Phenomenological Modelling of External Cloud Formation in Vented Explosions

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Abstract

Venting is a common method to mitigate damage caused by explosions in low strength buildings and industrial enclosures. External explosion caused by combustion of external cloud (formed by vented gases) plays a crucial role in internal pressure rise. However, there appears to be no modelling effort for external cloud formation in the existing literature. This paper presents a phenomenological model for the formation of the external cloud in vented explosions. This model employs experimental observation of flame propagation to formulate a correlation for flame velocity and prediction of the time for the internal flame to reach the vent. The model considers the enclosure geometry and mixture reactivity to account for cloud formation. It utilizes the theory of vortex bubble formation, based on pervious theoretical and experimental investigations. Detailed description of the modelling process and major assumptions involved are presented. The model is then validated with the cloud formation data obtained from experimental work reported in literature for hydrogen and methane, in enclosure volumes ranging from 1 m^3 to 100 m^3, for cylindrical and cuboidal geometries. Further predictions are made for various experimental configurations used for vented hydrogen explosions. Variation of cloud dimensions with enclosure geometry and mixture reactivity is studied in detail. Inferences on dependence of cloud shape on various parameters are discussed and the observed trends are explained.

Keywords: *hydrogen explosion, methane explosion, external cloud, vortex dynamics, vented explosions, aspect ratio*

1. Introduction

Low strength buildings and industrial containers/enclosures dealing with storage of gaseous fuels (or volatile liquid fuels) can potentially be subjected to the explosions. To mitigate this risk, enclosures and buildings are generally equipped with vents to reduce the damage caused by accidental explosions. When explosion occurs, these vents open to reduce the peak pressure attained inside the building by expelling out unburnt gases. During the venting process, a large percentage of the flammable mixture is expelled out which forms an external cloud. Explosion resulting from the combustion of this external cloud is referred to as external explosion, which poses serious risk to equipment and personnel in the near vicinity of the vent. However, most investigations on vented explosions focused on the internal flame and processes inside the enclosure and less effort has been devoted to the external explosions.

The earliest experimental observation on external explosion was reported by Harrison and Eyre (1987), who captured high speed images of the external explosions. They observed that the resulting overpressure in external explosions increases with the flame velocity. They have also studied the effect of external explosion on internal peak pressures and vent area. Another study focussed on external explosions has been carried out by Catlin (1991), who studied the effect of turbulence, gas exit velocity and mixture reactivity on external explosions and provided some useful scaling suggestions. After these pioneering works on external explosions, this phenomena remained largely unexplored and only recently there have been some experimental studies focussed on external explosion and visualization of the external cloud formation (Proust and Leprette, 2004, 2009; Daubech et al., 2013, 2017). In these studies, the unburnt gas was seeded with micro-particles of ammonium chloride to make the cloud visible to facilitate observation of its evolution. They observed that under certain conditions, the external explosion was more significant than the internal explosion, and pose more severe hazards to nearby installations. However, the phenomenon of gas venting and external cloud formation has not been studied theoretically and no phenomenological or mathematical models are available for calculating cloud parameters. Calculation of these parameters are critical to compute the overpressure generated by external explosions and its effect on pressure generated inside the enclosure.

The present study aims to theoretically investigate the formation of the external cloud and formulate a phenomenological model to predict the cloud shape and size for various conditions. Accurate prediction of the external cloud size is the first step in the current effort to better capture the effect of the external explosion on the maximum internal overpressure.

2. Modelling Details

The gas venting process is considered as an impulsively started jet, with the external cloud considered as a vortex bubble formed from the vented volume of the jet. The flame front is assumed to work similar to a piston and push the unburnt gases out of the vent. The modelling of this process can be carried out in two steps. Firstly, the speed of the equivalent piston needs to be determined, which expels the unburnt gases from the vent. Then using the parameters of the piston stroke and fundamental results from vortex dynamics, the dimensions of the external cloud can be computed.

