NUMERICAL INVESTIGATION OF A VERTICAL SURFACE ON THE FLAMMABLE EXTENT OF HYDROGEN AND METHANE VERTICAL JETS

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ABSTRACT

The effect of vertical surface on the extent of high pressure unignited jets of both hydrogen and methane is studied using computer fluid dynamics simulations performed with FLACS Hydrogen. Results for constant flow rate through a 6.35 mm round leak orifice from 100 barg, 250 barg, 400 barg, 550 barg and 700 barg compressed gas systems are presented for vertical jets. To quantify the effect of the surface on the jet, the jet exit is positioned at various distances from the surface ranging from 0.029 m to 12 m. Free jets simulations are performed for comparison purposes.

1.0 INTRODUCTION

The use of compressed hydrogen as fuel 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. The jet resulting from an accidental release of hydrogen, 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].

In a recent study [6], the effect of surfaces on the extent of high pressure horizontal unignited jets of hydrogen and methane was studied for constant flow rate through a 6.35 mm round leak orifice from 100 barg, 250 barg, 400 barg, 550 barg and 700 barg compressed gas systems. The objective of the work was 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. The present work continues this study for high pressure vertical unignited jets of hydrogen and methane using the same orifice diameter as well as storage pressure. To quantify the effect of the surface on the flammable extent of vertical jet, the jet exit is positioned at various distances from the surface ranging from 0.029 m to 12 m. Free vertical jet simulations are performed for comparison purposes.

2.0 MODELLING SCENARIO DESCRIPTION

The simulations are time-dependant with a constant mass flow rate. FLACS-Hydrogen from GexCon is used to perform the simulations. FLACS uses a rectilinear grid. 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. Figure 1 shows the direction of the jet with respect to the vertical surface and the orientation of gravity.

Figure 1. Direction of the jet (arrow) with respect to the position of the vertical surface.

The scenarios simulated for hydrogen and methane jets are presented in Table 1. Results for storage pressure of 100 barg, 250 barg, 400 barg, 550 barg and 700 barg are presented. For all scenarios, the exit diameter of the jet was 6.35 mm and the storage temperature was 293.15 K.

Table 1. List of scenarios for vertical hydrogen and methane jet

Gas	Storage pressure (barg)	Mass Flow rate (kg/s)	Jet exit distance from the surface (m)
H2	100	0.20	from 0.029 m to 10 m
	250	0.49	from 0.048 m to 10 m
	400	0.78	from 0.059 m to 10 m
	550	1.07	from 0.069 m to 10 m
	700	1.36	from 0.077 m to 12 m
CH4	100	0.54	from 0.029 m to 4 m
	250	1.34	from 0.048 m to 4 m
	400	2.14	from 0.059 m to 5 m
	550	2.94	from 0.069 m to 5 m
	700	3.74	from 0.077 m to 10 m

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 [7].

The compressible Navier-Stokes equations are solved on a three dimensional structured grid using a finite volume method. The numerical model uses a second order scheme for resolving diffusive fluxes and a second-order Kappa scheme (hybrid scheme with weighting between 2nd order upwind and 2nd order central difference, with delimiters for some equations) to resolve the convective fluxes. The time stepping scheme used in FLACS is a first order backward Euler scheme. 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 [8]. For all the scenarios studied, the simulations were run with constant mass flow rate as a function of time until steady-state was achieved.

3.0 MODELLING RESULTS

The centerline and maximum LFL extents are defined in Figure 2. Figure 3 and Figure 5 show plots of the maximum and centerline LFL extents as a function of the distance between the leak orifice and the surface for hydrogen and methane releases. As shown, both the hydrogen and methane clouds are greatly influenced by the proximity of the leak orifice to the surface.

