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Numerical investigation of the flammable extent of semi-confined hydrogen and methane jets

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ABSTRACT

The effect of surfaces on the extent of high pressure horizontal unignited jets of hydrogen and methane is studied using computer fluid dynamics simulations performed with FLACS Hydrogen. Results for constant flow rate through a 6.35 mm diameter pressure relief Device (PRD) orifice from 100 barg, 250 barg, 400 barg, 550 barg and 700 barg compressed gas systems are presented for both horizontal hydrogen and methane jets. To quantify the effect of a horizontal surface on the jet, the jet exit is positioned at various heights above the ground ranging from 0.1 m to 10 m. Free jet simulations are performed for comparison purposes. Also, for cross-validation purposes, a number of cases for 100 barg releases were simulated using proprietary models developed for hydrogen within commercial CFD software PHOENICS. It is found that the presence of a surface and its proximity to the jet centreline result in a pronounced increase in the extent of the flammable cloud compared to a free jet.

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1. Introduction

The use of compressed hydrogen and natural gas fuels holds significant potential for diversifying the world's energy mix, especially in the transportation and distributed power generation sectors. The deployment of an extensive high-pressure gaseous fuel infrastructure for hydrogen would benefit from specific, validated hazard assessment methods and engineering correlations. For conventional compressed gas systems operating at room temperature, the working pressures are in the range of 200–350 barg and potentially up to 700 barg on-board vehicles and 875 barg for ground storage for hydrogen. An accidental release of hydrogen typically arises from a failure of a piping component (e.g. a valve, a flange or a fitting). The resulting jet, which may potentially ignite could be harmful to personnel, equipment and property. High pressure jets are influenced by the presence of obstacles, either impinging surfaces or turbulence inducing structures. From hydrogen safety considerations, interest lays in characterizing the release of hydrogen jets and the determination of the extents of the flammable clouds, which are very important parameters in the establishment of the safety distances and sizes of hazardous zones for codes and standards [1–5].

Birch et al. [6] proposed a methodology to evaluate the decay of the mean concentration field along the centreline of a supercritical free jet. The distance taken for the mean mass fraction concentration to decay to a given value in such flows is proportional to the diameter of the source and inversely proportional to the square root of the density of the jet fluid. In their analysis they showed that the concentration field behaves as if it were produced by a larger source than the

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actual nozzle source diameter; this is referred to as the pseudo-source. Later in 1987, Birch et al. [7] reformulated their effective diameter definition based on the conservation of both mass and momentum. In a recent study, Houf et al. [8] used the Birch approach to determine the concentration decay of unignited hydrogen jets. In their implementation, Houf et al. reformulated the effective diameter of the pseudo-source by replacing the velocity at the end of the expansion region by an effective velocity originally suggested by Hess et al. [9] for under-expanded gas jets. They also removed the discharge coefficient in the effective diameter definition.

In recent studies [10,11], the extent of the flammable cloud for vertical and horizontal hydrogen and methane jets is determined as a function of time for a constant flow rate release from an 8.48 mm diameter round orifice of a 284 barg storage system for both hydrogen and methane. Effects of the proximity of the surface on the flammable extent along the axis of the jet and its impact on the maximum extent of the flammable cloud is explored and compared for both hydrogen and methane. The results were also compared to the predictions of the Birch correlations for flammable extents. It is found that the presence of a surface and its proximity to the jet centreline result in a pronounced increase in the extent of the flammable cloud compared to a free jet.

The objective of this work is to quantify the effect of surfaces on unignited hydrogen jets and if possible, find engineering correlations that could be used to establish the flammable extent of jet releases in the presence of surfaces. CFD simulations results, using FLACS Hydrogen software, for constant flow rate through a 6.35 mm PRD from 100 barg, 250 barg, 400 barg, 550 barg and 700 barg storage units are presented for horizontal hydrogen and methane jets. Surface effect on the flammable extent of the jet is explored by positioning the leak orifice at various heights above the ground ranging from 0.1 m to 10 m. Free jet simulations are performed for comparison purposes. Also, for cross-validation purposes, a number of cases for 100 barg releases were simulated using proprietary models developed for hydrogen within commercial CFD software PHOENICS.