Firstly, for the equivalent piston, the speed at which this spherical flame front expands in an enclosure is determined. Previous experimental investigations (Bauwens et al., 2011, 2012) have shown that the propagation velocity of the flame in vented explosions is much higher than its laminar flame speed, as the expansion of the burnt gases also increases the flame propagation velocity. Moreover, in the case of hydrogen flames, the flame-front is further accelerated due to flame wrinkling caused by instabilities which tend to increase in the flame front area. Considering the complex nature of flame acceleration and growth, it is not feasible to derive a simple expression based solely on theoretical considerations. It is hence decided to use experiments of spherical flame propagation from realistic geometries. Bauwens et al. (2012) have presented a detailed experimental study of hydrogen –air flames, for various concentrations for their 63.5 m^3 enclosure. This is the only flame propagation data available for vented explosions in a realistic geometry, and has been used in other studies as a standard data-set (Li and Hao, 2017). Bauwens et al. (2011, 2012) showed that the flame propagation velocities of different fuels at different concentration collapse to a single curve, if the flame propagation velocity is normalized by the laminar flame speed, expansion ratio, and a factor to account for the Lewis number effects. As this hypothesis is based on the fundamental mechanism of spherical flame propagation, it should be applicable to all relevant geometries. Taking average of the normalized velocity at each location from their data and approximating the resultant curve by a linear curve fit, the following linear expression can be obtained and plotted in Figure 1:

$$\frac{U_f}{\sigma S_L\, \Xi_{Le}} = 2.84x + 0.25 \tag{1}$$

where U_f is the flame propagation velocity, σ is the expansion ratio, S_L is the laminar flame speed, x is the distance between the flame-front and the ignition point, and Ξ_{Le} is the factor for Lewis number, which was defined by Bauwens et al. (2012) as:

$$\Xi_{Le} = \frac{0.9}{Le}$$

where Le is the Lewis number for the mixture.

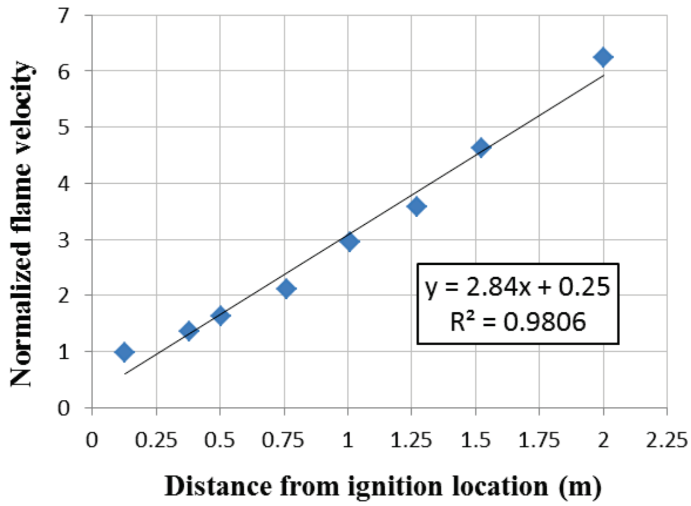


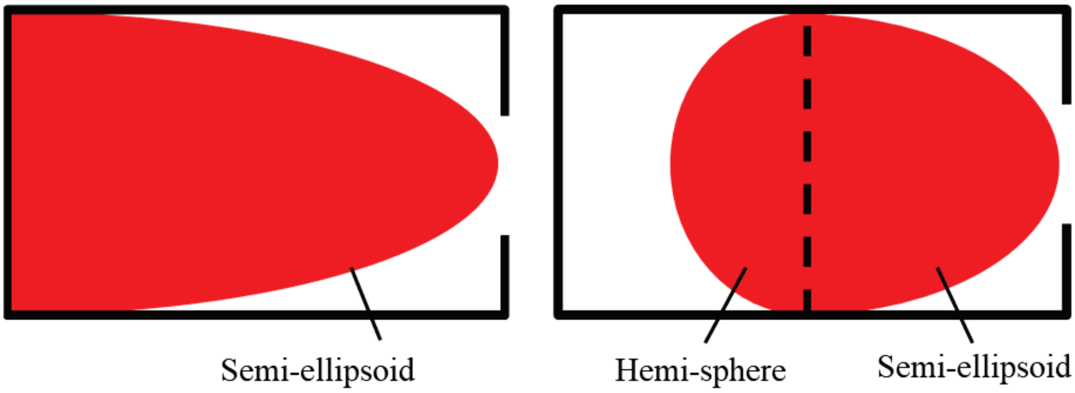
Figure 1. Curve-fit for average normalized flame propagation velocity data from Bauwens et al. (2012).

