

# WORST CASE SCENARIO FOR DELAYED EXPLOSION OF HYDROGEN JETS AT A HIGH PRESSURE: IGNITION POSITION

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## ABSTRACT

Delayed explosion of free field hydrogen releases at a high pressure is subject of multiple investigation performed by various authors in the past years. These studies considered various parameters such as pressures, flow rates etc., and their influence on the resulting overpressure. However, the influence of the ignition position on the maximum overpressure was not fully explored. Current investigation addressed by computational fluid dynamics (CFD) simulations and experimental measurement fills this gap. This work demonstrates that the ignition positions corresponding to 55%-65% of H<sub>2</sub>/air mixture give the maximum overpressure. This observation initially observed numerically and afterwards confirmed experimentally. A simple model is also suggested.

*High pressure releases, delayed explosion, experiments, numerical simulations, overpressure, worst case scenario, dispersion*

## 1.0 INTRODUCTION

Multiple recent works of Miller et al. [1], Daubech et al. [2], Jallais et al. [3] etc demonstrated a high importance of delayed explosions of high pressure H<sub>2</sub> release for risk assessment at production plants, filling centres, transportation pipelines, charging stations of FCEV etc.

The turbulence in the jets (especially having high momentum or high release pressure) strongly accelerate the flame, which can lead to higher overpressures due to vapour cloud explosion (VCE), see Jallais et al. [3].

Delayed explosion of high-pressure hydrogen jets was investigated experimentally by: Miller et al. [1], Daubech et al. [2], Grune et al. [4], Willoughby and Royle [5], Takeno et al. [6] and Chaineaux [7], numerically using computational fluid dynamics (CFD) approaches [2, 3, 8, 9, 10, 11]. An engineering model which uses the application of TNO Multi-Energy method for blast propagations was presented by see Vyazmina et al. [8] and Jallais et al. [3, 9].

Previous investigations of Daubech et al. [2], Vyazmina et al. [8], Jallais et al. [3] using a CFD code FLACS code [12, 13] demonstrated the CFD is able to correctly model high-pressure H<sub>2</sub> jet explosions. The comparison of simulations with the experimental measurements demonstrated a good match for the overpressure magnitude with the measurements [1, 2, 3, 8].

The objective of the current investigation is to predict the worst-case position of the ignition (the position that gives the highest overpressure) and to suggest an engineering assessment methodology for such cases.

This investigation is based on the results from CFD simulations and it has been confirmed by experimental measurements.

## 2.0 OVERPRESSURE VERSUS IGNITION POSITION

This work follows the investigations of the  $H_2$  release of 36bars (0.26kg/s) through the orifice of 12mm at the height of 1.5m above the ground, see Daubech et al. [2], Vyazmina et al. [8], Jallais et al. [3]. Simulations for this reference case with the ignition at 30% of  $H_2$ /air (Daubech et al. [2], Vyazmina et al. [8], Jallais et al. [3]) and Miller et al. [1] experiments (release of 1kg/s and 8kg/s) validated the basis for CFD modelling approach for the further analysis. The exact physical and numerical parameter values used in these simulations are given in reference Daubech et al. [2], Vyazmina et al. [8], Jallais et al. [3].

In the current work, a parametric study has been performed to identify the worst-case ignition position, which corresponds to the maximum overpressure. This parametric study has been done using software FLACS. The position of the ignition has been moved along the centreline (between 10% and 75% vol.  $H_2$ /air); the ignition location off the centreline are not considered in the current study. As shown on Figure 1, the overpressure is monitored along the centreline and at locations L2 (2m downstream of the ignition position).

