

Near Field Thermal Dose of Cryogenic Hydrogen Jet Fires

Cirrone D.*, Makarov D., Molkov V.

*Hydrogen Safety Engineering and Research Centre (HySAFER),
Ulster University, Shore Road, Newtownabbey, BT37 0QB, UK*

**Corresponding author's email: cirrone-dmc@ulster.ac.uk*

ABSTRACT

A competitive technique to store large quantities of hydrogen is the cryo-compression of the gas. A deeper understanding of the thermal hazards associated to ignited under-expanded cryogenic releases is fundamental to protect life and prevent property loss. The present study aims at the CFD modelling of thermal hazards beside jet fires with release temperature in the cryogenic range 48-78 K and pressure up to 4 bar abs. The harm level is assessed in terms of thermal dose. The CFD model employs realizable k- ϵ for turbulence modelling, along with Eddy Dissipation Concept for combustion and Discrete Ordinates model for radiation. The model has been previously validated against experiments by Sandia National Laboratories (SNL) on cryogenic hydrogen fires with release pressure up to 5 bar abs and temperature up to 82 K. Simulations were performed for three experimental tests conducted at SNL. The thermal dose was calculated for several exposure times in the near field to the jet fire. The harm criteria for people were defined according to the thermal dose thresholds for infrared radiation. The maximum exposure time to not be "harmed" at 0.5 m from the flame axis resulted to be lower than 30 s for all the 3 tests. In test 3 ($T = 78$ K, $P = 4$ bar abs, $m = 0.56$ g/s), 60 s exposure resulted in second degree burns within 0.5 m from the jet flame axis. At the same distance, 4 minutes is the maximum exposure time before third degree burns occurrence.

KEYWORDS: Thermal dose, cryogenic jet fires, hydrogen safety.

NOMENCLATURE

I	incident radiative heat flux (W/m^2)	x	distance (m)
L	length (m)	Greek	
k	turbulent kinetic energy (m^2/s^2)	ϵ	turbulence dissipation rate (m^2/s^3)
\dot{m}	mass flow rate (kg/s)	ρ	density (kg/m^3)
T	temperature (K)	Subscripts	
t	time (s)	<i>not</i>	notional nozzle
TD	thermal dose ($(\text{kW}/\text{m}^2)^{4/3}\text{s}$)	f	flame
v	velocity (m/s)		

INTRODUCTION

A competitive technique to store and transport large quantities of hydrogen is the cryo-compression of the gas [1]. In case of an unintended release or Thermally activated Pressure Relief Device (TPRD) opening, hydrogen is likely to ignite, producing a jet fire. The development of engineering tools capable of predicting thermal hazards from cryogenic jet fires and associated harm levels is needed to support a safer deployment of the hydrogen infrastructure. A predictive engineering tool has been developed in [2] to calculate hazard distances along the jet flame axis based on the

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temperature distribution and hot air currents in its surroundings. The “fatality” limit condition is achieved at a distance (x) equal to twice the flame length (L_f), the “pain” limit at $x = 3L_f$ and the “no harm” limit at $3.5L_f$. However, engineering tools able to predict the harm level on the sides of the jet fires are currently missing. This information may be of utmost importance to define first responders’ intervention strategy in the case of a fire involving a hydrogen-powered vehicle. The thermal dose is a comprehensive parameter to define such harm levels, as it considers the exposure duration in addition to the radiative heat flux from a source. Previous works calculated the safety distances for jet fires from a 60 l/min liquified hydrogen (LH₂) spillage [3]. It was found that a distance greater than 8.7 m from the flame extent (~5 m) should be maintained to avoid a harmful thermal dose for an exposure time up to 200 s. A distance equal to 7.6 m was found to be sufficient to reach the pain limit after 28 s exposure in high wind conditions (2.15 m/s), whereas a longer exposure time of 44 s was needed in low wind conditions (0.59 m/s). However, calculations are based on experimental measurements of radiative heat flux at 8.7 and 7.6 m along the jet axis, without provision of a tool to calculate thermal dose in arbitrary conditions. The present study aims at the development of a Computational Fluid Dynamics (CFD) model to predict distances beside the jet fire to harmful levels of thermal dose for humans. The CFD model is applied to jet fires with release temperature in the range 48-78 K, pressure up to 4 bar abs and orifice diameter equal to 1.25 mm. Only the near field to the jet fire is considered for the analysis in this study to assess the time available for first responders to act on an accident scene.