From this correlation for flame speed (Eq. 1), the flame propagation velocity for different composition of hydrogen-air mixtures can be calculated. As evident from Eq. 1, the flame speed inside the enclosure is increasing as a linear function of the distance from the source of ignition. The flame speed starts increasing from the ignition point to reach the maximum value at the vent location, which corresponds to the maximum value of distance x. Hence, the equivalent mean flame speed can be approximated as $0.5U_f$ where U_f is calculated at distance R, which is the distance of the ignition point to the vent location. R can be calculated using length of the enclosure (L) for different ignition locations as:

$$R = \begin{cases} L & \text{for Back} - \text{wall ignition (BWI)} \\ L/2 & \text{for central} - \text{ignition (CI)} \end{cases}$$

and the time taken for the flame to reach the vent (τ) can be calculated as:

$$\tau = \frac{R}{0.5U_f} \tag{2}$$



(a)Back-wall ignition (BWI) *(b) Central ignition (CI)*

Figure 2. Schematic of the flame-shapes for different ignition locations

To obtain the volume of the vented gases forming the cloud, the volume of the flame-ball inside the enclosure is required. Also, some simplifying assumptions for the flame shape are taken as: the flame-ball is considered to be a half ellipsoid for a BWI case (see Fig. 2) and a combination of a half ellipsoid and hemi-sphere for a CI case. These assumptions on flame-shape are based on experimental visualization of flame inside enclosure in previous investigations (Cooper, et al., 1986; Daubech et al., 2013). The schematic of these flame-shapes are shown in Figure 2. The flame-ball volume for the CI case –

$$V_b = V \text{ (semi-ellipsoid)} + V \text{ (semi-sphere)}$$

$$V_b = \left(\frac{\pi}{12} LBH\right) + \left(\frac{2}{3}\pi {R_{av}}^3\right) \tag{3}$$

where V_b is the volume of the burnt gases, L is the length of the enclosure, B is breadth, and H is the height, R_{av} is the equivalent radius of the semi-sphere, given by

$$R_{av} = \frac{B+H}{4}$$

while for the BWI case, the burnt volume can be estimated by calculating the volume of the semi-ellipsoid

$$V_b = \frac{\pi}{6} LBH \tag{4}$$

Finally, for both cases, the volume of cloud (V_c) can be calculated as:

$$V_c = V_b\left(1 - \frac{1}{\sigma}\right) \tag{5}$$

The formation of external cloud by vented gases can be calculated using the vortex ring theory given by Sullivan et al. (2008), who carried out experiments using piston gun in water. They considered inviscid equations for vortex ring in inviscid fluid and then modified those equations for viscous fluids to formulate their theoretical model. Their model is able to predict dimensions of the external vortex ring measured in their experiments and from literature reasonably well.

The present study aims to obtain the dimensions of the external cloud, which is formed by a similar process as the vortex ring in the study of Sullivan et al. (2008). . The steps of the calculation procedures are as follows. Firstly, for the piston, the equivalent radius (R_0) can be calculated by equating the piston surface area to the vent area (A_v)

$$R_0 = \sqrt{\frac{A_v}{\pi}}$$

Piston stroke length (L_P) using the cloud volume and equivalent piston area:

$$L_P = \frac{V_c}{A_v}$$

The radius of the bubble (R_b) can be calculated as:

$$R_b = \sqrt[3]{\frac{9\,\pi\,R_0^2\,L_P}{4\alpha^2\Lambda\,(1+k)}} \tag{6}$$

Various parameters used in the above equation can be calculated as:

$$a = \sqrt{4 \cdot \nu \cdot \tau}$$

where ν is the viscosity, and τ is the stroke time for the equivalent piston, or the time taken by the flame to reach the vent (Eq. 2). Radius (R_{Ring}) of the vortex ring:

$$R_{Ring} = \sqrt[3]{\frac{3\,R_0^2\,L}{4\alpha}}$$

$$\Lambda = \ln\left(\frac{8R_{Ring}}{a}\right) - B$$

where, α=1, B=0.558, and k=0.65. The external cloud has a complicated "mushroom" shape due to the rolling vortex core. Assuming it to be similar to a cylinder with radius R_b the length of the cloud can be calculated as:

$$L = \frac{V_c}{\pi {R_b}^2}$$

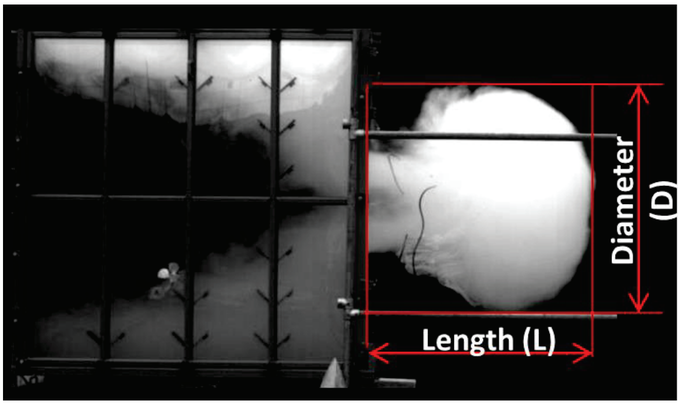


Figure 3. Experimental image of cloud visualization from Daubech et al. (2013). Also note the internal flame which has just reached the vent opening.

3. Results and Discussion

The theoretical framework developed in the previous section to calculate the dimensions and time of formation of the external cloud is now applied to various experimental configurations available in the open literature. Firstly, calculations are carried out for the 4 m^3 configuration used by Daubech et al. (2013). Detailed images of the cloud formation from those experiments can also be found in Vyazmina et al. (2017). These cloud shape images and time resolved images are used to measure the cloud diameter and time taken by the flame to reach the vent. The comparison of the calculated time and cloud dimensions with the experimentally measured data is shown in Table 1. As evident, a reasonably good match is found with both time and dimensions of the available experimental data sets.

Table 1. Comparison of the predicted and measured cloud dimensions and time for the flame to reach the vent from data of Daubech et al. (2013)

H_2 %	Vent area (m^2)	Measured diameter (m)	Predicted diameter (m)	Measured time (sec)	Predicted time (sec)
16.5	0.49	1.4	1.37	0.128	0.116
21.1	0.49	1.4	1.33	0.058	0.055

For further validation, cloud diameter data available from Proust and Leprette (2010) for methane explosion is used. To calculate flame propagation velocity of methane (where the Lewis number effects are not as important as hydrogen flames) a modified form of Eq. 1 is used, where the flame velocity is normalized using the initial flame speed (U_0) of Bauwens et al., 2011) for methane 2.9 m/s:

$$\frac{U_f}{U_0} = 2.84x + 0.25 \tag{7}$$

Proust and Leprette (2010) have used three enclosures having volumes 1 m^3, 10.5 m^3 and 100 m^3. The comparison of the predicted and measured cloud diameter for methane (Proust and Leprette, 2010) and hydrogen (Daubech et al., 2013) is shown in Figure 4 where reasonably good agreement is found between the predictions and measurements.

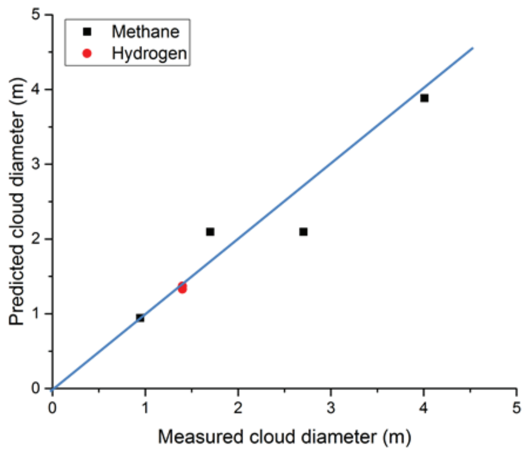
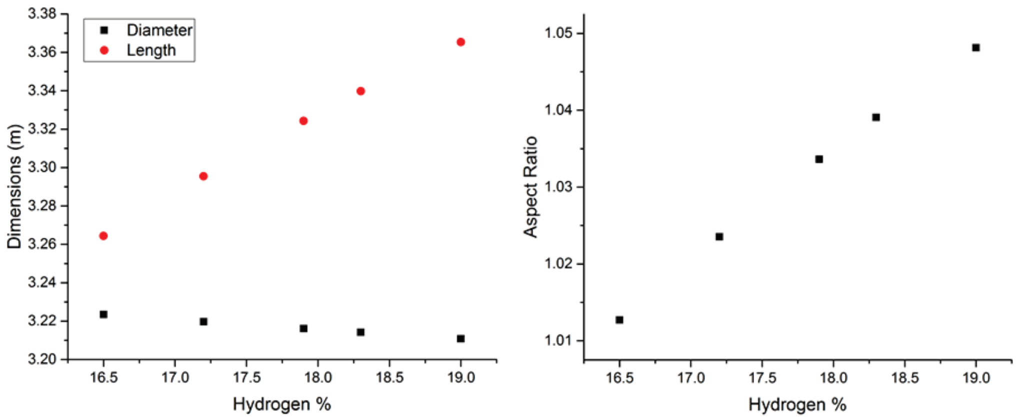