2. Modeling scenario and simulation description

Fig. 1 shows the direction of the horizontal jet (centreline along the x direction) with respect to the horizontal surface (ground) and the orientation of gravity for the scenario simulated.

The simulations are time-dependant with a constant mass flow rate. FLACS Hydrogen from GexCon is used to perform the simulations. Description of the FLACS CFD tool is reported in [12] and references therein. FLACS uses a structured grid made of rectangular cells. In the case of jet simulations, a zone made of cubic cells is defined right next to the leak origin. From that initial zone, the grid is stretched to a coarser rectangular grid away from the leak orifice. The cell size of the initial cubic zone is determined by the leak area. Grid sensitivity study was performed and showed that the results varied by less than 5%.

Fig. 1 – Direction of the horizontal jet with respect to the position of the surface “ground”.

Table 1 presents the different scenarios simulated for the hydrogen and methane jets. For each storage pressure, a constant flow rate from a 6.35 mm diameter orifice was studied numerically for both hydrogen and methane at different positions of the jet centreline from the ground.

For each scenario, the flow is choked at the jet exit. The jet outlet conditions, i.e. the leak rate, temperature, effective leak area, velocity and the turbulence parameters (turbulence intensity and turbulent length scale) for the flow, are calculated using an imbedded jet program in FLACS. FLACS can also calculate the time dependent leak and turbulences parameters data for continuous jet releases in the case of high pressure vessel depressurization. The estimation assumes isentropic flow conditions through the nozzle, followed by a single normal shock (whose properties are calculated using the Rankine–Hugoniot relations), which is subsequently followed by expansion into ambient air [13].

The conservation equation for mass, momentum, and enthalpy in addition to conservation equations for concentration, are solved on a structured grid using a finite volume method. The SIMPLE pressure–velocity correction method is used and extended for compressible flows with source terms for the compression work in the enthalpy equation. FLACS uses the k–ϵ turbulent model and the ideal gas equation of state. FLACS was extensively validated against experimental data and reasonable agreement was seen for hydrogen dispersion simulations for various release conditions [14]. For all the scenarios studied, the simulations were run with constant flow rate as a function of time until steady state was achieved.

All the simulations with PHOENICS were conducted with a transient CFD approach using the constant choked hydrogen release rate calculated based on the Abel–Nobel real gas equation of state (AN-EOS) under given storage pressure and

Table 1 – List of scenarios for horizontal hydrogen and methane jet.

Storage pressure (barg)	Gas	Mass flow rate (kg/s)	Jet exit distance from the ground (m)
100	H_2	0.20	0.029, 0.1, 0.5, 1, 1.5, 2, 2.5, 3, 3.5,
	CH_4	0.54	4, 5, 6, 7, 8, 9, 10, free jet
250	H_2	0.49	0.048, 0.5, 1, 1.5, 2, 3, 4, 6, 8, 10,
	CH_4	1.34	free jet
400	H_2	0.78	0.059, 0.5, 1, 1.5, 2, 3, 4, 6, 8, 10,
	CH_4	2.14	free jet
550	H_2	1.07	0.069, 0.5, 1, 1.5, 2, 3, 4, 6, 8, 10,
	CH_4	2.94	free jet
700	H_2	1.36	0.077, 0.231, 0.5, 1, 1.5, 2, 2.5, 3,
	CH_4	3.74	3.5, 4, 5, 6, 7, 8, 9, 10, free jet