CASES OF STUDY

Simulations were performed for three experimental tests conducted at Sandia National Laboratories (SNL) on cryogenic hydrogen fires [4]. The analysed scenarios involve hydrogen releases with temperature in the range 48-78 K and pressure 2-4 bar abs. The release temperature and pressure were maintained constant during each test and monitored upstream of the orifice, with a diameter equal to 1.25 mm. Operating conditions for each of the 3 tests are described in Table 1. The cases of study are part of the set of experimental tests selected for validation of the CFD model in [5], as described in the following section.

Table 1. Operating conditions at the release

Test No.	T , K	P , bar abs	\dot{m} , g/s
1	64	2	0.33
2	48	2	0.38
3	78	4	0.56

CFD MODEL AND NUMERICAL DETAILS

The CFD model employed in the present study has been previously validated against experiments by SNL on cryogenic hydrogen fires from storage with pressure up to 5 bar abs and temperature in the range 48-82 K [4]. For all the five tests, experimental radiative heat flux at 5 sensors along the jet flame was predicted within $\pm 15\%$ accuracy, with few exceptions [5]. The CFD approach is based on the Reynolds-Averaged Navier Stokes (RANS) conservation equations for mass, momentum, energy and species. The transport equations for turbulent kinetic energy, k , and turbulence dissipation rate, ε , are solved through the realizable k - ε model [6]. The Eddy Dissipation Concept [7] is employed to model hydrogen combustion in air, considering a subset of Peters and Rogg’s mechanisms with 18 elementary reactions and 9 species [8]. The Discrete Ordinates model is used to solve the Radiative Transfer Equation (RTE) [9]. Water vapour is the only emitting/absorbing

species considered in the study, and it is treated as a grey gas. The absorption coefficient is defined as a function of a control volume temperature and water vapour concentration according to Hubbard and Tien’s data [10]. Scattering is neglected, given that soot is not involved in hydrogen-air combustion. 10x10 angular divisions are employed to discretise the RTE, following the results of the parametric study performed in [5], along with 3x3 pixels. ANSYS Fluent is used as the platform for calculations.

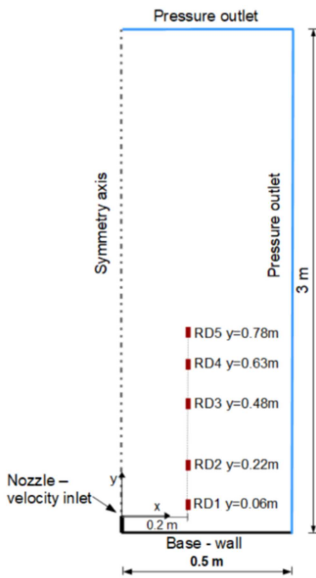


Fig. 1. Scheme of the release, sensors and domain set-up (domain height not in scale).

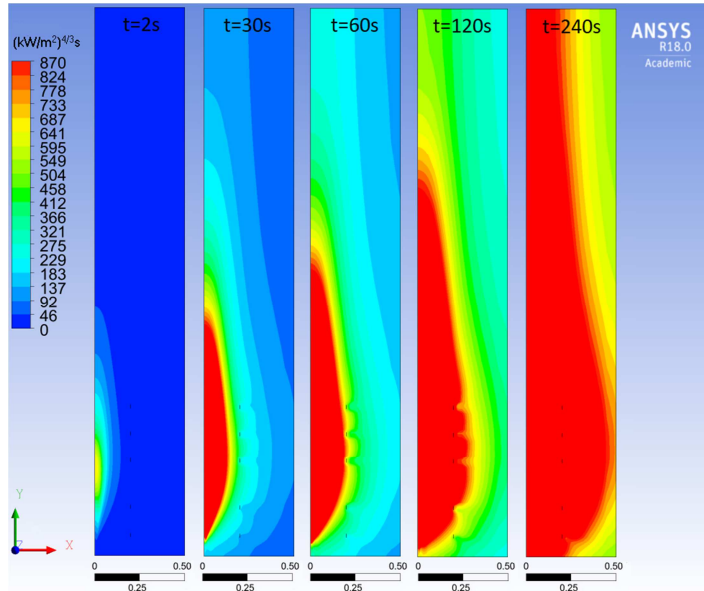


Fig. 2. Calculated thermal dose distribution for Test 3.

