EFFECTS OF SURFACE ON THE FLAMMABLE EXTENT OF HYDROGEN 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 CFD numerical simulations performed with FLACS Hydrogen. Results for constant flow rate through a 6.35 mm PRD from 100 barg and 700 barg storage units are presented for 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.

1.0 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 incidental release of hydrogen generally arises from a failure of a piping component (e.g. a valve, a flange or a fitting) on storage equipment. The resulting hydrogen fuel jet represents a potential for immediate or delayed ignition, which could be harmful to personnel, equipment and property. High pressure jets will also be influenced by the presence of obstacles in the immediate surroundings, 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 in the hydrogen 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 volume 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 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] reused the Birch method 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 a recent study [10], 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 orifice of a 284 barg storage unit 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 are 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. Results for constant flow rate through a 6.35 mm PRD from 100 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.

2.0 MODELING SCENARIO AND SIMULATION DESCRIPTION

Figures 1 show 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.

Figure 1. Direction of the horizontal jet with respect to the position of the surface "ground".

The simulations are time-dependant with a constant mass flow rate. FLACS-Hydrogen from GexCon is used to perform the simulations. 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%.

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.

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	Hydrogen	0.20	0.029, 0.1, 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 5, 6, 7, 8, 9, 10, free
	Methane	0.54	
700	Hydrogen	1.36	0.077, 0.231, 0.5, 1, 1.5, 2, 2.5, 3, 3.5, 4, 5, 6, 7, 8, 9, 10, free
	Methane	3.74	

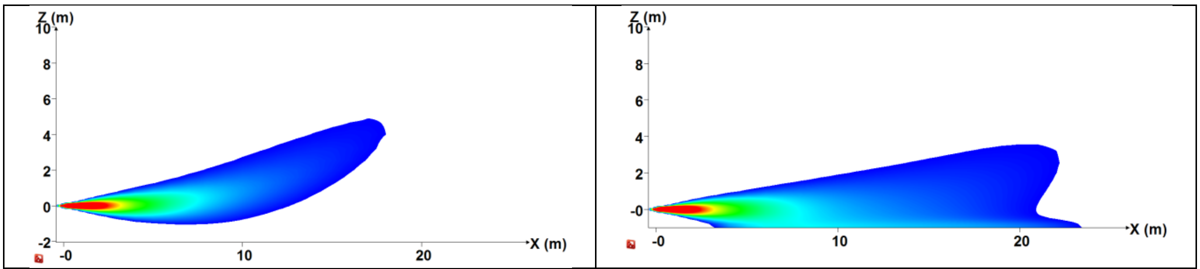
For each scenario, the flow is choked at the jet exit. The jet outlet conditions, i.e. the leak rate, temperature, effective leak area, velocity and the turbulence parameters (turbulence intensity and turbulent length scale) for the flow, are calculated using an imbedded jet program in FLACS. FLACS can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

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 [11]. For all the scenarios studied, the simulations were run with constant flow rate as a function of time until steady-state was achieved.

3.0 SIMULATION RESULTS

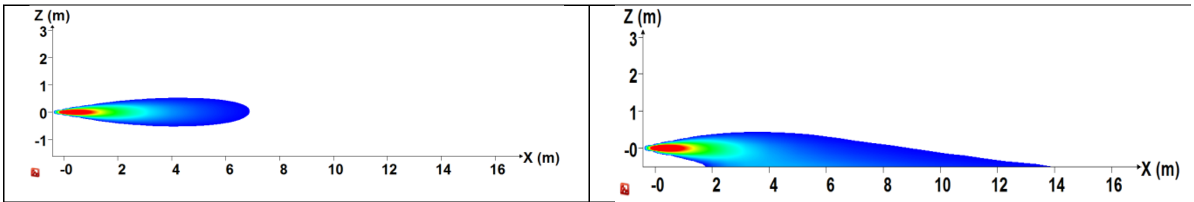
3.1 Simulation results: storage pressure=100 barg

Figures 2-3 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 jet for hydrogen and methane jets is included in each Figure correspondingly to show the impact of the ground proximity on the maximum LFL extent of the jet.



Free jet	Jet centerline at 1 m from the ground

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



Free jet	Jet centerline at 0.5 m from the ground

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

Figures 4-5 summarize the extents of the LFL cloud contour as a function of the distance of the jet centreline from the ground for the case where the storage pressure was set to 100 barg respectively for hydrogen and methane. As shown by the results, both the hydrogen and methane clouds are influenced by the height (the distance of the release point from the surface). In the case of hydrogen, for the first 1.5 m the centreline and maximum extent quickly drop as the distance of the leak orifice from the ground is increased. The jet is then slowly depleted until it reaches free jet extent. For methane, 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 jet practically disconnects itself from the ground and behaves like a free jet.