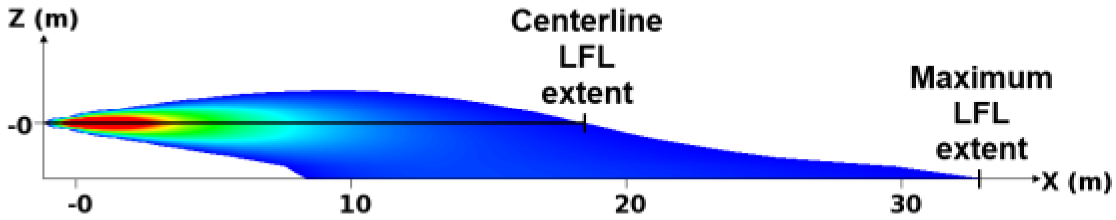

Figure 2. Centerline and maximum LFL extent definition

Figure 4 and Figure 6 show respectively the lower flammability limit (LFL) contours of hydrogen and methane jets as an example for the 700 barg release scenario (4% molar fraction in air for hydrogen and 5% molar fraction for methane) at steady state. The LFL contours of free jets for hydrogen and methane respectively are also displayed in these figures in order to show the impact of the surface proximity on the LFL extent of the jet.

3.1 Simulation results: hydrogen

As shown in Figure 3, for all scenarios, the centerline LFL extent drops smoothly as the distance between the leak orifice and the surface is increased, until the free jet extent is reached. At the same time the maximum LFL extent displays an erratic behavior. It initially quickly drops as the distance is increased up to about 0.5 m, then steadily decreases as the distance is increased further before rapidly converging toward the free jet extent. When the surface is right next to the leak orifice, the jet LFL extent is increased by 192% for 100 barg jet, 185% for 250 barg, 177% for 400 barg, 174% for 550 barg and 180% for 700 barg jet compared with that of the free jet. Furthermore, the increase of the maximum LFL extent drops below 5% before it reaches abruptly the free jet extent at a distance from the surface of about 3 m for 100 barg jet, 4 m for 250 barg, 5 m for 400 barg, 6 m for 550 barg and 7 m for 700 barg jet.

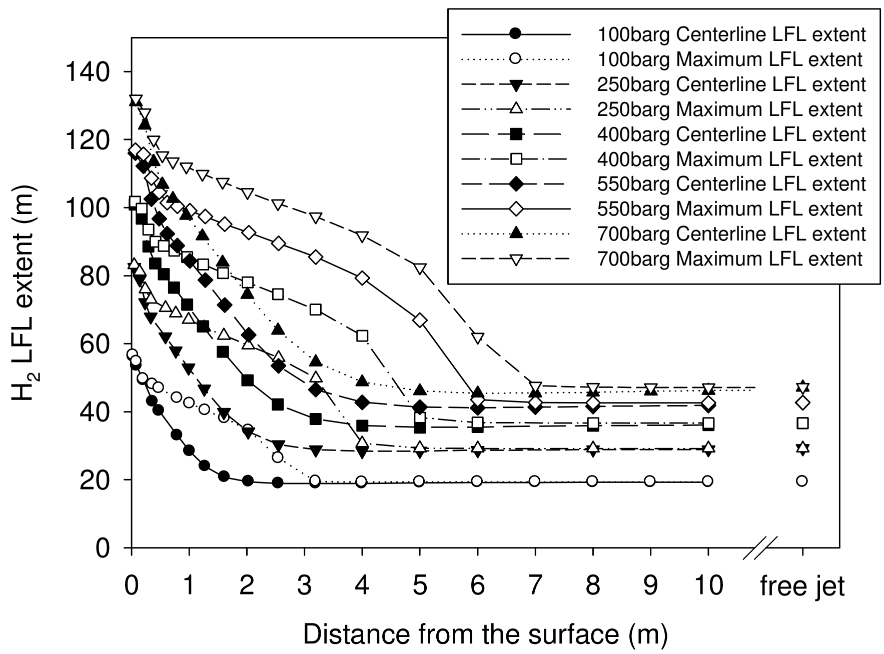

Figure 3. Lower flammable limit extent as a function of the leak proximity to the surface for hydrogen leaks with a storage pressure of 100 barg, 250 barg, 400 barg, 550 barg and 700 barg.

