SIMULATIONS OF HYDROGEN RELEASES FROM A STORAGE TANKS: DISPERSION AND CONSEQUENCES OF IGNITION

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ABSTRACT

We present results from hydrogen dispersion simulations from a pressurized reservoir at constant flow rate, in the presence and absence of a wall. The dispersion simulations are performed using a commercial finite volume solver. Validation of the approach is discussed. Constant concentration envelopes corresponding to the 2%, 4% and 15% hydrogen concentration in air are calculated for a subcritical vertical jet and for an equivalent subcritical horizontal jet from a high pressure reservoir. The consequences of ignition and the resulting overpressure are calculated for subcritical horizontal and vertical hydrogen jets and in the latter case, compared to available experimental data.

1.0 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. On the other hand, there have been comparatively fewer detailed investigations of the overpressure associated with the ignition of jets of hydrogen and other gaseous fuels. H. Seifert and H. Giesbrecht from BASF [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 [2]. The ultimate objective of this work is to eventually estimate the risks associated with the overpressure generated through numerical simulations of a jet of hydrogen from a high pressure reservoir (700 bars). We limit the scope of the present paper to simulations of constant subcritical outflow, for which experimental results are available, in order to validate the approach.

2.0 METHODOLOGY

The simulations were divided into two stages: simulation of the gaseous release and ignition of the release and overpressure calculation. The first stage was calculated using a commercial CFD solver. Ignition of the release and the overpressure calculation was performed using Autoreagas from Century Dynamics/TNO from the resulting calculated hydrogen release. Note that for a continuous release, we assume that the flame velocity close to the point of ignition in the hydrogen cloud is larger than the local velocity of the gases and that the overpressure wave velocity is larger than the outflow velocity at the nozzle. The 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 using the commercial finite volume solver FLUENT. The diffusion constant for hydrogen was set to $6.1\times10^{-}$

$^{5}m^2$/sec. Turbulence was modeled using the RNG k-ε model with the standard parameters. The choice of the modeling assumptions were validated using the data from hydrogen dispersion experiments of horizontal hydrogen jets from Michael Swain et al [3]. Overall agreement within 40% was obtained between simulations and experiments (typically 10%) for a 20 cm horizontal jet (Table 1, Fig. 1).

Table 1. Comparison of the experimental and simulation results at 45 seconds for the horizontal hydrogen jet.

Sensor position	Experimental H2 concentration (%)	Simulation H2 concentration (%)	Deviation(%) (*)
1	5.0-5.9	5.04	-8.13
2	5.6-7.0	6.96	10.48
3	9.4-10.8	13.99	38.50
4	8.1-9.4	8.25	-5.70
5	5.6-6.6	5.29	-13
6	3.5-4.6	5.37	32.60

(*) The deviation is computed using the average experimental value.

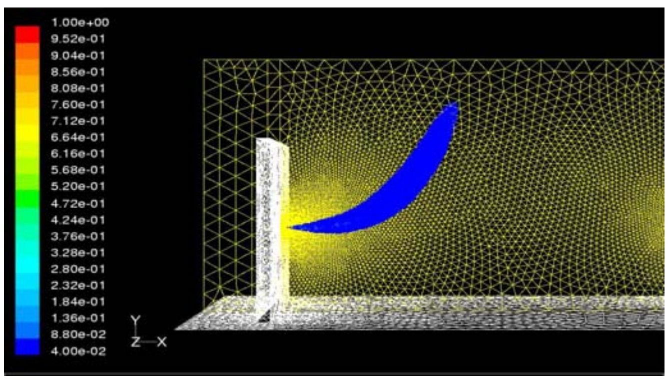

Figure 1. Simulation results 30 seconds after the leak began for the horizontal hydrogen jet. The mesh in the symmetry plane is also shown.