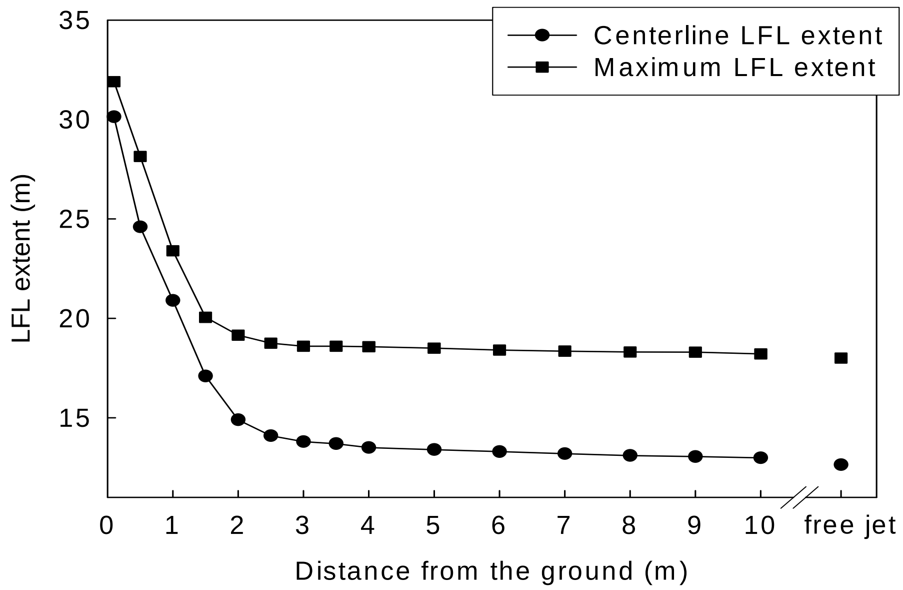


Figure 4. Lower flammablity limit extent as a function of the leak proximity to the ground for an hydrogen leak with a storage pressure of 100 barg.

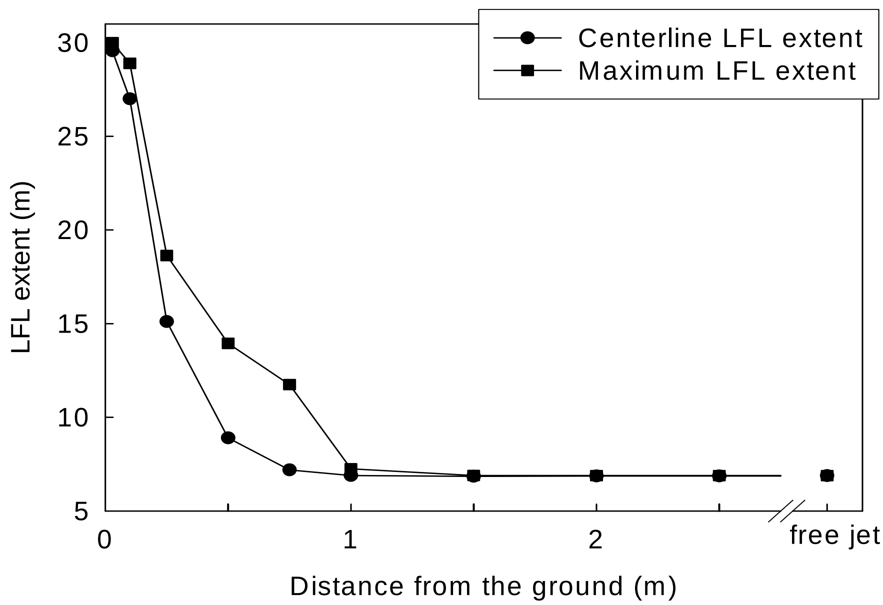


Figure 5. Lower flammability limit extent as a function of the leak proximity to the ground for a methane leak with a storage pressure of 100 barg.

3.2 Simulation results for a storage pressureof 700 barg

Figures 6-7 display the LFL cloud contour profile for the free jet and for the jet in the presence of the ground respectively for hydrogen and methane. It show the effects of the ground proximity on the LFL concentration envelop as well 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.