Figure 4. Comparison of the predicted and measured cloud dimensions for methane (Proust and Leprette, 2010) and hydrogen (Daubech et al., 2013)

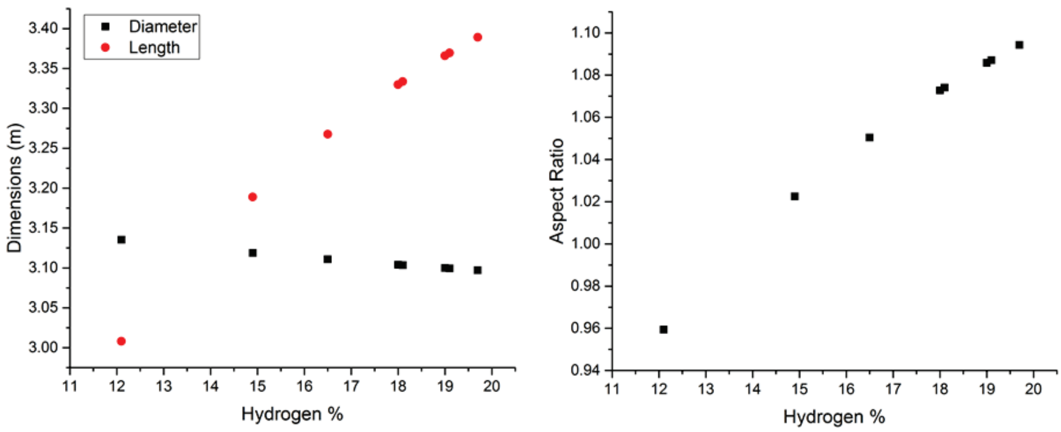
Predictions of the external cloud dimensions have also been performed for other configurations (Bauwens et al., 2012; Daubech et al., 2011; Kumar, 2006). These experimental investigations cover hydrogen concentrations ranging from 9% (for Kumar, 2006) to 27% (for Daubech et al., 2011). The enclosure volume used in these studies ranged from as small as 1 m^3 (for Daubech et al., 2011) to as large as 120 m^3 (for Kumar, 2006). More details about these experimental configurations can be found in the original papers quoting above. A brief summary of these experiments, their key findings and overpressure predictions can be found in our previous papers (Sinha et al., 2017a, 2017b).

Figures 5(a) and 6(a) show the predictions of cloud shape for the experiments of Bauwens et al. (2012). As observed, the cloud diameter decreases slightly with the increase in hydrogen concentration, but its length increases with the increase in hydrogen concentration. This observation can be explained as follows: with the increase in hydrogen concentration, the flame propagation velocity increases (see Eq. 1). Hence it is quicker for the flame to reach the vent. Also, the expansion ratio is higher for higher concentration of hydrogen. Equation 6 indicates that L_P in the numerator increases with the expansion ratio and Λ in the denominator increases with flame propagation velocity. The combining of these two opposite effects for a given geometry indicates that the cloud diameter is only weakly linked with the increase in hydrogen concentration for all the experimental configurations considered here. However, the length of the cloud, which is controlled by the expansion ratio, is observed to increase with the increase in hydrogen concentration. This trend is also the same for all the cases examined in this study. It is also observed that the cloud diameter in cases for BWI is generally larger than that in cases with CI. This can be attributed to larger burnt volume in the BWI cases and consequently larger vented cloud volume, which results in larger cloud diameter.