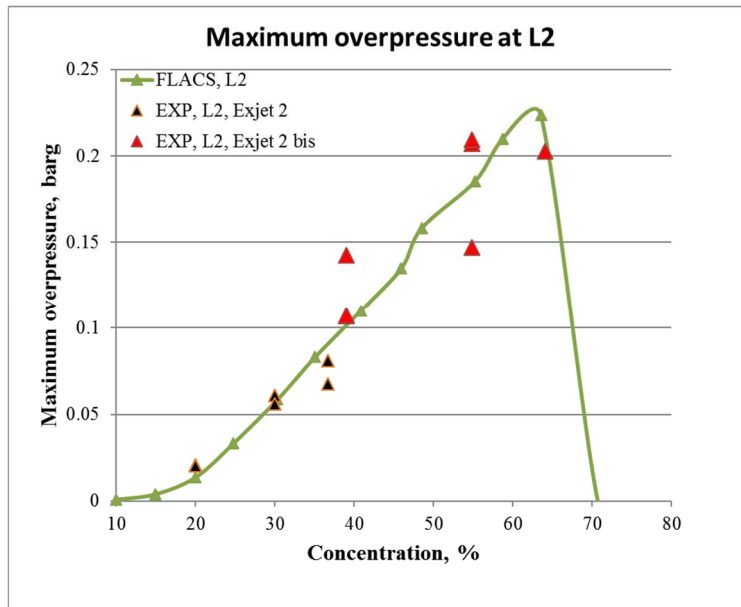


Figure 1: Parametric study: the maximum overpressure versus the ignition position corresponding to different concentrations. Green line with triangles corresponds to FLACS CFD results, black triangles represent the experiments of Daubech and al. [3] (release at 1.5m height above the ground), red triangles shows the results of the current work (the release is at 1m height above the ground).

The ignition located in the lean region of the cloud leads to very low overpressures. As one can see, simulations are in good agreement with experiment for ignition at 20%, 30% and 40%. Simulations have predicted that the worst ignition is not in the most reactive region of the cloud (30-40%  $H_2$ ). The maximum overpressure has been obtained for ignition at 65%  $H_2$ .

Based on the simulation prediction, the second experimental campaign has been performed to validate this conclusion (red triangles on fig 1). Experimental measurements have demonstrated the similar trend, which gives the maximum overpressure for the ignition position corresponding to the 55-65%  $H_2$  not for 30%-35% !

Parametric study to define the worst-case scenario has been also performed for releases with mass flow from 1 kg/s up to 8 kg, see figure 2. According to simulations, in all cases the maximum overpressure corresponds to the ignition at concentration in the range 55-65% H<sub>2</sub>.

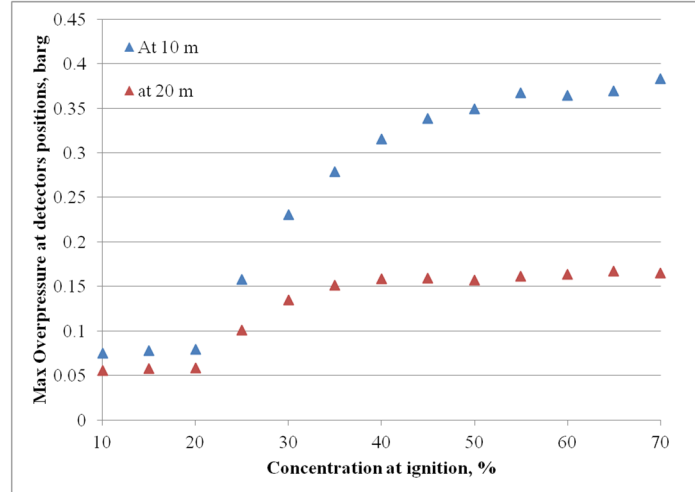


Figure 2: Parametric study: the maximum overpressure versus the ignition position corresponding to different concentrations for the release of 8kg/s. Overpressure is measured at 10m and 20m perpendicular to the jet axis, 23m downstream of the release point, 2m and 3m from the ground respectively.

This behavior can be explained by a simple phenomenological model, which assumes that:

- flame propagates with the same velocity in all 3 directions, hence its shape is an inserted sphere;
- the overpressure is proportional to the average flame velocity propagation in the sphere;
- the average flame velocity is proportional to the average concentration in the inserted sphere.

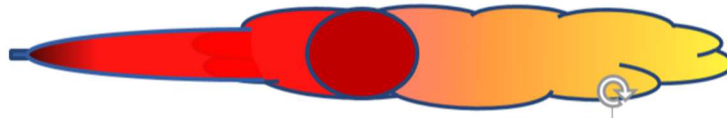


Figure 3: Scheme of the flame propagation in a high-pressure H<sub>2</sub> jet: red circle corresponds to the spherical flame.

Concentration decay in the radial and axial directions can be written in the following form:

$$C(x, r) = C(x, 0) \exp \left[ -\frac{K r^2}{(x - x_0)^2} \right],$$

$$\frac{C(x, 0)}{C_j} = \frac{K_0 D_{fic}}{x - x_0}$$

where  $C(x,0)$  in the concentration along the centreline in the downstream direction  $x$ ,  $x_0$ - the position of the fictive source,  $D_{fic}$  is the diameter of the fictive source and  $K_0$  and  $K$  are constants,  $C_j$  is the concentration at the release position.