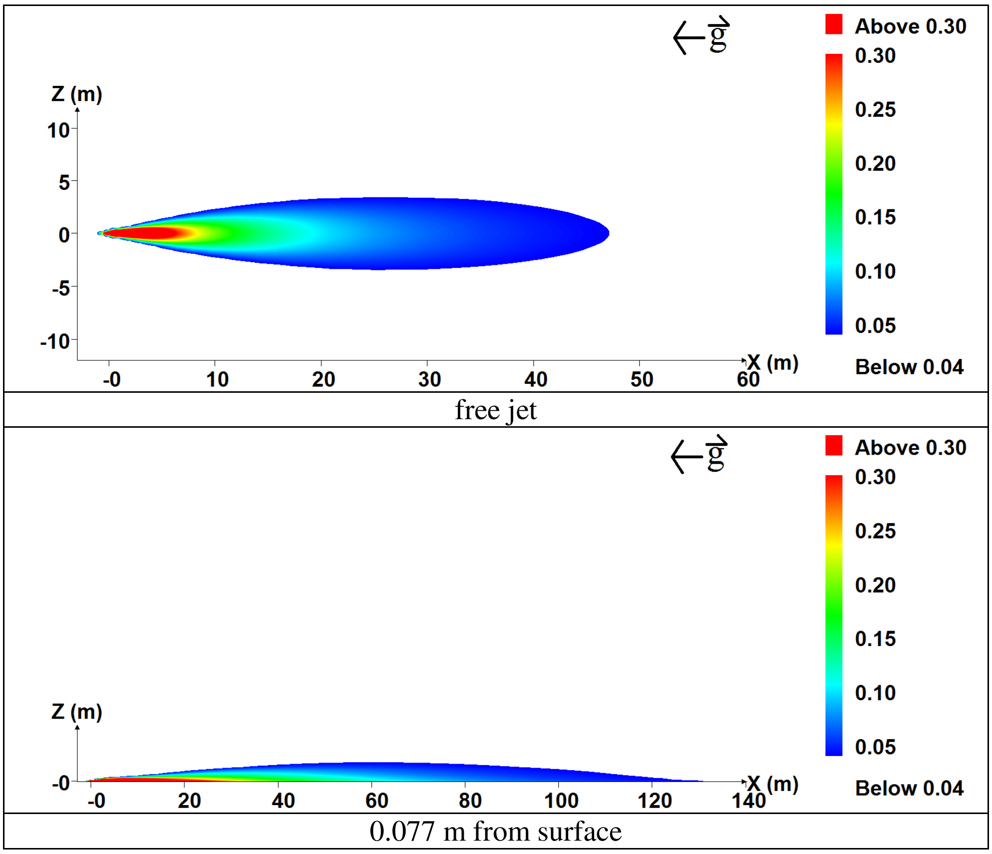

Figure 4. Hydrogen concentration distribution within the lower flammability limit (4% (vol) for hydrogen) contour along the jet direction for a storage pressure of 700 barg.

3.2 Simulation results: methane

As shown in Figure 5, the same behavior that was observed for the hydrogen jets can be seen for the centerline and maximum extents of the methane jets with the noted difference that the surface effect subsides much more rapidly as the distance between the leak orifice and the surface is increased. When the surface is closest to the leak orifice, the jet extent is increased by 300% for 100 barg jet, 297% for 250 barg, 290% for 400 barg, 284% for 550 barg and 283% for 700 barg jet compared with that of the free jet. Moreover, at a surface distance of about 1 m for 100 barg jet, 1.6 m for 250 barg, 2 m for 400 barg, 2.5 m for 550 barg and 3.2 m for 700 barg, the increase of the maximum LFL extent drops below 12% and the extent of the jet quickly converges to free jet extent.

