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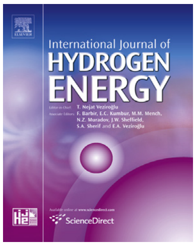

Adjacent surface effect on the flammable cloud of hydrogen and methane jets: Numerical investigation and engineering correlations

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ABSTRACT

The effect of an adjacent surface on the lower flammability limit cloud extents of high pressure horizontal and vertical unignited jets of both hydrogen and methane is studied using Computational Fluid Dynamics (CFD) simulations performed with FLACS Hydrogen. Two jet directions (horizontal and vertical) and two surface positions (horizontal or ground, vertical or side wall) were studied: horizontal jets along a horizontal surface, vertical and horizontal jets along a vertical surface or side wall. Results for constant flow rate through a 6.35 mm round leak orifice from 101 bar, 251 bar, 401 bar, 551 bar and 701 bar compressed gas systems are presented. The effect of the surface on the flammable extents is studied systematically by positioning the jet exit release at various distances from the surface ranging from 0.029 m to 10 m. Free jets simulations were performed for comparison purposes. Our results were quantified by establishing engineering correlations that could be used to predict the flammable extent of hydrogen and methane jet releases in the presence of surfaces. These correlations were validated using experiments conducted for horizontal hydrogen jets in the vicinity of horizontal surfaces, carried out at the facilities of Defence Research and Development Canada (DRDC) in Val-Belair, Québec.

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 [1,2]. From

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Abbreviations: CFD, Computational Fluid Dynamics; DRDC, Defence Research and Development Canada; 0G, zero gravity; LFL, lower flammability limit.

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hydrogen safety considerations, interest lies in characterizing the release of hydrogen jets [3–6] and the determination of the extents of the flammable clouds [7], which are very important parameters in the establishment of the separation distances and sizes of hazardous zones for codes and standards. The calculation of the cloud extent of hydrogen–air mixture encompassing the lower flammability limit or a fraction of the latter can be used to set separation distances between reservoirs, vehicles, and public areas or defining 'zones' as in the Electrical code. Knowledge of the dynamics of a hydrogen cloud is also required to evaluate the proper location of hydrogen sensors in vehicles or refuelling stations.

The behaviour of the expanded region of free vertical jets is well understood and can be treated analytically. Concentration envelopes of a vertical jet release can be calculated from the storage conditions using [8,9] or Sandia [7] correlations which evaluate the decay of the mean concentration field along the centreline of the supercritical free jet. However, the presence of a surface in the vicinity of the jets will significantly alter these predictions.

Previously, Hourri et al. [10] have preliminary investigated the effect of horizontal and vertical surfaces on the flammable extent of high pressure horizontal and vertical hydrogen and methane jets. This study was carried out for constant flow rate from a round leak orifice of a 285 bar storage unit for both hydrogen and methane. Two jet directions (horizontal and vertical) and two surface positions (horizontal or ground, vertical or side wall) were studied: horizontal jets along a horizontal surface, horizontal and vertical jets along a vertical surface or side wall. For each scenario, effect 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 was investigated by positioning the release orifice at only three distances from the surface, namely 0.5 m, 1 m and 2 m. The results were also compared to the predictions of the Birch [8] correlations for flammable extents. It was 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.

In this work, a systematic study on the effect of an adjacent surface on the lower flammability limit cloud extent of hydrogen and methane jets is being reported, but for each scenario, the CFD simulations were carried out for specific storage pressures ranging from 101 bar to 701 bar with constant flow rate from 6.35 mm orifice. To quantify the effect of the surface on the jet maximum flammable extent, the release orifice was positioned, for each storage pressure, at various distances from the surface ranging from 0.029 m to 10 m. Free horizontal and vertical jet simulations were performed for comparison purposes. In order to assess the impact of gaseous buoyancy on the flammable extents, jets along a surface in the absence of gravity were also studied. Simulation study for the scenario describing horizontal hydrogen and methane jets in the presence of horizontal surface was presented earlier by Hourri et al. [11] where for cross validation purposes results obtained with two commercial CFD softwares FLACS and PHOENICS agree well with each other for considered leak scenarios with most deviations within 10% and all within 20%. For a complete analysis, in conjunction with the other surface orientation scenarios, results from Hourri et al. [11] are reported again in this work with a primary objective to quantify the surface effect on unignited hydrogen jets and to establish engineering correlations that could be used to predict the lower flammability limit cloud extent of hydrogen jets in close proximity to a parallel surface.

Modelling scenario description

Fig. 1 shows the different scenarios related to the direction of the jet (centreline along the x direction) with respect to each surface position as indicated by the orientation of gravity $\vec{g}$.

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 by Middha [12] and references therein. 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. Grid sensitivity study was performed and showed that the results varied by less than 5%.

The scenarios simulated for horizontal and vertical hydrogen and methane jets are presented in Table 1. 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 centerline from the parallel adjacent surface. 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.

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