Once the outflow of hydrogen was calculated, the resulting steady-state velocity and concentration profile was exported for use in the gas explosion modeling solver Autoreagas. The laminar combustion model is based on a one step irreversible reaction using a laminar reaction rate calculated from the ratio of the burning velocity produced, during one cycle, and the burning velocity specified. The same one step irreversible reaction using a turbulent reaction rate calculated from the Bray turbulent flame velocity described in more details in reference [4] is used for the turbulent combustion. Transition of laminar to turbulent flame propagation is allowed in locations where the turbulent burning corresponding with local turbulence properties exceeds the laminar burning [4]. Turbulence is modeled using the standard k-epsilon approach.

$$S_t = 1.8 u'^{0.412} L_t^{0.196} S_L^{0.784} \nu^{-0.196}, \tag{1}$$

where S_t is the turbulent burning speed, m/s; u' is the turbulence intensity; L_t is the turbulence characteristic length scale (integral scale); S_L is the laminar burning velocity flammable mixture, m/s and v, the kinematic viscosity of the flammable mixture.

$$R_c = -C_t \rho \frac{S_t}{\delta} \mathrm{Min}\left(m_{fuel}, \frac{M_{O_2}}{s}, \frac{M_{Product}}{1+s} \right), \tag{2}$$

where R_c is the combustion rate; C_t is a modelling constant; ρ is the local density of the flow field; m_{fuel} is the fuel mass fraction; m_{O2} is the mass fraction of oxygen; $m_{Product}$ is the mass fraction of the products of the reaction and finally s is the stoichiometric ratio. Here δ is the thickness of the combustion front:

$$\delta = \frac{D_{fuel}}{S_t}, \tag{3}$$

where D_{fuel} is the turbulent diffusion coefficient. The thickness of the combustion front is modelled to take into account numerical diffusion when the thickness of the combustion zone is smaller than the cells of the mesh [4].

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) as well as using the laminar burning velocity of hydrogen as an adjustable parameter. 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), and is not representative of the average concentration of the hydrogen within the flammable mixtures considered here.

The blast solver of Autoreagas based on the multi-dimensional Euler equations was used in certain cases to calculate the far field overpressures waves. It was only used when the combustion solver was unable to give results at long range due to faster combustion rate.

Calculation of the consequences of ignition of the hydrogen release was performed using a version of Autoreagas customized for this project, which takes into account the initial velocity distribution of the release. The concentration and velocity profiles obtained from Fluent were averaged over the coarser grid used in Autoreagas and imported into the latter. 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.

The ignitions of both the horizontal and vertical jets were done 0.5 m away from the pressure relief device (PRD) at the center of the cloud region. The timing of the ignition was not important in the studied cases since we were considering steady-state clouds.

3.0 RESULTS

The approach was tested by simulating a vertical jet from a 10 mm diameter pipe with the following outflow velocities: 140, 190 and 250 m/sec, experimentally studied in [1]. The jet was simulated using Fluent. The size of the domain used in the simulations was 5 by 5 by 11 meters. The PRD was 1 m above the ground. An unstructured mesh with 205,263 cells and a symmetry plane at y=2.5 meters was used. The size of the simulated flammable cloud is given in Table 2 below.

Table 2. Size of the simulated flammable cloud for a vertical jet as a function of flow velocity.

Flow velocity (m/s)	Extension of the hydrogen cloud along the x axis (m) perpendicular to the jet at concentrations of			Extension of the hydrogen cloud along the y axis (m) perpendicular to the jet at concentrations of			Extension of the hydrogen cloud along the z axis (m) parallel to the jet at concentrations of		
	2%	4%	15%	2%	4%	15%	2%	4%	15%
140	0.52	0.36	0.12	0.50	0.33	0.11	5.88	4.15	1.04
190	0.58	0.39	0.12	0.58	0.36	0.11	6.27	4.63	1.11
250	0.60	0.41	0.12	0.60	0.36	0.12	6.82	4.89	1.16