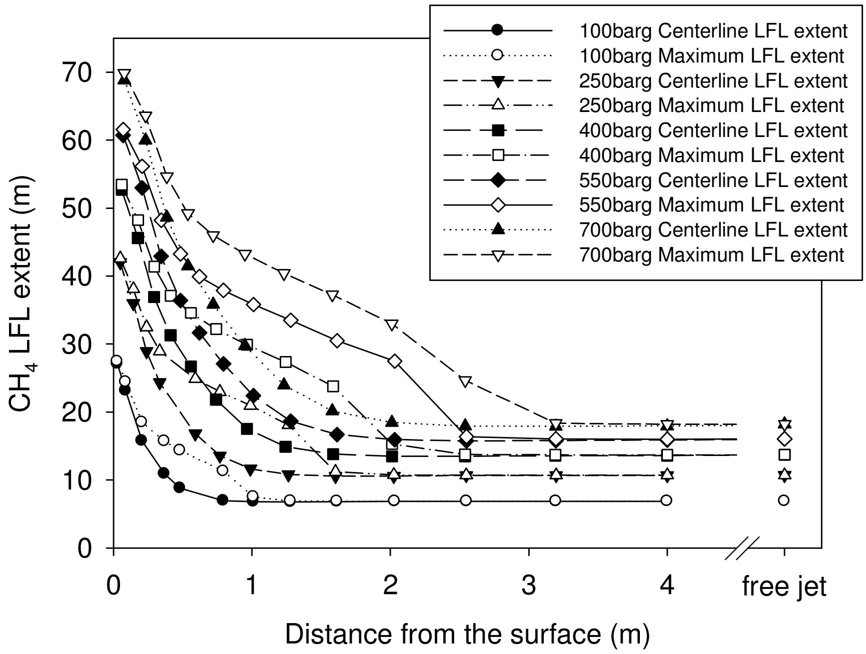

Figure 5. Lower flammable limit extent as a function of the leak proximity to the surface for methane leaks with a storage pressure of 100 barg, 250 barg, 400 barg, 550 barg and 700 barg.

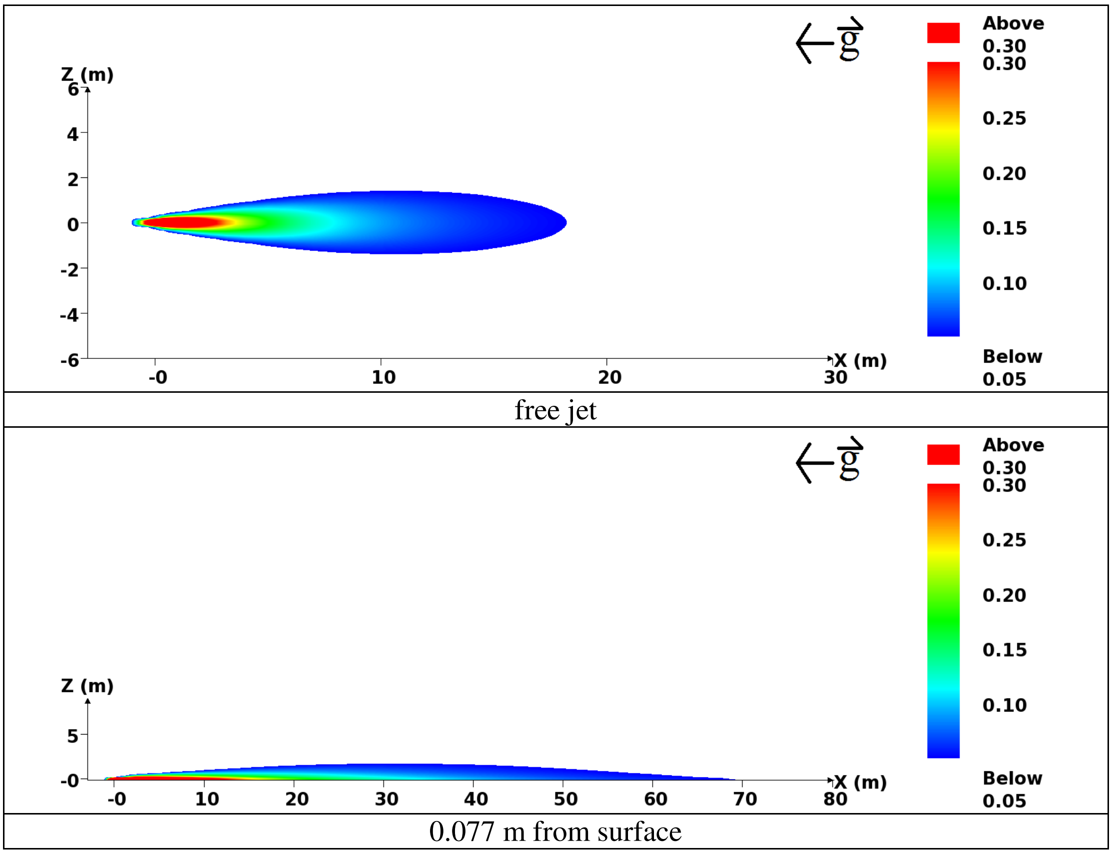

Figure 6. Methane concentration distribution within the lower flammability limit (5% (vol) for methane) contour along the jet direction for a storage pressure of 700 barg.