Table 2. Calculated notional nozzle conditions for the simulated tests

Test No.	T , K	v , m/s	ρ , kg/m ³	d_{not} , mm	\dot{m} , g/s	Variation \dot{m} from experiment, %
1	53	554.9	0.461	1.27	0.326	-1.26
2	40	480.6	0.614	1.27	0.376	-1.10
3	65	612.6	0.378	1.80	0.589	4.93

The Ulster’s notional nozzle theory [11] is used to model the release source, as it was validated also for the investigated cryogenic jets with release pressure up to 4 bar abs [5]. The conditions calculated at the notional nozzle are reported in Table 2 and they are imposed as inlet conditions in simulations, along with turbulent intensity and turbulent length scale equal to 25% and 0.07D_{eff} respectively, according to the LES study on hydrogen under-expanded jet fire [12]. The releases are assumed to be steady-state, given that the experimental set-up was arranged to maintain constant release parameters. A quarter of the domain is considered, and it has dimensions L x W x H=0.5 m x 0.5 m x 3 m. Figure 1 shows the scheme of the release and the computational domain with specification of the imposed boundary conditions. The scheme includes the 5 sensors (rd) measuring the radiative heat flux in the experiments used for validation of the CFD model in [5]. The domain is initialised with temperature and pressure equal to 288 K and 1 atm respectively. Moist air with 74% relative humidity is considered, according to the average meteorological data for SNL location

[13]. However, relative humidity may be lower in environments where controlled air ventilation systems are present, such as combustion or chemical laboratories. The effect of relative humidity was assessed in [5], considering as limiting case dry air. The absence of water vapour in air caused up to 13% increase of radiative heat flux at the sensors. The boundaries are modelled as pressure outlets with gauge pressure equal to 0. A second order upwind scheme is employed to discretise convective terms, and SIMPLE procedure for velocity-pressure coupling.

THERMAL DOSE AND HARMFUL EFFECTS ON HUMANS

Jet flames originated by pressurised hydrogen ignited releases can cause life threatening conditions in their surroundings, i.e. injury or death of the exposed subject. It could be conservatively assumed that the direct contact with the flame can result in fatality, whereas exposure to the radiative heat flux of the flame can have as consequent injury harm levels: first, second or third degree burns. The potential damage depends on the vulnerability of the target, which is determined by age, health conditions, etc. The resulting level of harm is a function of the exposure duration in addition to the incident thermal flux. Therefore, it is usually expressed in terms of thermal dose (TD):

$$TD = \int_0^t I^{4/3}(t) dt, \quad (1)$$

where I is the incident radiative heat flux (kW/m^2) and t is the exposure time (s). The thermal dose unit (TDU) is equal to $1 (\text{kW/m}^2)^{4/3} \text{s}$. Thermal dose harm levels are different depending on whether emitted radiation is included in the ultraviolet or infrared range of the spectrum. Table 3 reports the thresholds provided by [14] for both spectrum ranges. Exposure to infrared radiation results to be more dangerous, as shown by the lower and more conservative TD limits. Furthermore, water vapour is the dominant emitting species in hydrogen combustion in air and the emitted thermal radiation is mainly included in the infrared range [15]. Therefore, the associated TD thresholds are selected for calculation of hazard distances. The range $86\text{-}103 (\text{kW/m}^2)^{4/3} \text{s}$ was employed in [3] to identify the pain limit for infrared radiation. Given that the thresholds are within the range reported for first degree burns (see Table 3), only the latter will be considered in the study as it is valid also for the pain limit.