The velocity field and the concentration profile were averaged over the grid used in AutoReaGas and then imported. The mixture was ignited by defining a burned region in the center of the flammable mixture. The resulting overpressure for the lowest and largest flow velocities are given in Table 3 below for three distances and two hydrogen laminar burning velocity values. As discussed above, the first velocity considered is the maximum value 3.5 m/s (at 42% H_2 in air by volume), which corresponds to the default value of the laminar burning velocity in Autoreagas. This value leads to larger values of the overpressure as shown in Table 3. To obtain agreement with the experimental data, the value of the laminar flame velocity must be lowered as shown in Table 3. The adjusted values obtained would be representative of the laminar burning velocity in the hydrogen cloud. The other parameters were not changed from their default values. A sensitivity analysis of their effects on the overpressure showed that they had much less influence than the laminar velocity.

A comparison with the data from reference [1] in Table 4 shows that the calculated overpressures at 2, 5 and 10 meters are overestimated if the default parameters are used in Autoreagas.

Table 3. Simulated overpressure as a function of distance and laminar burning velocity for a vertical hydrogen jet.

Flow velocity (m/s)	Laminar burning velocity (m/s)	Overpressure at 2 m (Pascal)	Overpressure at 5 m (Pascal)	Overpressure at 10 m (Pascal)
140	3.50	236.7	140.9	50.2
	1.00	57.3	25.8	12.9
190	3.50	418.1	202.8	66.9
	1.15	64.3	31.6	15.6
250	3.50	429.7	214.1	70.0
	1.35	87.6	40.2	19.1

Table 4. Experimental Overpressure as a function of distance for a vertical hydrogen jet.

Flow velocity (m/s)	Overpressure at 2 m (Pascal)	Overpressure at 5 m (Pascal)	Overpressure at 10 m (Pascal)
140	57 ± 22	19 ± 8	12 ± 4
190	61 ± 22	25 ± 7	16 ± 4
250	75 ± 25	35 ± 10	22 ± 6

The rise time is essentially constant and equal to 0.01 sec for the 250 m/sec outflow. It was about three times larger than the value observed experimentally in reference [1] when the burning velocity was taken as an adjustable parameter. A similar value was found for the 140 m/sec outflow. When the flame velocity was set to 3.5 m/sec, the rise time was about twice as large as the values obtained experimentally in reference [1].

Simulations of horizontal jets due to a leak through a 6 mm PRD device were also performed on a high pressure storage cylinder, corresponding to the outflow velocities used in the validation runs discussed above. There are not as of yet any experimental data pertaining to those simulations. The size of the simulation domain was 8 by 8 by 8 meters. The PRD was 0.5 m above the ground. An unstructured mesh with 279,026 cells was used. The extent of the cloud for the two outflow velocities discussed previously are given below. Fig. 2 show the 2%, 4% and 15% molar fraction contours of hydrogen in air obtained for an outflow velocity of 250 m/sec. Fig. 3 shows by comparison the same contours obtained form a critical sonic outflow from the same cylinder in the presence and absence of an obstacle.

Table 5. Size of the simulated flammable cloud for a horizontal jet as a function of flow velocity.

Flow velocity (m/s)	Extension of the hydrogen cloud along the x axis (m) parallel to the jet at concentrations of			Extension of the hydrogen cloud along the y axis (m) perpendicular to the jet at concentrations of			Extension of the hydrogen cloud along the z axis (m) perpendicular to the jet at concentrations of		
	2%	4%	15%	2%	4%	15%	2%	4%	15%
140	1.74	1.35	0.24	0.62	0.37	0.10	1.91	0.82	0.07
190	2.03	1.55	0.27	0.49	0.29	0.09	2.05	0.78	0.06
250	2.35	1.77	0.27	0.79	0.39	0.09	2.11	0.80	0.07

Table 6 shows the size of the incident overpressure peak as a function of distance for the horizontal jets. For comparison purposes, the simulations were performed using two values of the burning velocity: a conservative value of 3.5 m/sec and the values obtained from the parametric study of the vertical jets discussed above. Note that that the different shapes of the releases for the horizontal and vertical jets may lead to different values of the laminar burning velocity that should be used for horizontal jets.   Both set of simulations show a substantially smaller value of the overpressure for the horizontal jets.