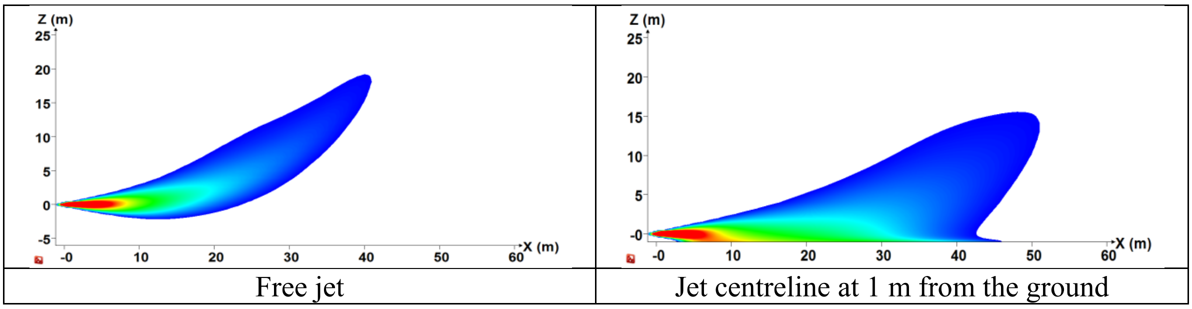


Figure 6. Contour of constant concentration (4% volume) of hydrogen in air at steady state for the storage pressure of 700 barg.

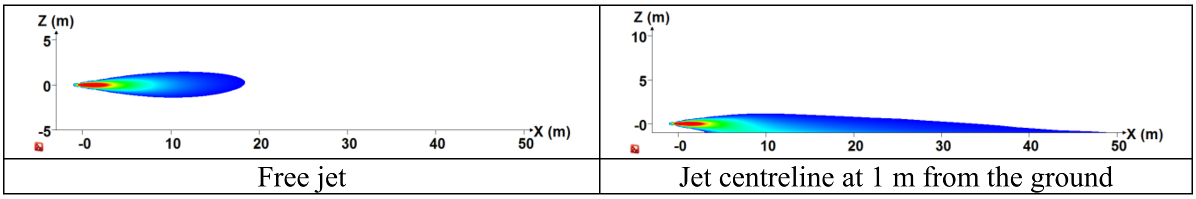


Figure7. Contour of constant concentration (5% volume) of methane in air at steady state for the storage pressure of 700 barg.

Figures 8-9 below show plots of the LFL extents as a function of the distance of the leak orifice from the ground respectively for hydrogen and methane for the case where the storage pressure is set to 700 barg. As shown previously for the 100 barg storage case, the results for both hydrogen and methane clouds are influenced by height. In the case of hydrogen, the maximum LFL cloud extent reached 60.9 m when the jet exit is located at 0.077 m from the ground, the height studied. At this distance, the maximum extent increased by 48% compared with the maximum extent of the 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 reach the corresponding free jet extents. For the methane jet, i.e. Figure 9, the maximum LFL extent is reached when the leak orifice is at the lowest distance from the ground, which is 0.077m. At this height, compared to the free jet, the maximum LFL extent is increased by 303%. The maximum and centreline LFL extents both drop sharply as the distance from the ground increase up to around 2.5 m where it is shown that the jet practically disconnects itself from the ground and behaves like a free jet.

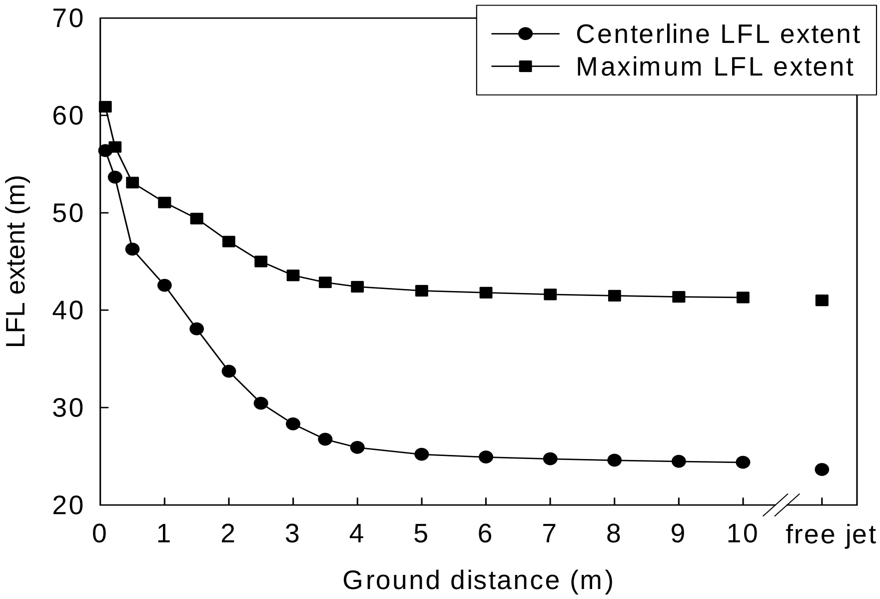


Figure 8. Lower flammability limit extent as a function of the leak proximity to the ground for the hydrogen leak with a storage pressure of 700 barg.