3.3 Normalized relative extent (NRE)

We're looking at comparing the variation of the flammable extent as a function of the proximity to the surface for different inlet conditions. Figure 7 and Figure 8 show the behavior of the normalized relative extent (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 surface is smallest). The distance of the orifice from the surface is normalized by the corresponding distance at 50% NRE.

To illustrate the NRE approach, consider the case of the hydrogen release at 700 barg. We calculate the NRE for all distances:

$$NRE(h) = (X_{max}(h) - X_{free\_jet})/(X_{abs\_max} - X_{free\_jet}) \quad (1)$$

where $X_{max}(h)$ is the maximum LFL extent of the jet with the orifice at a distance h from the surface, X_{free_jet} is the maximum LFL extent of the corresponding free jet and X_{abs_max} is the maximum extent of the jet at the smallest distance from the surface. In this case, $X_{max}(h)$ will vary from 132 m (at h = 0.077 m) to 47.2 m (at h = 12 m). Thus X_{free_jet} = 47.2 m and X_{abs_max} = 132 m (at h = 0.077 m). We then find the two distances h from the surface bracketing NRE = 0.5 (for 700 barg this corresponds to h = 4 m and h = 5 m with NRE(4) = 0.53 and NRE(5) = 0.42). A linear regression is then performed to find the distance h where NRE(h) = 0.5, which in our example yields a value of 4.23 m. The original distances h are then normalized by this value. The resulting data is shown on Figure 7. The values used to find NRE of the maximum extent for vertical hydrogen releases are shown in Table 2.

Table 2. Values used to calculate NRE of the maximum extent for vertical hydrogen releases

Pressure (barg)	X_{free_jet} (m)	$X_{abs\_max} - X_{free\_jet}$ (m)	h (m) at NRE(h) = 0.5
100	19.4	37.3	1.63
250	29.2	53.9	2.51
400	39.7	65.0	3.28
550	42.7	74.2	3.93
700	47.2	84.8	4.23

The behavior of the NRE along the centerline is similar for all the cases studied which suggest form of scaling behavior. Although in our case, the scaling is linked to the distance between the orifice and the surface which corresponds rather to a boundary condition. Furthermore, to plot the NRE as a function of the corresponding distance require the knowledge of the whole curve. The distance corresponding to 50% NRE is not a fundamental physical property of the system.

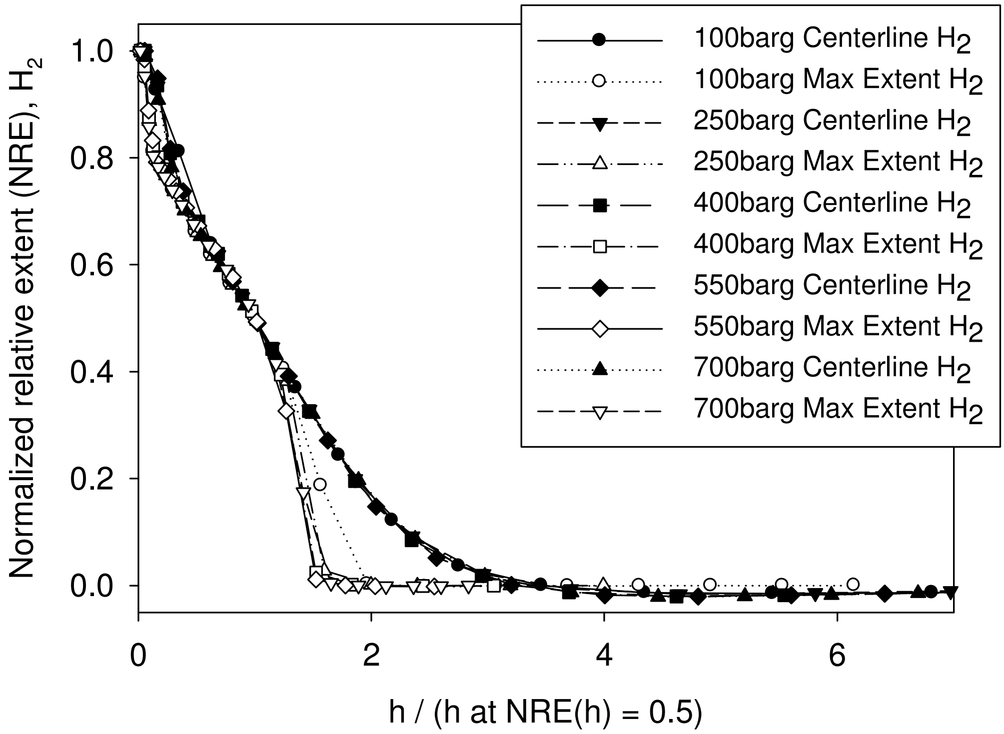

Figure 7. Centerline extent and maximum extent normalized axes for 100 bar, 250 bar, 400 bar, 550 bar and 700 bar hydrogen release.