Table 6. Amplitude of the incident overpressure peak as a function of distance for a horizontal hydrogen jet as obtained from Autoreagas.

Flow velocity (m/s)	Laminar burning velocity (m/s)	Overpressure at 2 m (Pascal)	Overpressure at 5 m (Pascal)	Overpressure at 10 m (Pascal)
140	3.50	72.0*	26.5*	9.0*
	1.00	13.5	4.8	1.9
190	3.50	118.4*	44.62*	14.4*
	1.15	25.4	9.71	3.9
250	3.50	138.0*	52.0*	16.3*
	1.35	35.1	13.8	6.1

*Reflected peaks were larger

Secondary peaks of higher amplitude from a reflected wave were observed in the three cases where the laminar burning velocity used was 3.5 m/s. These peaks came from reflections off the floor and other obstacles. At 2 m for a velocity of 140 m/s, 190 m/s and 250 m/s secondary peaks of 188 Pa, 211.4 and 155 Pa were observed respectively.

A three dimensional representation of the overpressure as a function of distance caused by the ignition of the flammable cloud from a 250 m/sec outflow from a 6mm PRD device of a cylinder using a laminar burning velocity of 3.5 m/s is shown in Fig. 4, 0.036 seconds after ignition. The clear gray patterns show overpressures with stronger magnitude than darker patterns as displayed in the scale shown on the right side of the figure.

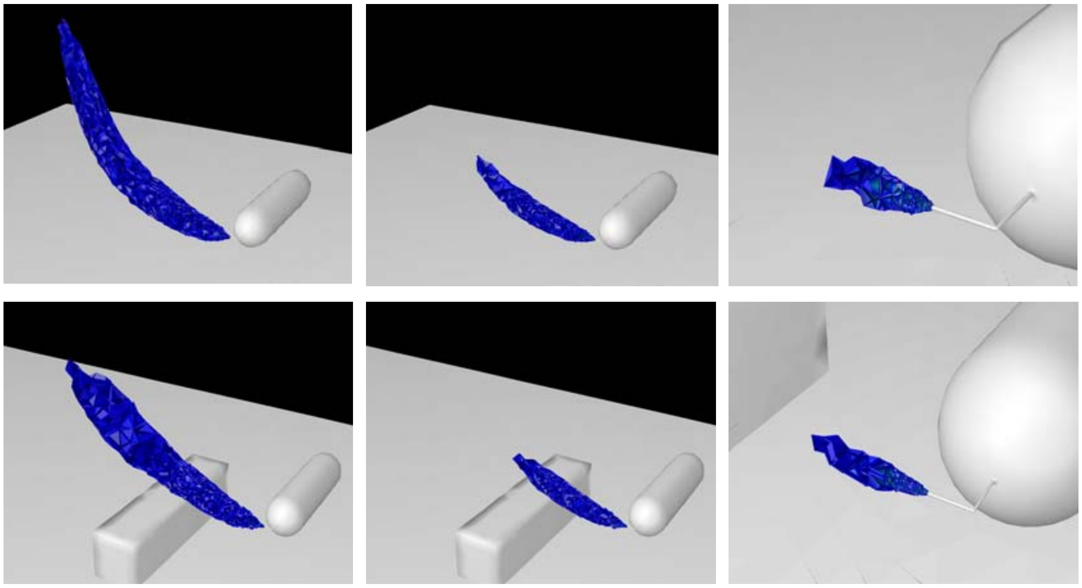

Figure 2. Molar fraction contours arising from a 250 m/sec leak from the pressure relief device of a pressurized cylinder in the absence (top) and presence (bottom) of a wall. From left to right, the molar fractions are 2%, 4% and 15%.