Since for  $H_2$  LFL is 4% (and explosion limit is 10%) it is necessary to take into account the concentration down to 4% or 10%:

$$C(x, R) = C(x, 0) \exp \left[ -\frac{KR^2}{(x - x_0)^2} \right] = A.$$

Here  $A$  is the concentration of interest (4% or 10%), hence the radii corresponding to  $A$  can be found as

$$R = (x - x_0) \left[ \frac{1}{K} \ln \left( \frac{C(x, 0)}{A} \right) \right]^{0.5}$$

For each  $x$  it can find an integral of  $C(x,r)$  of the inserted sphere (the sphere is indicated at fig 3), the integral of the concentration in the inserted sphere is

$$C_{total} = \pi \frac{C_j}{K} D_{fic} (x - x_0) \left[ 1 - \frac{A(x - x_0)}{C_j K_0 D_{fic}} \right]$$

Hence the average concentration in this sphere is

$$C_{av} = \frac{C_{total}}{Vol} = \frac{\frac{3}{2} C_1^3 \left( \frac{1}{C_1} - \frac{A}{C_1^2} \right)}{\ln \frac{C_1}{A}}, \quad \text{where } C_1 = C_j K_0 \frac{D_{fic}}{x_1 - x_0}.$$

The average concentration in the inserted sphere (see fig 3)  $C_{av}$  vs  $C(x,0)$  is shown on fig 4.

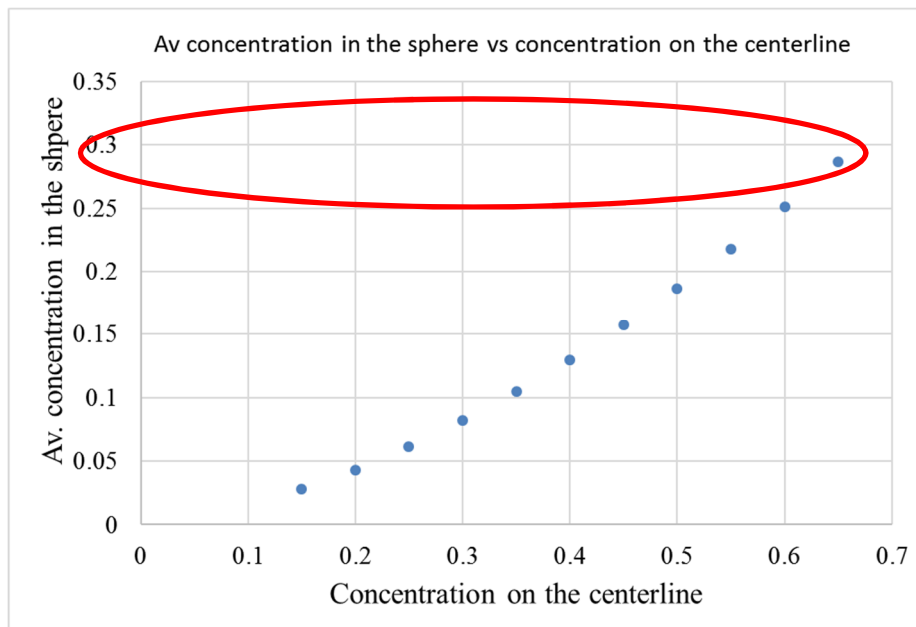


Figure 4: The average concentration versus the concentration on the centerline (ignition position) for the limit corresponding to 10% vol.  $H_2$  in air.

In this case, the average concentration approaches 30%, when the concentration on the centerline is close to 65% H<sub>2</sub>/air. Since, the maximum flame velocity corresponds to 30%, the maximum flame velocity will be observed at for the ignition located at 65% vol H<sub>2</sub> on the centerline. Therefore, the maximum overpressure is obtained at the ignition at 65%. This result is similar to the CFD and experimental observations (see fig 1).

Jallais et al. [9] states that the worst case scenario corresponding to 65% vol H<sub>2</sub> can be explained by the “high turbulence of the jet which increases the flame velocity before reaching the most reactive region”. Since the turbulence intensity is proportional to the velocity (see Daubech et al.[2]), this adds an additional flame acceleration to the flame. That means that at 65% the average concentration corresponds to the most reactive region with a high turbulence. These both reasons causes the worst case corresponding to 65% vol H<sub>2</sub>.