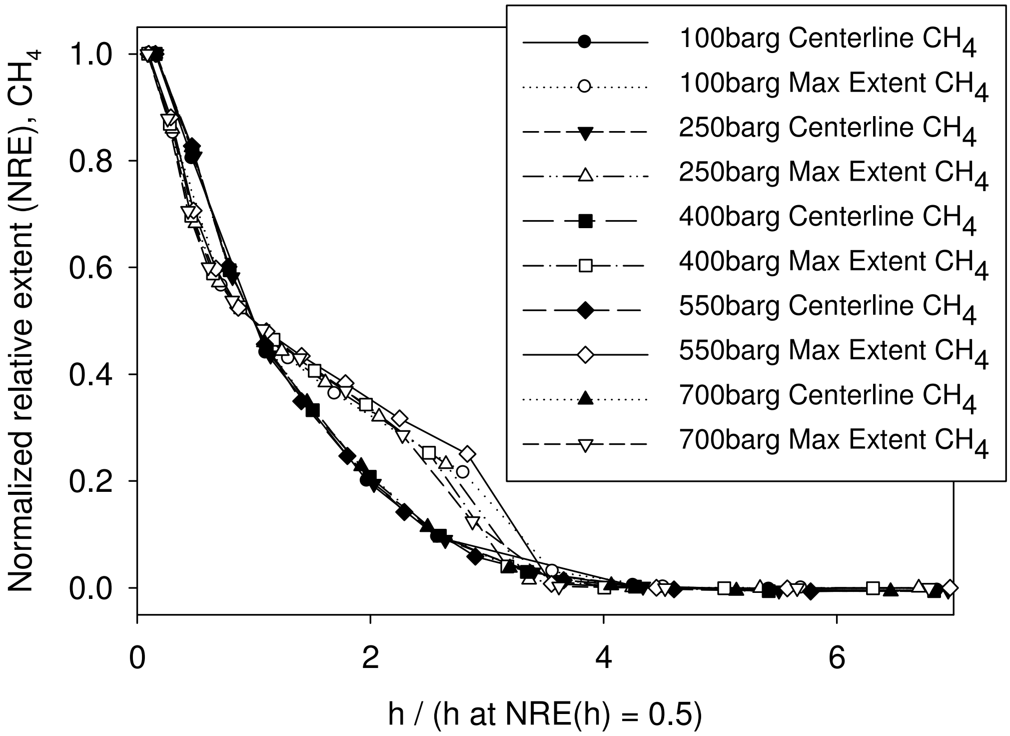

Figure 8. Centerline extent and maximum extent normalized axes for 100 bar, 250 bar, 400 bar, 550 bar and 700 bar methane release.

4.0 CONCLUSION

Surface effect on the flammable extent of vertical jet was explored by positioning the leak orifice at various distances from a surface ranging from 0.029 m to 12 m. Free jet simulations were performed for comparison purposes. For all the scenarios studied, when the leak orifice is right next to the surface, the maximum extent of the jet is increased by an average of 182% for hydrogen and 291% for methane compared to the free jet extent. These results are qualitatively consistent with earlier obtained and reported results for horizontal jets [6]: hydrogen jets appear to be less sensitive to the effects of a surface than methane jets under similar release conditions. Surface effects on the flammable extent of the jet is significantly reduced, i.e. the extent increase is under 15%, when the orifice distance from the surface is around 3 m for 100 barg jet and around 7 m for the 700 barg jet for the hydrogen releases, and around 1 m for 100 barg jet and around 3.2 m for the 700 barg jet for the methane leaks. The results show that the presence of a wall can significantly enhance the flammable extent of hydrogen and methane jets. This has consequences on the safety of hydrogen systems as to the location of ignition sources and detectors and suggests avenues for mitigation, such as minimum distances from surfaces.

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