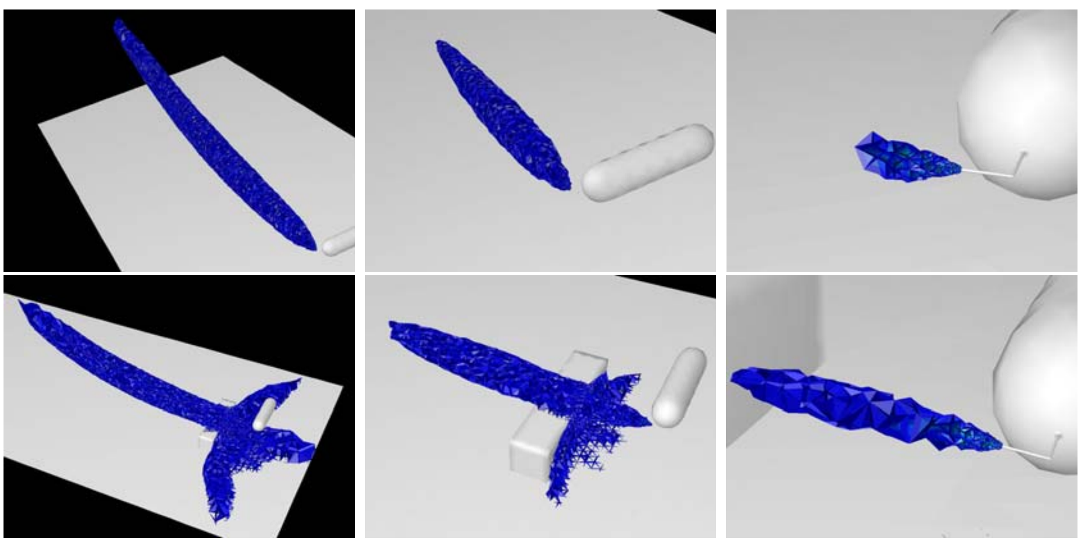

Figure 3. Molar fraction contours arising from a critical flow from a cylinder in the absence (top) and presence (bottom) of a wall. From left to right, the molar fractions are 2%, 4% and 15%.