Table 3. Thermal dose thresholds for people

Burn Severity	Threshold Dose, $(\text{kW/m}^2)^{4/3} \text{s}$	
	Ultraviolet	Infrared
First degree	260-440	80-130
Second degree	670-1100	240-730
Third degree	1220-3100	870-2640

RESULTS AND DISCUSSION

A first analysis involves the calculation of distances along the jet fire axis to the harmful effects for exposure of people to hot air currents according to [2]. The average of the calculation for temperature 1300 K and 1500 K was considered, as this is the region on the jet axis where the flame tip is generally located [16]. Results for the 3 tests are presented in Table 4. It is shown that the distance from the release point indicated for “no harm” of people can vary from 2.43 m for test 1 to 3.08 m for test 3.

A second analysis addresses the calculation of separation distances on the sides of the jet fire through evaluation of the thermal dose. Figure 2 shows the thermal dose distribution at several

times of exposure for Test 3, including representation of the five 2x2 cm sensors where radiative heat flux was measured for validation of the CFD model in [5]. Maximum thermal dose was recorded inside the flame and it varied from 684 to $8.2 \cdot 10^4$ (kW/m²)^{4/3}s in the range of time 2-240 s. The graph legend is limited to a maximum value 870 (kW/m²)^{4/3}s, to represent distinctively the range of values characterising the thresholds reported in Table 3. Higher thermal doses are represented in red as for 870 (kW/m²)^{4/3}s. It is noticeable that 60 s exposure would result in first degree burns within 0.5 m from the jet flame axis.

Table 4. Distances to harm levels for people considering the jet fire flame length

Test No.	1	2	3
Average calculated flame length, m	0.70	0.75	0.88
“no harm” limit, m <i>70°C for any exposure duration</i>	2.43	2.63	3.08
“pain” limit, m <i>115°C for 5 minutes exposure</i>	2.09	2.25	2.64
“fatality” limit, m <i>309°C, third degree burns for 20 s exposure</i>	1.39	1.50	1.76
Maximum calculated flame width, m	0.09	0.09	0.11

Figure 3 provides the thermal dose classified by the associated harm criteria, as function of distance and exposure time for Tests 1, 2 and 3. As shown in Fig. 2, the thermal dose is not uniformly distributed around the jet fire due to the changing properties and width along the flame axis, and its radial distribution depends on the distance from the release point. The values of thermal dose presented in Fig. 3 are maximum thermal dose at a particular radial distance recorded among all distances along flame axis. The maximum exposure time to not reach the pain limit and to not incur in first degree burns at 0.5 m from the flame axis was found to be lower than 30 s for all the 3 Tests. In Test 3, an exposure longer than 60 s resulted in second degree burns within 0.5 m from the jet flame axis, whereas 4 minutes is the maximum exposure time before third degree burns occurrence. The same harm level is reached in only 20 s of exposure at 0.7 m from the flame tip along the jet axis. However, it must be considered that this study does not include convective heat flux and deals with comparatively small-scale vertical jet fires, whereas conclusions may be different for horizontal fires due to the effect of buoyancy on combustion products and for releases from larger orifices and higher pressures. Furthermore, one radiation level in the surroundings of the jet is affected by the presence of water vapour in the atmosphere, which corresponds to a mass fraction equal to 0.008 in the present case of SNL location.

The considerations above are for people not wearing protecting clothes. The same conclusions on hazard distances can be withdrawn for operators wearing standard workwear, as they are characterised by similar tolerance to radiative heat flux [17]. In case of an accident involving hydrogen ignited releases, fire fighters responding to the scene will wear thermal protective clothing, increasing significantly the tolerable levels of radiative heat flux for short term activities (~2 minutes) in the near field of the jet fire, such as opening or closing valves [17]. Emergency operations can be performed for a maximum duration of 3 minutes when exposed to heat fluxes up to 4.6 kW/m², which agrees with the intensity indicated as tolerable for emergency personnel in [18]. Simulation results have shown that for Test 3 fire fighters can stay as close as 0.27 m from the jet axis for up to 3 min, receiving a thermal dose of approximately 1380 (kW/m²)^{4/3}s. A limit of 6.3 kW/m² is given for an operating time of 5 minutes if fire fighters are wearing aluminised clothing (TD ≈ 3490 (kW/m²)^{4/3}s), reducing further the distance from the jet axis to about 0.20 m. A radiation level of approximately 3.8 kW/m² is recorded 5 cm upstream the release point, allowing

fire fighters to act to open or close valves at this distance behind the release, whereas first responders not wearing protecting clothes can be exposed less than 13 s to prevent first degree burns occurrence.