For calculations of the explosive mass, it is recommended to use the mass of hydrogen between 10% and 75% vol. in air

### 3.0 TNO MULTI ENERGY STRENGTH INDEX FOR FREE JETS

Using this the conclusion from the previous section that the worst-case scenario corresponds to the ignition at 65% vol. H<sub>2</sub>. The engineering approach suggested by Daubech et al. [2] can be extended.

In previous investigations, Dorofeev et al. [14] showed that for hydrogen the threshold concentration of 11%vol splits the slow flame propagation mixtures from the fast ones. Daubech et al [3] confirmed this experimentally: no flame propagation in jets for concentration lower than 10% of hydrogen. Hence, in the current engineering model the mass of hydrogen, which undergoes a fast deflagration, is limited by 10% and 75% vol. H<sub>2</sub>. Using different experiments and CFD results, the strength index for the multi-energy is defined. Daubech et al. [2] defined it for the ignition position corresponding to 30%, see figure 5.

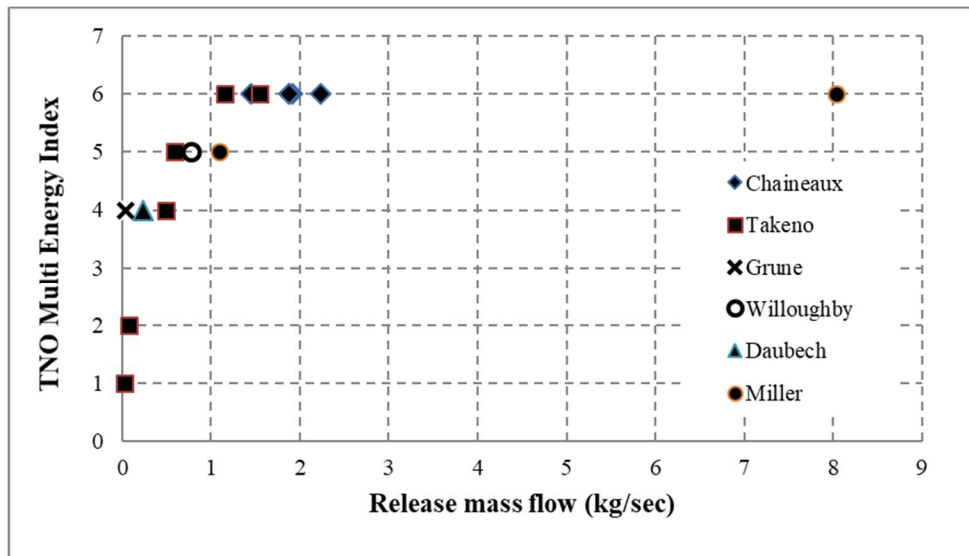


Figure 5: TNO multi energy strength index versus the mass flow rate for ignition located at 30% vol. H<sub>2</sub>/air.

It is recommended to use for 30% vol. H<sub>2</sub>/air ignition position

- index of 4 for H<sub>2</sub> releases with the mass flow < 0.5 kg/s, flame velocity of 100m/s, max overpressure <100mbars;

- index of 5 for H<sub>2</sub> releases with 0.5kg/s < mass flow < 1 kg/s, flame velocity of 140m/s, 100mbar < max overpressure < 200mbar;
- index of 6 for H<sub>2</sub> releases with 1kg/s < mass flow < 10 kg/s, flame velocity of 240m/s, 200mbar < max overpressure < 200mbar.

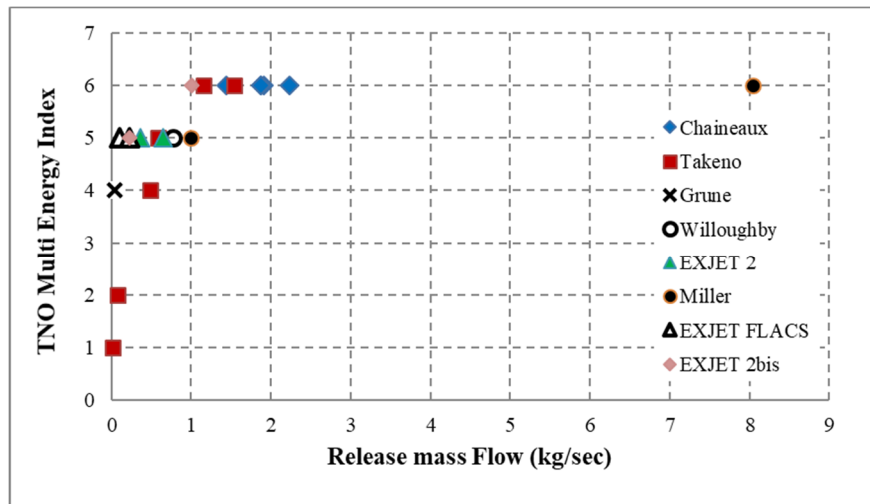
These correlations are valid only for high-pressure free field releases (no impact of the ground, no obstacles) of H<sub>2</sub> from 10 up to 400 bars. The correlation cannot be applied to cases, where the interaction with the ground takes place.