(a) Diameter and Length (b) Aspect Ratio

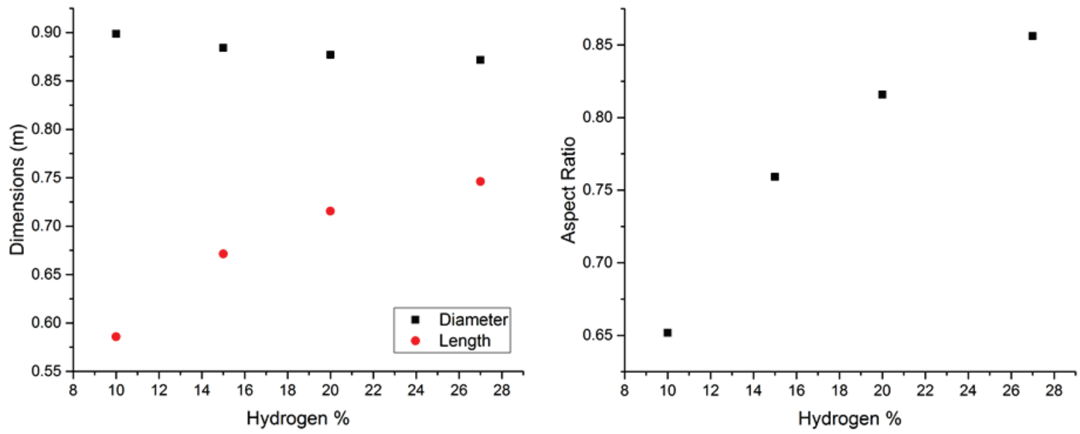
Figure 5 Dimensions and aspect ratio of the external cloud for the configuration of Bauwens et al. (2012) for Back-wall ignition (BWI).



(a) Diameter and Length *(b) Aspect Ratio*

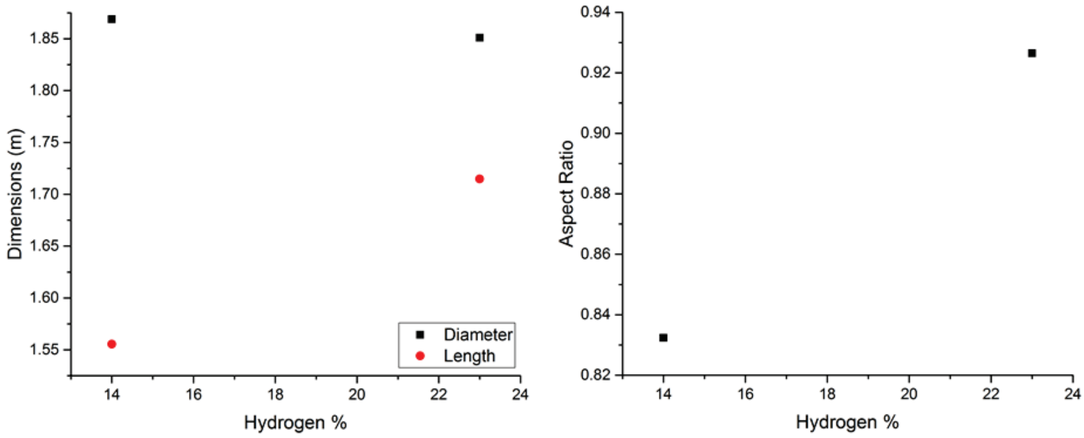
Figure 6. Dimensions and aspect ratio of the external cloud for the configuration of Bauwens et al. (2012) for Central ignition (CI).

Figures 5(b) and 6(b) show the variation of the aspect ratio of the cloud with hydrogen concentration for the configuration used by Bauwens et al. (2011). Here the aspect ratio is defined as the ratio of the length to diameter of the cloud. It can be seen that the aspect ratio of the cloud increases with the increase in hydrogen concentration. This is expected as the cloud diameter decreases and its length increases with the increase in hydrogen concentration.