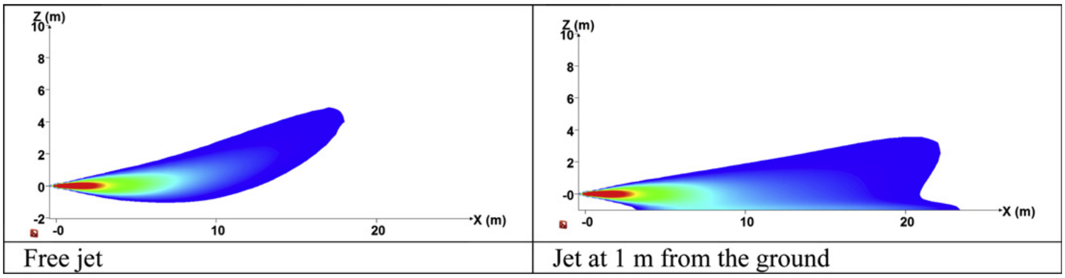

Fig. 2 – Contour of constant concentration (4% volume) of hydrogen in air at steady state for the storage pressure of 100 barg.

temperature at 293.15 K. Hydrogen convection, diffusion, buoyancy and transience were modeled based on the 3-D compressible Navier–Stokes equations and hydrogen mass conservation.

The CFD real gas model used thermodynamic relations derived based on the AN-EOS. The PHOENICS 2008 CFD software was utilized with adding customized gas properties correlations. The LVEL turbulence model, which is available in PHOENICS, was applied and the transient runs were conducted until reaching the steady state solution. The LVEL model allows for both laminar and turbulent flow conditions to be considered within one model. It computes local Reynolds numbers in every cell of the computational mesh and applies the local effective viscosity based on this number. A detailed description of the CFD tool PHOENICS is given in [15,16]. The same computational domain of 100 m $\times$ 18 m $\times$ 25 m was considered in all the runs and the grid of $40 \times 20 \times 30$ was used in the reported six-tank configuration.

3. Simulation results

3.1. Simulations with FLACS hydrogen

Figs. 2 and 3 show respectively the lower flammability limit (LFL) contours of hydrogen and methane as an example for a given scenario (4% molar fraction in air for hydrogen and 5% molar fraction for methane) at steady state. The LFL contour of free jets for hydrogen and methane is included in these figures correspondingly as well in order to show the impact of the ground proximity on the maximum LFL extent of the jet, as well as the upward bending of the flammable hydrogen cloud further away from the leak point which is a consequence of the strong buoyancy effect of hydrogen.

Figs. 4 and 5 show plots of the LFL extents as a function of the distance of the leak orifice from the ground for hydrogen and methane releases. Both the hydrogen and methane clouds are influenced by the height of the release (defined as the distance of the release point from the surface). In the case of hydrogen at 100 barg, for the first 1.5 m the centreline (CL) and maximum (ME) extents quickly drop as the distance of the leak orifice from the ground is increased. The centreline extent is defined as the maximum LFL extent along the horizontal line parallel to the normal to the surface of the jet orifice, whereas the maximum extent is the overall maximum LFL extent along the orientation of the jet. The jet is then slowly depleted until it reaches free jet extent. For methane at 100 barg, the jet is greatly affected by the ground for distances below 0.5 m. Compared to a free jet, the LFL extent is increased by 330% at a distance of 0.03 m. On the other hand, the ground has no more effect on the LFL extent for distances above 1.5 m. At about 1 m, the flammable concentration contour of the jet is no longer influenced by the presence of the surface and behaves like a free jet. In the case of hydrogen at 700 barg, the maximum LFL cloud extent reached 60.9 m when the release is located closest to the surface, i.e., 0.077 m from the ground. At this distance, the maximum extent is increased by 48% compared with that of free jet. The centreline and maximum extents quickly decrease as the distance of the leak orifice from the ground is increased up to around 4 m where the effect of the ground is nearly absent and both the maximum and centreline extents compare to the corresponding free jet extents. For the methane jet at 700 barg, the maximum LFL extent is reached when the leak orifice is at the closest distance from the ground, which is 0.077 m. At this height, compared to the free jet, the maximum LFL extent is increased by 303%. The maximum and centreline LFL extent both drop sharply as the distance from the ground is increased up to around

