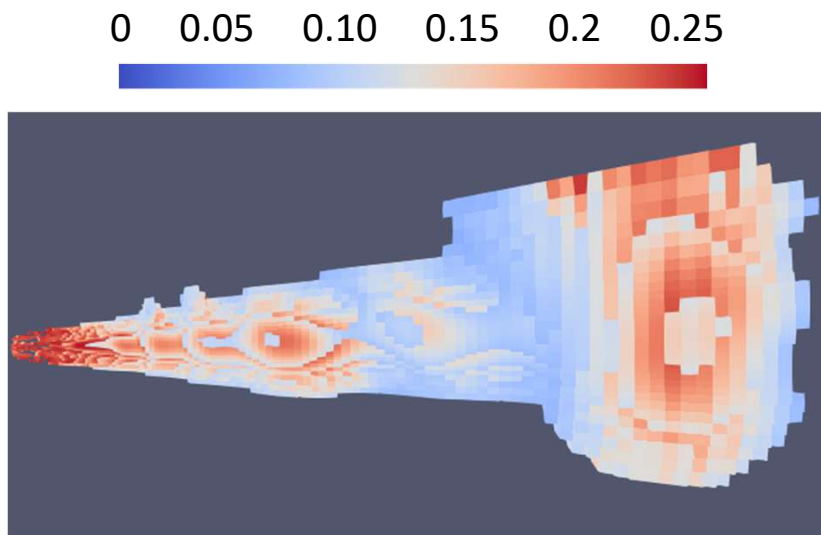
- A colder, hydrogen-rich region can be detected within the core of the flame, reaching a distance of 3.5 m from the releasing point on the horizontal axis (red arrow);
- A wider hot region can be observed, especially in the proximity of the ground (black circle)
- The maximum temperature is obtained in the proximity of the outer layer in the colder case (green box), probably because of local oxygen deficiency



Results (3): Flame Geometry – Side View

The tools integrated in OpenFOAM allow for the direct visualisation of the temporal and spatial distribution of temperature, pressure, composition (e.g. water vapour).

Considering a threshold value for the estimated temperature (800 °C), the flame geometry and its composition can be extracted for all the investigated conditions.