(a) Diameter and Length *(b) Aspect Ratio*

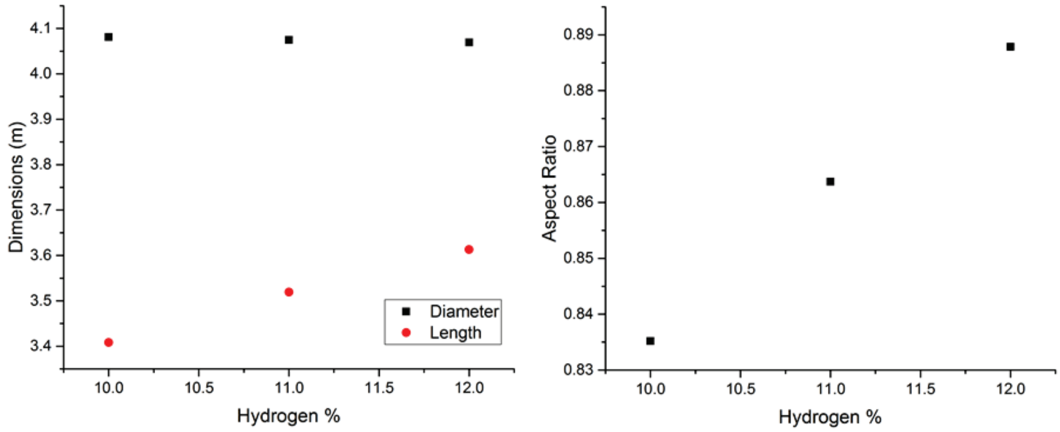
Figure 7. Dimensions and aspect ratio of the external cloud for the configuration of Daubech et al. (2011) for 1 m3 enclosure.



(a) Diameter and Length *(b) Aspect Ratio*

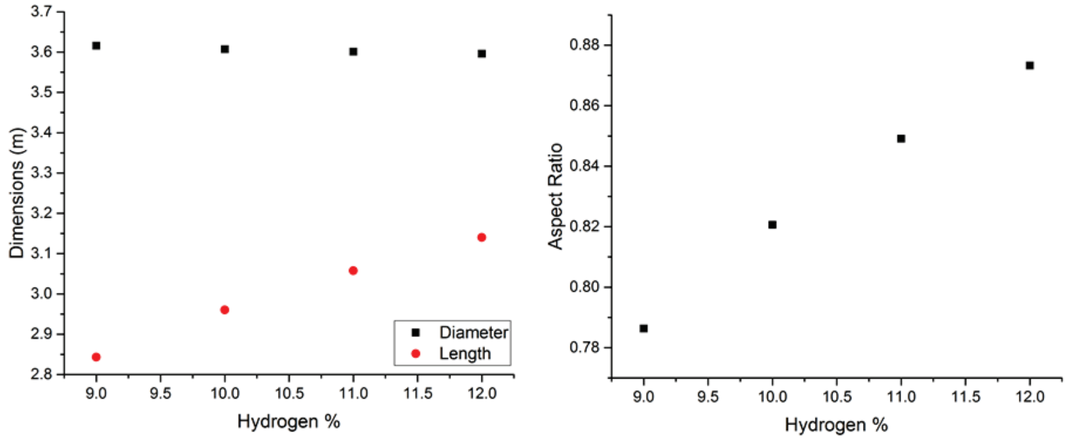
Figure 8. Dimensions and aspect ratio of the external cloud for the configuration of Daubech et al. (2011) for 10.5 m3 enclosure.

Figures 7 and 8 show the dimensions and aspect ratio of the cloud formed in the experiments of Daubech et al. (2011) for their enclosures with volumes 1 m^3 and 10.5 m^3, respectively. Similar trends can be observed in these results as were seen in Figures 5 and 6. The cloud diameter decreases and its length increases with the increase in hydrogen concentration while the aspect ratio increases with the increase in hydrogen concentration. Also, as expected, a larger cloud is formed with an enclosure with larger volume.



(a) Diameter and Length *(b) Aspect Ratio*

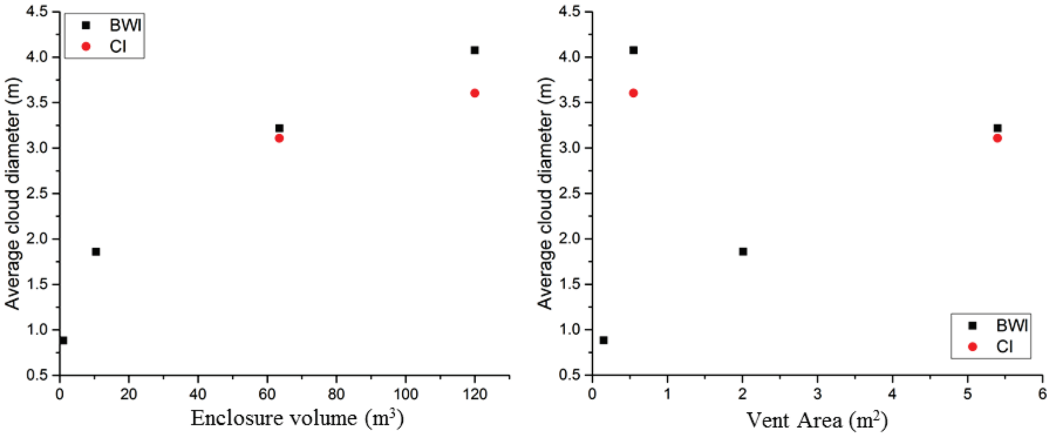
Figure 9. Dimensions and aspect ratio of the external cloud for the configuration of Kumar (2006) for for the BWI.