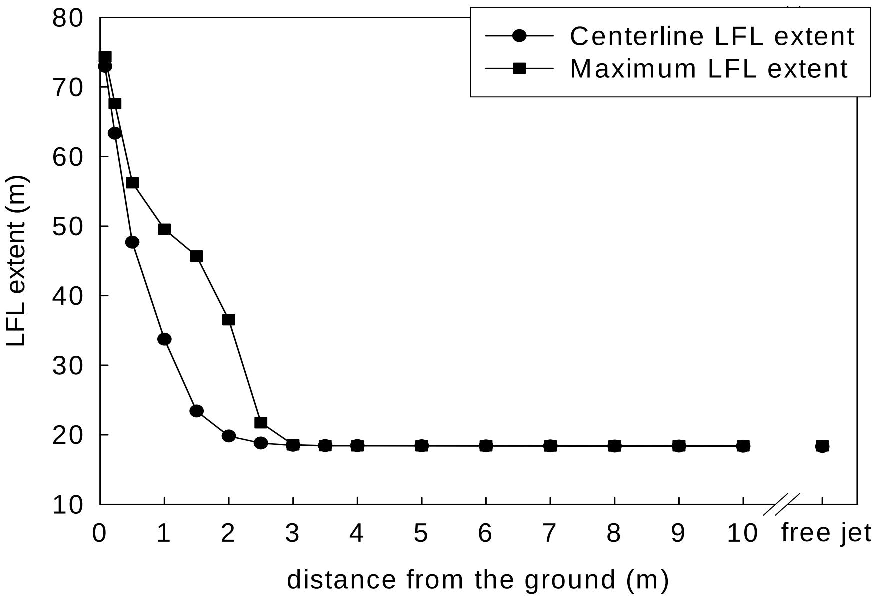


Figure 9. Lower flammability limit extent as a function of the leak proximity to the ground for a methane leak with a storage pressure of 700 barg.

Figure 10 shows the behaviour of the normalized relative extent (NRE) as a function of the distance normalized by the distance 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 at 100 barg and 700 barg are following the same trend. Figure 10 shows that 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.

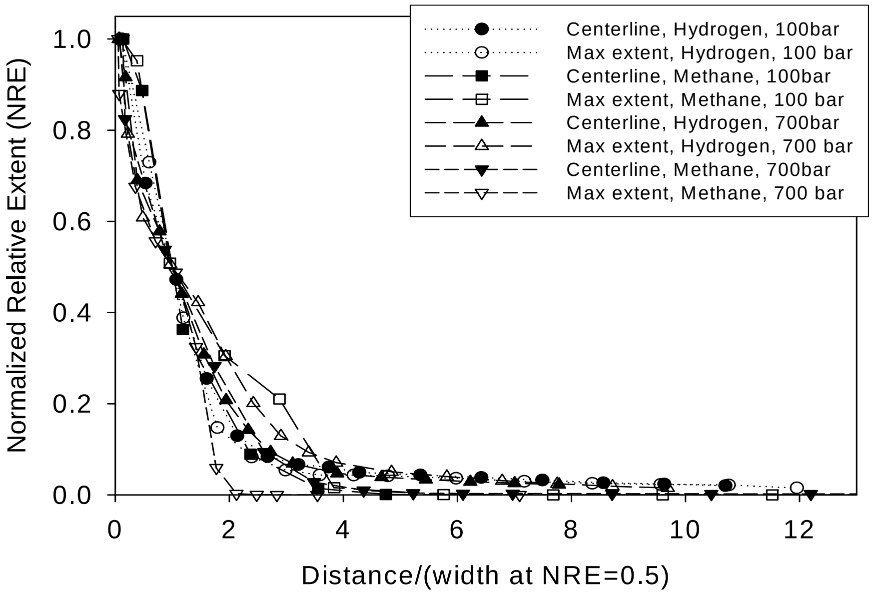


Figure 10. Normalized Relative Extent (NRE) as a function of the distance normalized by the distance at 50% NRE.

4.0 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. 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. The results are likely to depend on the specific turbulence model used, especially in view of the reduced symmetry of the problem. Simulations are currently being run to that effect with a second compressible solver in subsonic regime to avoid the use of effective diameter approaches. Experiments are also required to validate these results: experimental studies are planned as part of the H2Can network particle velocimetry activities on hydrogen safety.

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