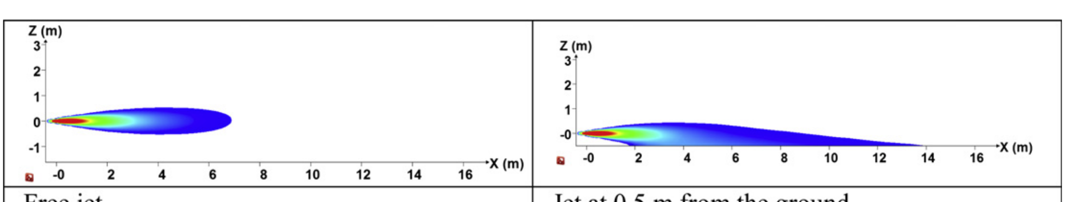

Fig. 3 – Contour of constant concentration (5% volume) of methane in air at steady state for the storage pressure of 100 barg.

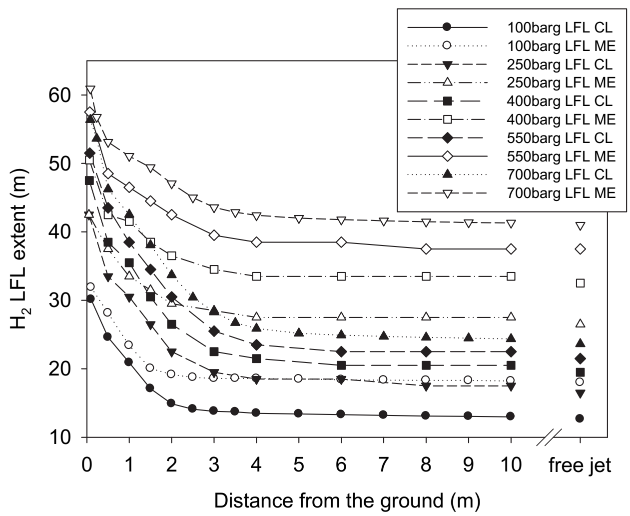

Fig. 4 – Lower flammability limit extent as a function of the leak proximity to the ground for hydrogen leaks (CL: Centerline extent; ME: Maximum Extent).

2.5 m where the jet practically disconnects itself from the ground and behaves like a free jet.

3.2. *Simulations with PHOENICS and comparison with FLACS hydrogen results*

While the geometrical set up in modelling with FLACS considered only a simple round orifice, a realistic 6-tank set up was applied in modelling with PHOENICS (see Fig. 6) to predict the LFL hydrogen clouds at the 100 bar hydrogen storage pressure, 6.35 mm orifice size, no wind conditions and various orifice heights above the grounds: 0.029 m, 0.5 m, 1 m, 1.5 m and 3 m. The LFL clouds for the maximum (ME) and centreline (CL) extents were measured using the PHOENICS VR Viewer capabilities at different times.

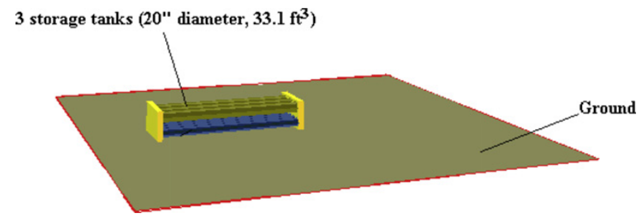

Fig. 6 – Storage geometry for hydrogen releases in PHOENICS at 100 barg.

Table 2 – Dependence of 'steady state' maximum and centreline extents on distance to the ground at 100 bar storage pressure.