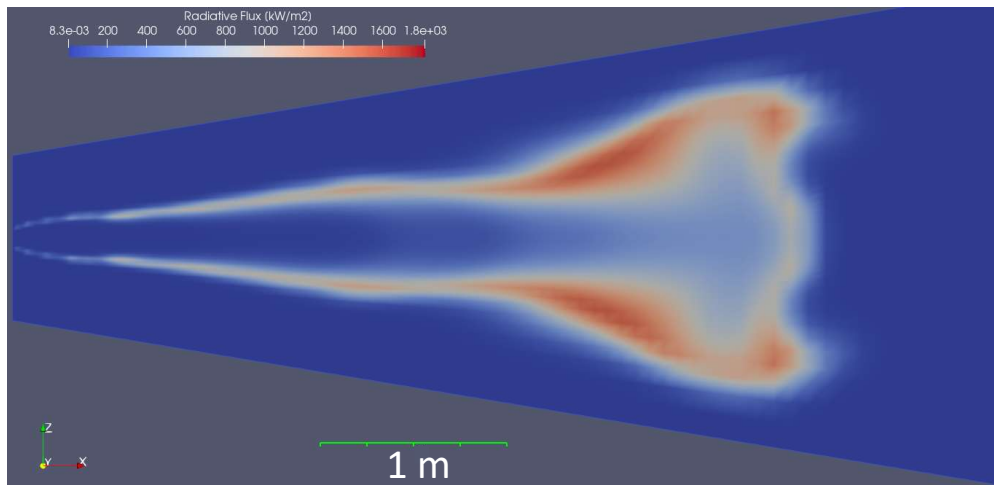


Results (4): Flame Geometry – Top View

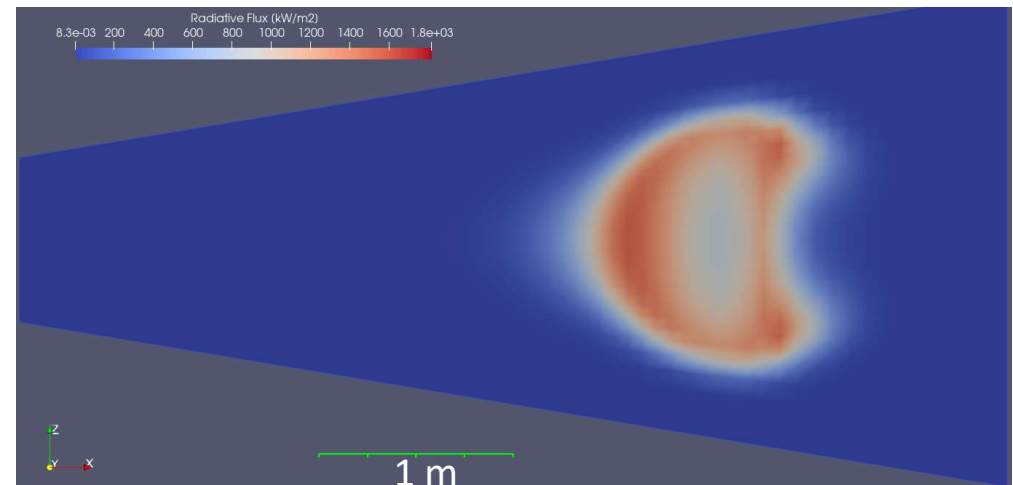
Based on the obtained values, the emitted radiative flux can be obtained by considering the local conditions and compositions.

However, radiative fluxes received by a given target are not calculated by the available tools.

Case ID #1 at Y = 1.5 m



Case ID #1 at Y = 2.0 m

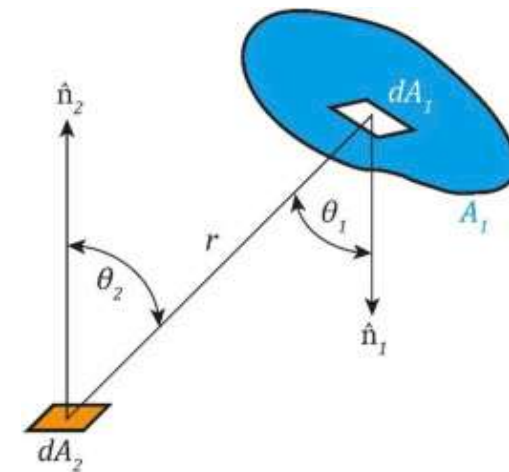
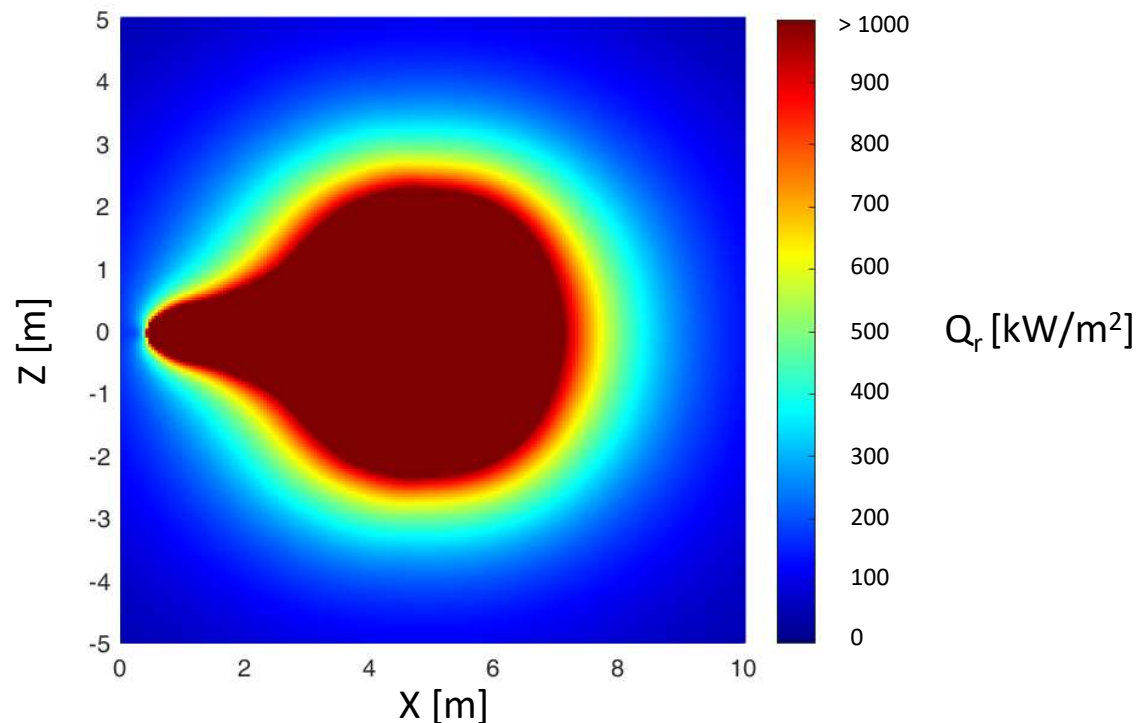


Results (5): Emitted Radiation – Top View

The obtained three-dimensional geometry of the flame was used in a specifically developed external tool, which allowed the calculation of view factors for a given target surface, assuming a radiative fraction of 20%.