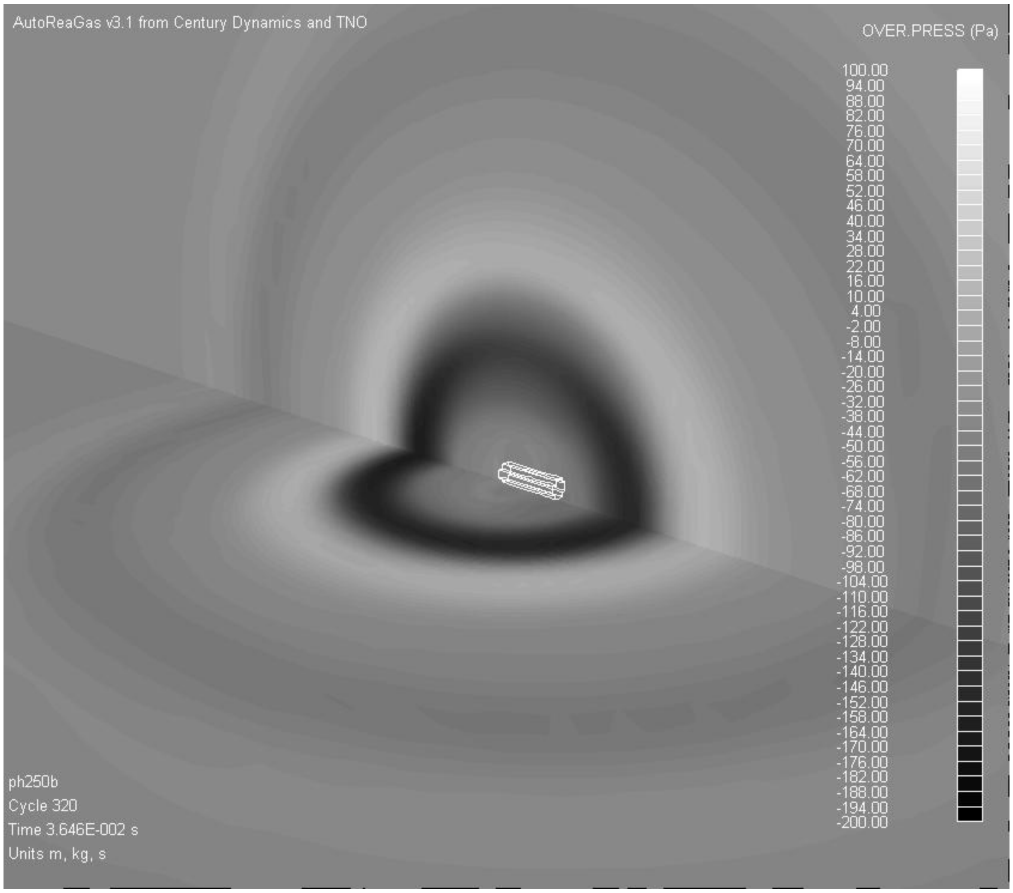

Figure 4. Overpressure generated by the ignition of the flammable cloud from a 250 m/sec outflow from a 6mm PRD device of a cylinder as a function of distance.

4.0 CONCLUSIONS

We presented simulations of the overpressure resulting from the ignition of a hydrogen jet. Validation runs were performed to compare the overpressures obtained from Autoreagas with available experimental data from subsonic vertical jets reference [1]. For vertical jets, the use of the standard values in Autoreagas (burning velocity=3.5 m/sec) leads to larger overpressure peaks than experimentally observed by a factor of 4 to 8. Good agreement with the available experimental data from jets could be obtained by adjusting the burning velocity to lower values. Note that an important effect of the mesh was also observed in our simulations. Meshes effects occur when the concentration profile is imported into the coarser mesh used in Autoreagas through averaging, or when the mesh that covers an area that at least encompasses the burned zone is not detailed enough. A thorough analysis of mesh effects in this problem is critical. For small exit diameters (below the limiting blow out diameter, 45 mm for methane according to reference [1]) the possibility of a blowout of the flame should be considered. Note also that the initial outflow through a 6 mm diameter pressure relief device from a high pressure hydrogen reservoir is sonic (an estimate of the isentropic flowrate shows that it can be higher than 1 kg/sec for a 700 bar cylinder). The validity of the approach described here is limited to situations where the flow has become subcritical. In the case of a 700 bars reservoir, this would correspond to an ignition delay of the order of 5 seconds after the beginning of the outflow for an isentropic flow when calculated using the equations for gas outflow through holes reported in reference [5]. The next stage of this project is to estimate the size and concentration profile from the release through a PRD of a fully filled hydrogen tank, as well as the overpressure resulting from its ignition.

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REFERENCES

1. Seifert H. and H. Giesbrecht, Safer design of inflammable gas vents, Loss prevention and safety promotion in the process industries: 5th International symposium of the European Federation of Chemical Engineering, 1986.
2. Gundelach, V.G., Fortschritte der Sicherteknik II: Berichte aus der Arbeit der Dechema-Fachhausschusse im Jahre 1987, Dechema-Monographien, No 11, 1987.
3. Swain, M., Codes and standards analysis, 2004 annual program review meeting of the hydrogen, fuel cells & infrastructure program of the US Department of Energy, 2004.
4. AutoReaGas version 3.1 Theory Manual, Century Dynamics & TNO, 2002.
5. Yellow Book: Methods for the calculation of physical effects, CPR 14E, Third Edition 1997.