Distance to ground (m)	0.029	0.5	1	1.5	3
ME (m)	36.06	30.36	26.57	24.22	19.02
CL (m)	28.83	22.00	19.56	18.60	15.79

Both ME and CL increase substantially with the decrease of the distance from the ground from 3 m to 0.029 m as shown in Table 2.

The steady state maximum extent decreases from 36.06 m for 0.029 m–19.02 m for 3 m. The maximum extents are larger than the corresponding centreline extents at all the orifice proximities to ground considered.

Comparison of PHOENICS results with FLACS Hydrogen predictions is shown on Fig. 7. As it can be seen, there is generally good agreement between the two. PHOENICS predictions for the maximum extent (ME) seem to be consistently higher than FLACS's, although remaining within 10–20% of the latter, while the centerline predictions were crossing over staying within ±10% of each other. Also, PHOENICS predicted a bit wider gap between ME and CL than FLACS. The difference between FLACS and PHOENICS results

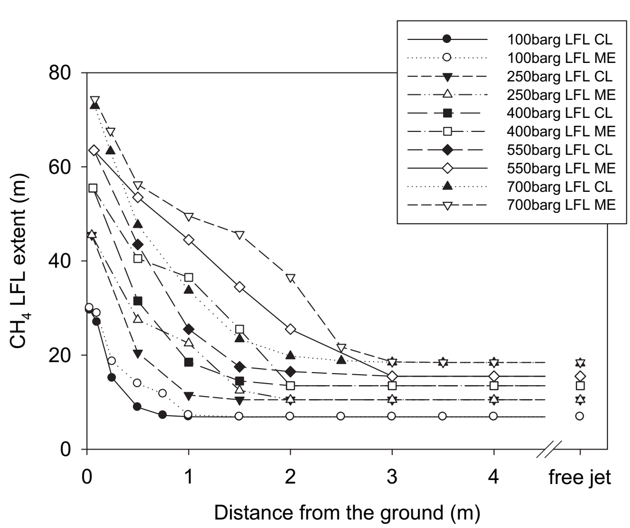

Fig. 5 – Lower flammability limit extent as a function of the leak proximity to the ground for methane leaks (CL: Centerline extent; ME: Maximum Extent).

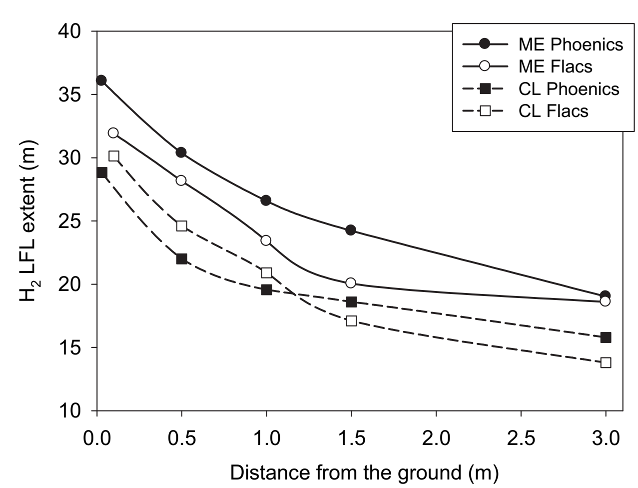

Fig. 7 – Comparison of PHOENICS and FLACS Hydrogen results for 100 barg leaks (CL: Centerline extent; ME: Maximum Extent).

