Simulations of hydrogen releases from high pressure storage systems

Benjamin Angers\textsuperscript{a}, Pierre Bénard\textsuperscript{a}, Ahmed Hourn\textsuperscript{a}, Pascal Tessier\textsuperscript{b} and Jérôme Perrin\textsuperscript{c}

\textsuperscript{a}Institut de recherche sur l’hydrogène, Université du Québec à Trois-Rivières, Trois-Rivières, Québec, Canada, G9A 5H8
\textsuperscript{b} MEDAL, 305 Water Street, Newport, Delaware, 19804-2410, USA
\textsuperscript{c} Centre de Recherche Claude-Delorme, 1 Chemin de la Porte des Loges, Les Loges-en-Josas, B.P. 126 – 78354 Jouy-en-Josas Cedex – France

ABSTRACT:
We present results from hydrogen dispersion simulations from a time dependent choked horizontal release through a 6 mm PRD of a 700 bar storage unit. The properties of the release (concentration profile, velocity field) are discussed shortly after initiation. Critical constant concentration envelopes are calculated. The consequences of ignition shortly after initiation of the release are discussed.

KEYWORDS: Safety, dispersion, gaseous hydrogen

Introduction

The thermal hazards associated with flares arising from the ignition of jets of gaseous fuels, perhaps the most likely hazard associated with leaks of gaseous fuels from pressurized tanks, have been investigated in some degree of details. There have been comparatively few detailed investigations of the overpressure associated with the ignition of jets of hydrogen and other gaseous fuels. H. Seifert and H. Giesbrecht from BASF \cite{1} have studied the pressure waves immediately following the ignition of hydrogen, propane and methane jets resulting from subsonic outflows, and proposed a model to describe the overpressure as a function of fuel properties. Specifically, they performed experimental studies of hydrogen jets with outflow velocities of 140, 190 and 250 m/sec from a 10 mm diameter outlet and observed a maximum overpressure of 80 Pascals at a distance of 2 meters from the ignition point. They proposed a model which predicts a peak overpressure of 3 mbars at a distance of 10 meters resulting from the ignition of a 100 m/sec hydrogen outflow from a 100 mm outlet. V.G Gundelach also studied the overpressure resulting from the ignition of propane jets and observed overpressures of 50 mbars for a 80 mm diameter outlet \cite{2}. Very recently, Takeno et al have performed experimental measurements of the overpressure resulting from the ignition of hydrogen releases from 400 bar reservoirs through a 10 mm nozzle \cite{3}. The objective of this work is to simulate the release of hydrogen through a 6 mm PRD as a function of time from a 700 bars reservoir, and to perform a qualitative estimate of the risks associated with the ignition of a jet of hydrogen.

Methodology

The simulations were performed into two steps: simulation of the gaseous release and ignition of the release and overpressure calculation. The release was simulated using the finite volume solver Fluent. Ignition of the release and overpressure calculations were performed using Autoreagas from Century Dynamics/TNO based on the release cloud obtained from Fluent.

The time-dependent hydrogen density profile in air was obtained from CFD dispersion simulations performed by solving the steady-state Navier-Stokes equations in the presence of turbulence with the finite volume solver Fluent, using its standard coupled solver and first order discretization. The diffusion constant for hydrogen was set to 6.1×10^{-5} m\(^2\)/sec. Turbulence was modeled using the RNG k-\varepsilon model with the standard parameters. The choice of the modeling assumptions were validated using the data from subsonic hydrogen dispersion experiments of horizontal hydrogen jets from Michael Swain et al \cite{4}. To the best of our knowledge, validation data for sonic releases of hydrogen in air was not available. Overall agreement was obtained between simulations and experiments (typically 10\%, at worst 40\%) for a 20 cm horizontal jet.

The configuration considered in this paper is a horizontal jet from a high pressure cylinder. This reservoir is assumed to have a volume of 150 liters and a rated maximum storage pressure of 700 bars. Its size is 413 x
1534 mm (diameter and length respectively) and the internal dimensions are 372 x 1381 mm (diameter and length respectively). The reservoir has hemispherical extremities. The reservoir is set horizontally and located 500 mm above ground.

**Figure 1.** High pressure reservoir geometry used in the simulations.

The outflow is assumed to come from a pressure relief device (PRD) with a 6 mm diameter. The pressure relief device is located 100 mm from the symmetry axis and 100 mm from the tip end of the cylinder, perpendicular to the symmetry axis. The ambient temperature and pressure are respectively set to 293 K and 101.3 kPa. The Fluent release simulation was performed in a 27 m x 8 m x 8 m domain using an unstructured mesh with 1 079 876. Refinement of the grid was used during the simulation.

**Dispersion simulation results**

The time-dependent mass flow rate from the PRD device was calculated using a lumped parameter approach assuming an ideal gas law described in reference [6]. The mass flow rate as a function of time is given in Figure 2.

**Figure 2.** Mass flow rate as a function of time from a leak through a 6 mm nozzle from a 700 bars reservoir (obtained assuming an ideal gas equation of state).

Because ignition shortly after release is considered, the concentration profile at 0.082 seconds after initiation is used in the calculation. The overall shape of the flammable contour of hydrogen is shown in Figure 3.
Due to the large pressure difference, the flow is choked at the nozzle. The molar concentration profile 0.082 seconds after the release obtained from Fluent is shown in figure 4 below. At this stage of the expansion, the diffusion of hydrogen in air remains limited and its concentration remains fairly high throughout the cloud (Figure 5), in qualitative agreement with reference [3]. The extent of the flammable cloud is given in table 1 below.