The figure represents the radiation (Q_r) received by targets on a horizontal plane at the elevation of the release obtained for Case ID #1.

Similar values are obtained for Case ID #2 and Case ID #5, resulting as the worst-case conditions.



Results (6): Received Radiation – Model Comparison

Based on the obtained radiative heat flux distribution, safety distances were calculated for different threshold values and compared with estimations from HyRAM+6.1.0 and PHAST 9.11.

CFD data are in good agreement with results from other approaches.

HyRAM+ tends to provide lower distances, because of higher flame bending and faster lift-off, resulting in lower view factors and less intense radiations on the jet axis.

Test ID #	Distance at 3 kW/m ² [m]			Distance at 5 kW/m ² [m]			Distance at 8 kW/m ² [m]		
	CFD	HyRAM+	Phast	CFD	HyRAM+	Phast	CFD	HyRAM+	Phast
1	70	48	76	56	36	65	45	26	57
2	53	34	57	42	24	49	34	17	45
3	9.3	5.5	10.6	8	4.2	9.7	7.1	3	8.7
4	18	13	22	14.7	9.5	20	12.5	7	18
5	81	61	85	64	47	73	51	35	64

Results (7): The effects of jets on insulation assemblies

The expected temperature profile in insulation assemblies impinged by unignited and ignited jets was modeled by means of **1D simulation**.

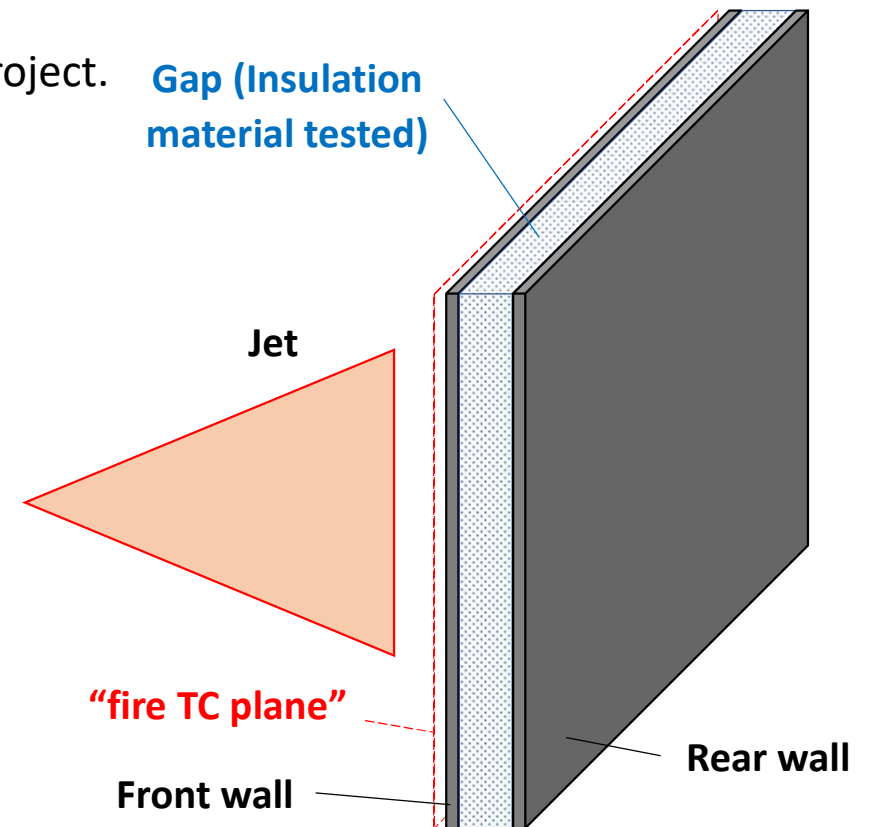
Results supported design on jet experiments in WP4 of the project.

Two walls of stainless steel with thickness within 2 – 5 mm.