(a) Diameter and Length *(b) Aspect Ratio*

Figure 10. Dimensions and aspect ratio of the external cloud for the configuration of Kumar (2006) for the CI.

Figures 9 and 10 show the cloud dimensions and aspect ratio for the configuration used by Kumar (2006). This configuration represents the largest volume of enclosure considered in this study and consequently the largest cloud diameters are formed in these cases. These cases also show an increase in cloud diameter and decrease in cloud length with increase in hydrogen concentration. The aspect ratio also increases monotonously with hydrogen concentration for both the BWI and CI cases.



(a) *(b)*

Figure 11. Variation of the average cloud volume with (a) enclosure volume and (b) vent area. Different symbols are shown for different ignition locations.

As observed in Figures 5-10, the cloud diameter for a fixed geometry and ignition location varies within a small range with the change in hydrogen concentration. This indicates that using an average cloud diameter for all hydrogen concentrations will be a reasonable approximation. Average cloud diameter is obtained for various geometries considered in this study. The variations of average cloud diameter with enclosure volume and vent area are shown in Figure 11. In Figure 11(a), it is observed that the cloud dimeter increases with increase in enclosure volume. The same trend is observed for both BWI and CI cases, and the trend is monotonous. Figure 11 (b) shows the variation of average cloud diameter with vent area. In general, the cloud diameter increases with the increase in the vent area but there is an anomaly for vent area of 0.55 m^2. This vent area corresponds to the large enclosure used by Kumar (2006). Hence, from these observations, it can be inferred that the cloud diameter increases with increase of both vent area and enclosure volume, but the role of volume is more dominant. This can be attributed to the role of head vortex which expands with the cloud bubble, and makes it larger than the vent dimensions (see Fig. 3, Krueger and Gharib, 2003; Didden, 1979). This expansion makes it primarily dependent on the total vented volume rather than only the vent area. The vented volume depends on the total volume of the enclosure (cf. Equation 5). The dominance of total volume in determining the external cloud diameter is indeed evident in Figure 11.

4. Conclusions

External explosion is an important phenomenon in vented explosions, which occurs from the combustion of the external cloud. This paper presents a model to calculate the time for the internal flame to reach the vent and dimensions of the external cloud. Correlations based on published experimental observation of flame propagation are used to estimate flame propagation velocity and the time taken for the flame to reach the vent. The theory for vortex bubble formation is then used to estimate the dimensions of the cloud. The model predictions for the cloud diameter and the time for the flame to reach the vent are found to be in reasonably good agreement with experimentally measured values. Further observations are made on the aspect ratio of the external cloud. It is observed that the cloud diameter decreases slightly with the increase in hydrogen concentration, while the cloud length increases with increase in hydrogen concentration. Hence, the aspect ratio, which is the ratio of cloud length to diameter, increases with the increase in hydrogen concentration. However, the aspect ratio is generally close to 1 and varies within a small range. It is also observed that the cases with back-wall ignition produce larger clouds as compared to central ignition cases with the same geometry. Further, the effects of volume and vent area on the cloud dimensions are discussed. It is observed that the cloud diameter increases with the increase in both volume and vent area. For the experiments of Kumar (2006), which involved a small vent area for a large enclosure volume, cloud formed is still found to be larger than other cases, irrespective of the small vent area. It appears that the role of enclosure volume is more dominant in determining the cloud shape as compared to the vent area.

Work is underway to extend the model for predicting the over pressure generated by the external explosion as well as to formulate a physics based model to predict the maximum internal over-pressure. The standard flame speed data used in this study can also be used for internal pressure predictions for empty enclosures. Prediction for cases with obstacles, which represent more realistic accidental scenarios, will be a major challenge for the further development of the present approach. Further effort will focus on modifying the spherical flame propagation velocity in this study to account for flame acceleration caused by obstacles.

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