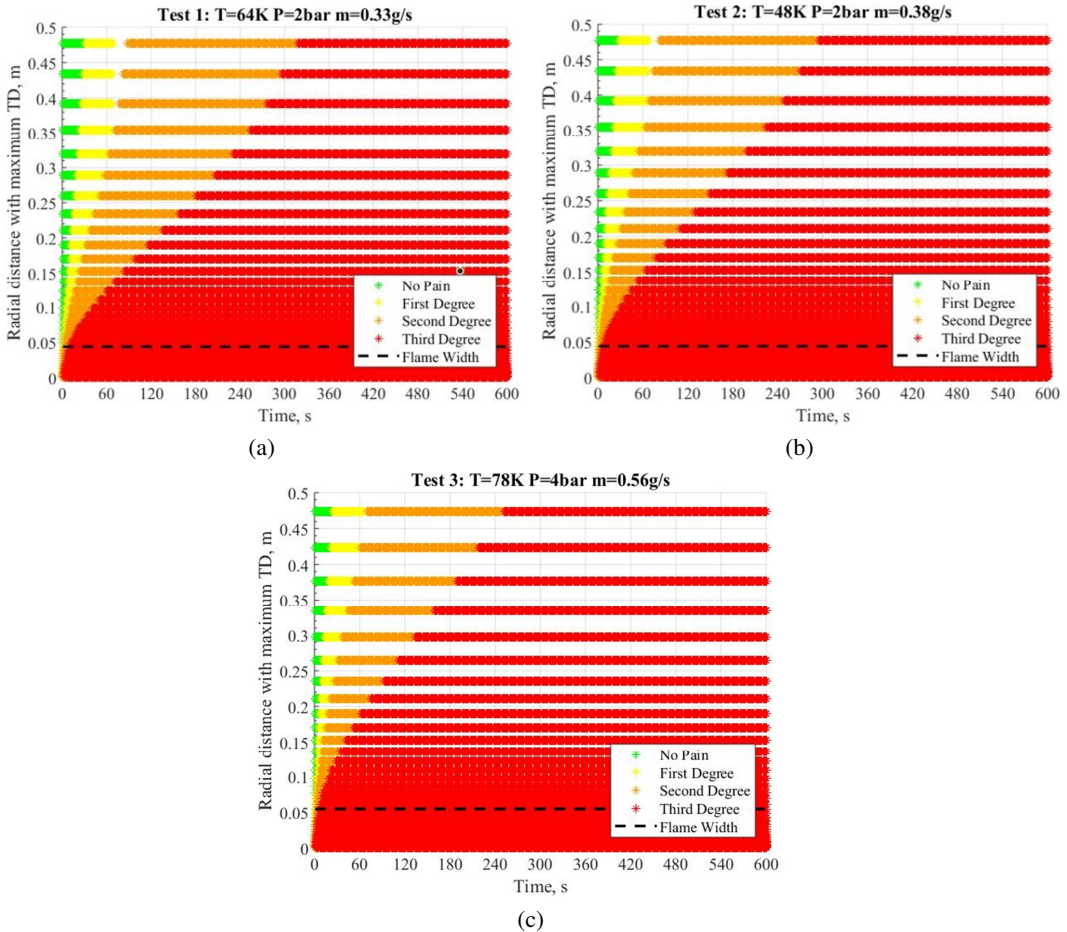


Fig. 3. Thermal dose harm levels: time versus radial distance with maximum TD for Test 1 (a), Test 2 (b) and Test 3 (c).