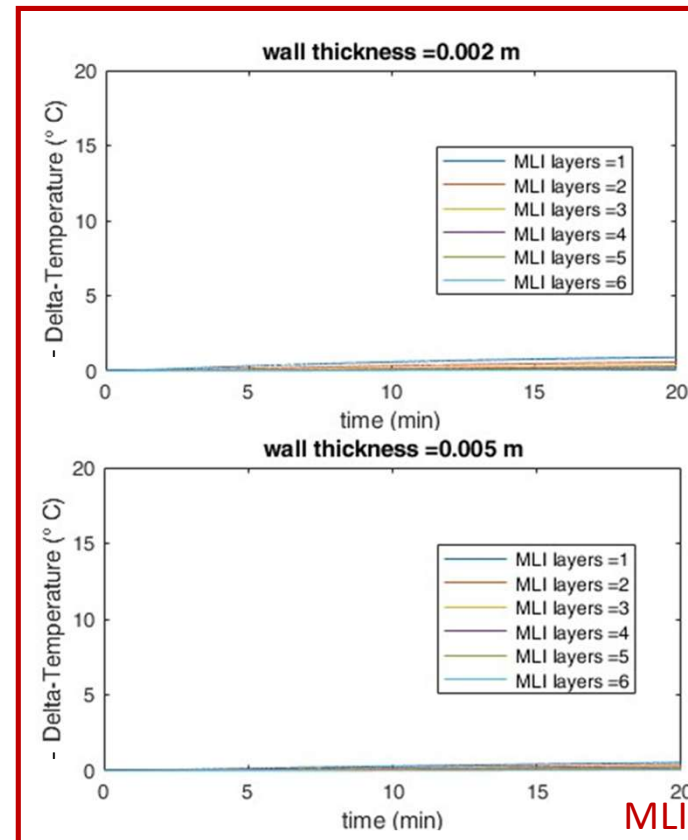
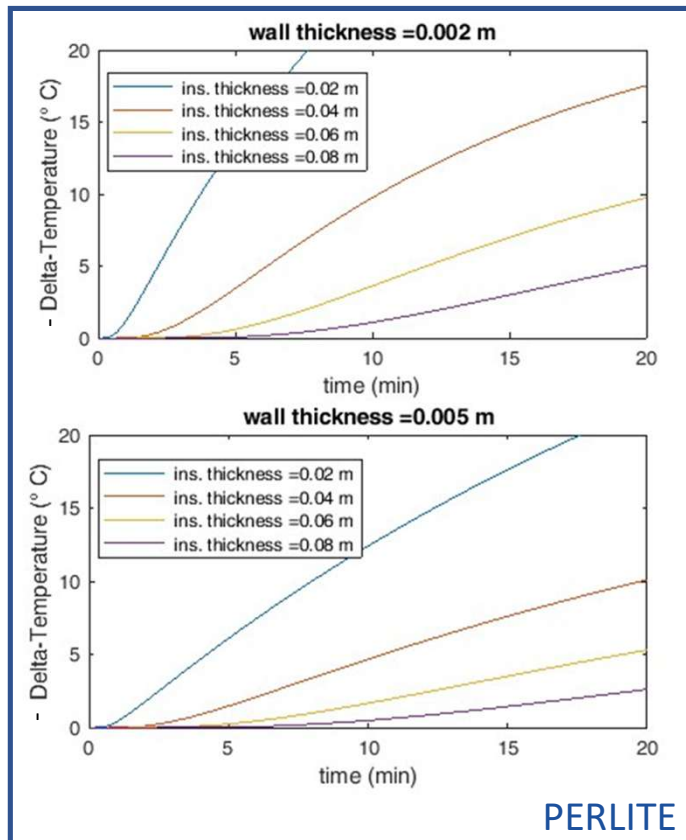
Perlite and Multi layer insulation (MLI) were considered

Modeling of 20 minutes transient in case of:

- **cold jet** (non-ignited, 20 K)
- **jet fire** (ignited, 1100 K)