Similar analysis can be extended to the ignition position corresponding to at 55%-65% of H<sub>2</sub>. Fig. 6 shows the dependence of the TNO multi energy index on the mass flow rate for the ignition located at 55% -65%.

It is recommended to use for 55%-65% H<sub>2</sub>/air ignition position

- index of 4 for H<sub>2</sub> releases with the mass flow < 0.1 kg/s, flame velocity of 100m/s, max overpressure < 100mbar;
- index of 5 for H<sub>2</sub> releases with 0.1kg/s < mass flow < 1 kg/s, flame velocity of 140m/s, 100mbar < max overpressure < 200mbar;
- index of 6 for H<sub>2</sub> releases with 1kg/s < mass flow < 10 kg/s, , flame velocity of 240m/s, 200mbar < max overpressure < 200mbar.

The major difference of the TNO index concerning the ignition position is observed for releases with the mass flow rate lower than 0.5kg/s.



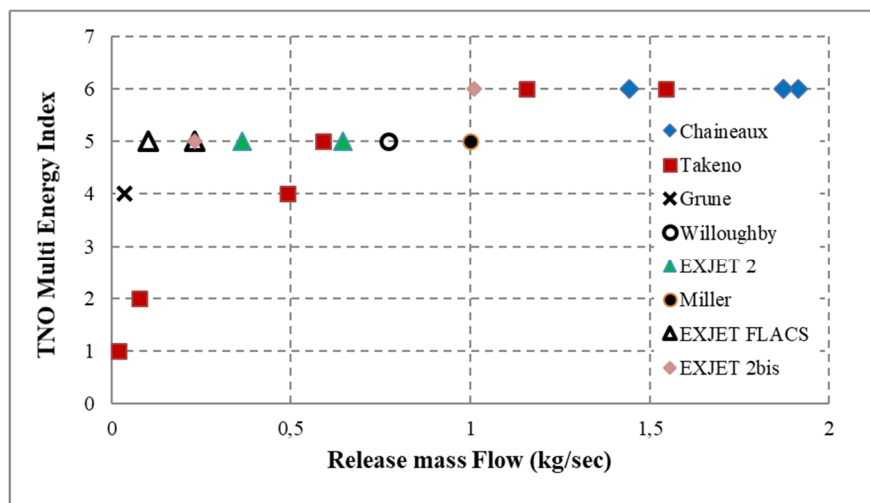


Figure 6: TNO multi energy strength index versus the mass flow rate for ignition at 55% - 65%: top frame - mass flow rates up to 8kg/s, bottom frame - close-up on mass flow rate up to 2kg/s.

It is recommended to use the worst case (55%-65%vol H<sub>2</sub>/air) ignition scenario for risk assessment, since à priori the location of the ignition source is unknown.

#### 4.0 CONCLUSION

Simulation and experimental investigation demonstrated the ignition position corresponding to 55-65% vol. H<sub>2</sub>/air at the centreline of free jets gives the more conservative results in terms of the maximum overpressure. The suggested simple analytical model also confirms the same trend.

TNO multi energy index is updated and extended for the ignition position located at 55% -65%:

- index of 4 for H<sub>2</sub> releases with the mass flow < 0.1 kg/s, flame velocity of 100m/s, max overpressure <100mbar;
- index of 5 for H<sub>2</sub> releases with 0.1kg/s< mass flow< 1 kg/s, flame velocity of 140m/s, 100mbar< max overpressure<200mbar;
- index of 6 for H<sub>2</sub> releases with 1kg/s< mass flow< 10 kg/s, , flame velocity of 240m/s, 200mbar< max overpressure<200mbar.

Since à priori the location of the ignition source is unknown, for risk assessment studies it is recommended to use the worst case (55%-65%vol H<sub>2</sub>/air) ignition scenario.

#### 5.0 REFERENCE

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