**Figure 4.** Molar fraction of hydrogen (0.082 seconds after the release)

**Table 1.** Size of the flammable cloud 0.082 second after initiation of the leak as obtained using Fluent.

<table>
<thead>
<tr>
<th>Extent of the hydrogen cloud along the x axis (m) perpendicular to the jet at concentrations of</th>
<th>Extent of the hydrogen cloud along the y axis (m) perpendicular to the jet at concentrations of</th>
<th>Extent of the hydrogen cloud along the z axis (m) parallel to the jet at concentrations of</th>
</tr>
</thead>
<tbody>
<tr>
<td>2%</td>
<td>30%</td>
<td>70%</td>
</tr>
<tr>
<td>4.37</td>
<td>4.1</td>
<td>0.25</td>
</tr>
</tbody>
</table>
Figure 5. Molar concentration of hydrogen along the axis of the jet.

The velocity profile close to the nozzle is shown in Figure 6. The supersonic region, due to the rapid expansion of the chocked flow can be clearly seen, as well as a rapid transition to a very low velocity subsonic region immediately after the Mach disk. Figure 7 shows the velocity along the axis of the jet.

Figure 6. Absolute velocity (in m/sec) of hydrogen (0.082 seconds after the release) close to the nozzle.
The overall structure of the jet is very similar to that reported in reference [4] for a choked flow from a slightly larger (1 cm) diameter orifice and a 10 bar release using the k-omega model.

**Ignition and consequences**

Calculation of the consequences of ignition of the hydrogen release was performed using the commercial explosion modeling solver AutoReaGas. Because AutoReaGas does not perform dispersion calculations, the concentration profile obtained from Fluent was averaged over the coarser structured grid used in AutoReaGas and imported into the latter. The AutoReaGas mesh had 904,200 cells in a domain 85.5 m × 82.8 m × 41.8 m. Thus each cell in the mesh used in AutoReaGas has its own value of hydrogen mass fraction. This is a departure from typical uses of AutoReaGas, which is calibrated for methane, and relies on uniform mixtures of gaseous fuels and air in coarser mesh cells. A detailed calibration for hydrogen would be required: the results obtained here should be considered as estimates based on a conservative value of the hydrogen laminar flame velocity.

The concentration profile at the last time step of the dispersion simulation was averaged over the coarser grid used in AutoReaGas. The mixture was ignited by defining a burned region in the center of the flammable mixture 4 m after the PRD. The simulations were performed using the standard values of the model (3.5 m/sec and the standard values of the adjustable parameters for AutoReaGas) The standard value 3.5 m/sec corresponds to the maximum value of the flame velocity of hydrogen which occurs at high hydrogen concentrations in air (specifically ~42% by volume, which is close to the average molar concentration of the release within the flammable bounds). Note that the laminar flame velocity depends on the local...
concentration of hydrogen. In this case, early ignition was assumed which lead to a dense cloud with slowly decreasing molar fraction as discussed below.

To study the possible consequences of accidental ignition the hydrogen jet was ignited shortly after release. At this stage of the simulation the cloud could not be ignited when the velocity field was taken into account using a custom version of AutoReaGas that could import the velocity field. Because the blow-out velocity of hydrogen is quite high, ignition is still expected to occur and the standard version of AutoReaGas was used (which neglects the velocity field) to obtain typical estimates of the overpressure. Note that it was observed when validating the approach with subsonic releases (Reference [6]), that taking into account the velocity field tends to lead to larger values of the overpressure. Using the standard parameters of AutoReaGas (3.5 m/sec for hydrogen), the overpressure obtained is shown in figure 8. The time dependence of the maximum overpressure recorded (close to the ignition point) is shown in figure 9. The maximum overpressure obtained is 23 kPa, which is smaller than in reference [3], who observed a maximum overpressure of 100 KPa from igniting mixtures from a 400 bar reservoir through a 10 mm nozzle. The smaller value is not a surprise because the cloud is ignited earlier in this case and the effects of the velocity field is neglected. Figure 10 shows the time dependence of the maximum overpressure observed, whereas Figure 11 shows the directionality of the overpressure 25 milliseconds after ignition.

Figure 9. Maximum overpressure peak as a function of distance from the PRD, as obtained from AutoReaGas.

Figure 10. Maximum overpressure as a function of time at 2.5 meters from the PRD along the jet.
Conclusions

We have presented results from a finite volume simulation of a time dependent chocked horizontal release through a 6 mm PRD of a 700 bar storage unit. The properties of the release (concentration profile, velocity field) have been discussed shortly after initiation of the release. Despite the wide difference in length scales, the basic structure of the chocked flow close to the nozzle has been obtained. Critical constant concentration profiles have been obtained early in the transient regime. The consequences of ignition shortly after initiation of the release have been estimated using AutoReaGas. A maximum overpressure of 0.23 bars was obtained 2.5 meters from the PRD.

Acknowledgements

We gratefully acknowledge the support of the Auto 21 Network of Centres of Excellence and of Air Liquide. We wish to thank Ed Draper from Century Dynamics who provided invaluable support to adapt AutoReaGas to the specifics of this project.

References