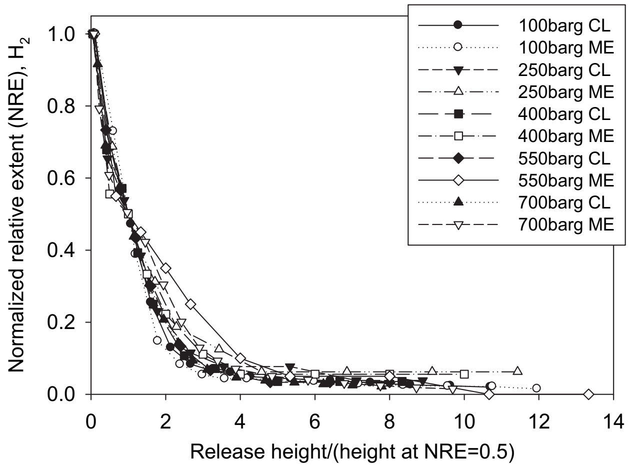

Fig. 8 – Normalized Relative Extent (NRE) as a function of the release height normalized by the height at 50% NRE for hydrogen jets (CL: Centerline extent; ME: Maximum Extent).

are due in large part to the different turbulent models used by both softwares and also to the fact that FLACS uses the ideal gas equation of state while PHOENICS used the Abel–Nobel real gas equation of state.

3.3. *Normalized relative extent*

Figs. 8 and 9 show the behaviour of the normalized relative extent (NRE) as a function of the release height normalized by the height at 50% NRE. The Normalized Relative Extent is defined as the difference between the maximum extent of the flammable cloud and the maximum extent of the free jet, divided by the maximum value of this difference (typically obtained when the distance from the ground is smallest). For hydrogen and methane jets, both the centreline and max extents are following the same trend. Figs. 8 and 9 show that

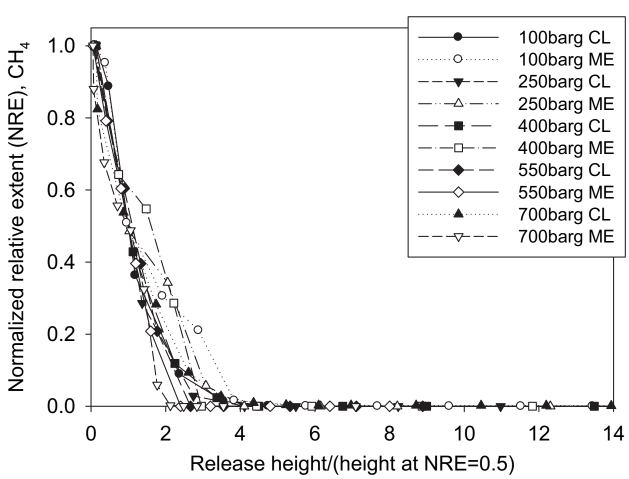

Fig. 9 – Normalized Relative Extent (NRE) as a function of the release height normalized by the height at 50% NRE for methane jets (CL: Centerline extent; ME: Maximum Extent).

the behaviour of the NRE as a function of the normalized distance from the ground is similar for all cases studied, although no definitive scaling behaviour can be ascertained from our results. The NRE plot represents a useful comparison between jets according to a boundary condition (the height of the jet) and not according to the intrinsic properties of a given jet or to the general properties of the turbulent length scales (in a direct sense). For instance, the functional dependence of the relative extent on the dimensional height requires knowledge of the width of the distribution function involving jets located at different heights. In addition, a model predicting the absolute maximum extent (as a function of height) of the flammable cloud close to the ground would be required.

4. Conclusion

Surface effect on the flammable extent of the jet is explored by positioning the leak orifice at various heights above the ground ranging from 0.1 m to 10 m. Free jet simulations are performed for comparison purposes. Also, for cross-validation purposes, a number of cases for 100 barg releases were simulated using proprietary models developed for hydrogen within commercial CFD software PHOENICS. Simulation results obtained by FLACS and PHOENICS agree well with each other for considered leak scenarios with most deviations within 10% and all – within 20%. The presence of a surface for horizontal hydrogen and methane jets has a major impact on the flammable cloud extent at steady state. For free hydrogen horizontal jets, the difference between the maximum extent at steady state and the centreline extent is attributed to the strong buoyancy effect observed towards the end of the flammable cloud, noticeably reducing its centreline extent. For methane, this effect is not observed.

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