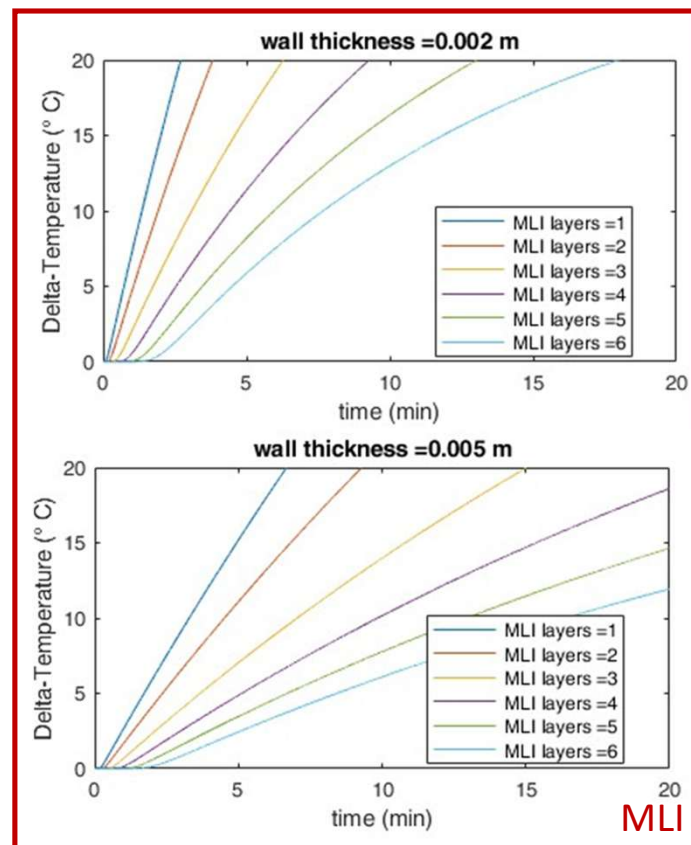
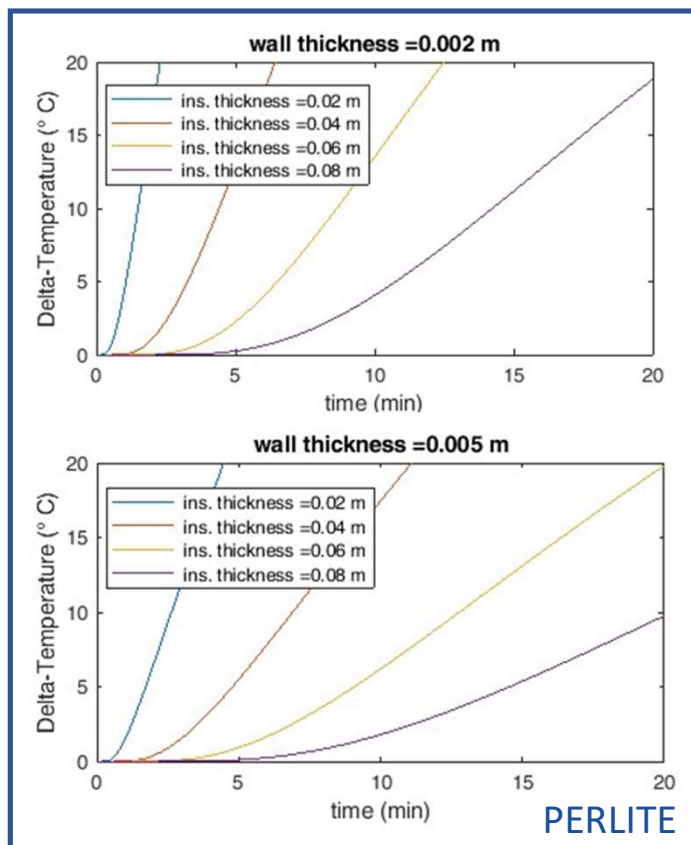
Results (8): The effects of jets on insulation assemblies



In the case of exposure to **cold jets**:

- A wall thickness of 5 mm does not allow the complete development of temperature profile for most of the insulation thickness tested in the case of perlite.
- Regardless of the wall thickness, negligible variations in estimated temperature can be observed in the case of MLI, no matter the number of layers.

Results (9): The effects of jets on insulation assemblies



In the case of exposure to a **jet fire**:

- In case of perlite small insulation thickness (e.g. 2 mm) leads to abrupt change in temperature
- In case of MLI, wall thickness > 2 mm and a number of layers > 4 does leads to temperature changes < 20°C in 20 mins

Conclusions

- Preliminary analyses indicate reactingFOAM as the most suitable solver for the analysed scenarios;
- The comparison with available experimental data and empirical correlations indicates that the existing models in OpenFOAM are suitable for the characterisation of hydrogen jetfires;
- The effects of initial pressure, temperature, and releasing size were investigated;
- Spatial and temporal distributions of temperature and composition obtained numerically were integrated to assess the radiative heat flux emitted and determine the flame geometry;
- An external tool was developed and implemented for the evaluation of received radiative fluxes as a function of distance, showing excellent agreement with existing tools;
- An insulation layer of 0.4 m and wall thickness lower than 5 mm are advised to test perlite effectiveness either in the case of cold jets or jet fires;
- Four insulation layers in 0.4 m vacuum gap and wall thickness lower than 5 mm are advised to test MLI effectiveness in the case of jet fires.



Thank you for your attention

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