CONCLUSIONS

The present study aimed at the CFD modelling of thermal dose in the near surroundings of cryogenic jet fires with release temperature in the range 48-78 K and pressure 2-4 bar abs from 1.25 mm orifice. The engineering tool for prediction of harmful thermal effects on the sides of the jet fires was developed. It can be integrated to the existing tool for calculation of hazard distances along the jet axis provided in [2]. The employed CFD model had been previously validated [5] against experiments by SNL on cryogenic hydrogen fires [4]. For example, it was found that at 0.5 m distance from the flame axis, the time of exposure should be lower than 30 s to not incur first degree burns for all the Tests. For a release with $\dot{m} = 0.56 \text{ g/s}$ (Test 3), an exposure time longer than 60 s resulted in second degree burns within 0.5 m from the jet flame axis, whereas 4 minutes led to the occurrence of third degree burns.

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REFERENCES

- [1] DOE, Technical Assessment: Cryo-Compressed Hydrogen Storage for Vehicular Applications, 2006.
- [2] V. Molkov, Fundamentals of Hydrogen Safety Engineering I, www.bookboon.com, 2012.
- [3] J.E. Hall, P. Hooker, D. Willoughby, Ignited Releases of Liquid Hydrogen: Safety Considerations of Thermal and Overpressure Effects, *Int. J. Hydrogen Energy* 39 (2014) 20547–20553.
- [4] P.P. Panda, E.S. Hecht, Ignition and Flame Characteristics of Cryogenic Hydrogen Releases, *Int. J. Hydrogen Energy* 42 (2016) 775–785.
- [5] D.M.C. Cirrone, D. Makarov, V. Molkov, Thermal Radiation from Cryogenic Hydrogen Jet Fires, *Int. J. Hydrogen Energy* (2018) in press.
- [6] T.H. Shih, W.W. Liou, A. Shabbir, Z. Yang, J. Zhu, A New Eddy-Viscosity Model for High Reynolds Number Turbulent Flows – Model Development and Validation, *Comput. Fluids* 24 (1995) 227–238.
- [7] B. Magnussen, On the Structure of Turbulence and a Generalized Eddy Dissipation Concept for Chemical Reaction in Turbulent Flow, In: 19th Aerospace Sciences Meeting, 1981, doi:10.2514/6.1981-42.
- [8] R.B. Peters N, Reduced Kinetic Mechanisms for Applications in Combustion Systems, Berlin, 1993.
- [9] J.Y. Murthy, S.R. Mathur, A Finite Volume Method for Radiative Heat Transfer Using Unstructured Meshes, *J. Quant. Spectrosc. Radiat. Transf.* 12 (1998) 313–321.
- [10] C. Hubbard, G.L. Tien, Infrared Mean Absorption Coefficients of Luminous Flames and Smoke, *J. Heat Transfer* 100 (1978) 235–239.
- [11] V. Molkov, V. Makarov, M.V. Bragin, Physics and Modelling of Underexpanded Jets and Hydrogen Dispersion in Atmosphere, In: *Physis of Extreme States of Matter*, Institute of Problems of Chemical Physics, Russian Academy of Sciences, Chernogolovka, 2009, pp. 146–149.
- [12] S. L. Brennan, D. V. Makarov, V. Molkov, LES of High Pressure Hydrogen Jet Fire, *J. Loss Prev. Process Ind.* 22 (2009) 353–359.
- [13] Current Results Weather and Science Facts, California Average Relative Humidity, available from www.currentresults.com/Weather/California/humidity-annual.php.
- [14] J. Lachance, A. Tchouvelev, A. Engebo, Development of Uniform Harm Criteria for Use in Quantitative Risk Analysis of the Hydrogen Infrastructure, *Int. J. Hydrogen Energy* 36 (2010) 2381–2388.
- [15] J.R. Howell, Mengüç M.P., Siegel R., Thermal Radiation Heat Transfer, 6th Ed., Taylor and Francis Group, 2016.
- [16] R. Schefer, B. Houf, B. Bourne, and J. Colton, Experimental Measurements to Characterize the Thermal and Radiation Properties of an Open-flame Hydrogen Plume, In: *Proceedings of the 15th annual hydrogen conference and hydrogen expo*, 2004.
- [17] R. Heus, Maximum Allowable Exposure to Different Heat Radiation Levels, *Instituut Fysieke Veiligheid*, 2016, 29 p.
- [18] S. Tretsiakova-McNally, D. Makarov, Lecture – Harm Criteria for People and Environment, Damage Criteria for Structures and Equipment, 2015.