PERFORMANCE EVALUATION OF EMPIRICAL MODELS FOR VENTED LEAN HYDROGEN EXPLOSIONS

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ABSTRACT

Explosion venting is a method commonly used to prevent or minimize damage to an enclosure caused by an accidental explosion. An estimate of the maximum overpressure generated though explosion is an important parameter in the design of the vents. Various engineering models (Bauwens et al., 2012, Molkov and Bragin, 2015) and European (EN 14994) and USA standards (NFPA 68) are available to predict such overpressure. In this study, their performance is evaluated using a number of published experiments. Comparison of pressure predictions from various models have also been carried out for the recent experiments conducted by GexCon using a 20 feet ISO container. The results show that the model of Bauwens et al. (2012) predicts well for hydrogen concentration between 16% and 21% and in the presence of obstacles. The model of Molkov et al. (2015) is found to work well for hydrogen concentrations between 10% and 30% without obstacles. In the presence of obstacles, as no guidelines are given to set the coefficient for obstacles in the model, it was necessary to tune the coefficient to match the experimental data. The predictions of the formulas in NFPA 68 show a large scatter across different tests. The current version of both EN 14994 and NFPA 68 are found to have very limited range of applicability and can hardly be used for vent sizing of hydrogen-air deflagrations. Overall, the accuracy of all the engineering models was found to be limited. Some recommendations concerning their applicability will be given for vented lean-hydrogen explosion concentrations of interest to practical applications.

Keywords: Vented explosion, Hydrogen, engineering models, overpressure, obstacles

1.0 INTRODUCTION

Explosion venting is one of the most widely and simplest methods to reduce overpressure developed in a low-strength building or enclosure due to accidental explosions. With the growing interest in hydrogen as an energy source, its storage and safety becomes important concern. The objective of research in this area is to assess the effect of various operating parameters and to provide safety guidelines and recommendations for its storage in building or enclosure design. The engineering models available consider various operating parameters and calculate venting area required for a given enclosure. These models can also be used to calculate the maximum overpressure generated for a given configuration and fixed vent area. Vented deflagration is a complicated process. The pressure peaks and maximum overpressure developed depend upon the interplay of several physical processes like external explosion, flame-acoustic interaction, coupling of resonant modes of the enclosure walls and the flame. The objective of this present study is to review engineering models available, and compare their predictions for available experimental data. Another aspect particularly important in practical situations is the effect of obstacles on the overpressure. This is also investigated and recommendations have been made to account for it. First the experimental studies relevant are discussed. The engineering models are briefly described and then comparison between their predictions and experimental results is shown. The experimentally measured pressure is denoted as P-exp and pressure calculated by using model is denoted as P-mod in the subsequent discussion.

2.0 EXPERIMENTAL STUDIES

There are several experimental investigations reported on vented deflagrations, observing the pressure traces, maximum overpressure values generated, and effect of various operating parameters like vent area, fuel concentration, enclosure geometry, presence of obstacles, etc. Studies pertaining to hydrogen deflagration, relevant for this project are discussed in detail. These results are later compared with model predictions to assess their applicability for various conditions.

2.1 Bauwens et al. (2012) – Bauwens et al. [1] have carried out a series of experiments using a 63.7 m^3 enclosure. The experiments are focused on using different hydrogen concentrations, ignition locations, vent size, and presence of obstacles. The hydrogen concentrations used are in the range 12% to 17% of hydrogen by volume. The ignitor locations used are center ignition, back wall ignition, and front wall ignition. They have used two vent areas of 2.7 m^2 and 5.4 m^2. The results confirmed the significance of maximum flame area, burning velocity, obstacles, external explosion, and their interplay in determining the overpressure in the enclosure. Some recent improvements in this model have also been accounted for in this study [25]

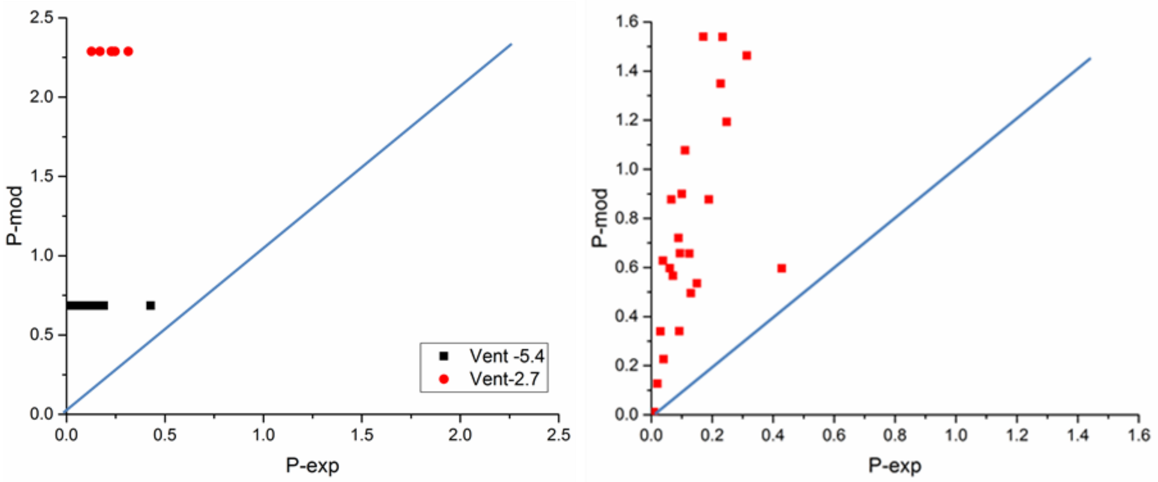
2.2 Kumar (2009) - Kumar [2] carried out experiments in a cuboidal enclosure with internal volume 120 m^3. It remains one of the largest enclosures used in vented explosion studies with hydrogen as a fuel. Lean hydrogen mixtures having hydrogen concentrations in the range 6% to 11% are used. Vent area used are 0.55, 1.09, and 2.19 m^2. Igniter is located at the geometric center of the enclosure. The objective of this study was to study the effect of initial turbulence on combustion. Turbulence is generated by using eight fans rotating at 1000 RPM. It is observed that much higher overpressures are developed with turbulent mixtures as compared to studies with quiescent mixtures. The double peak structure for overpressure generally observed in vented deflagration is not obtained in this study and a single peak is found. It is inferred that the instabilities generated in laminar flames are responsible for double pressure peak and oscillatory combustion. If the mixture is already turbulent, those instabilities will not grow. This work has presented a case where new models are required, or existing models need to be improved to account for initial turbulence in the test chamber and its effect on flame structure and over-pressure.

2.3 Kumar (2006) - Kumar et al. [3] has undertaken experiments in a large cuboidal enclosure with internal volume 120 m^3. Lean hydrogen mixtures having hydrogen concentrations in the range 6% to 12% are used. Different vent sizes are also tested. The objective of the experiments is to evaluate the effect of ignition locations with different hydrogen concentrations. The mixture is ignited at the center, back wall and front wall. A major difference with the study mentioned in the previous paragraph is that this study was carried out at quiescent conditions. A non-monotonous behavior of pressure rise is also observed with variation of hydrogen concentrations. Similar non-monotonous behavior is also observed in a recent study by Schiavetti and Carcassi [5]

2.4 Daubech et al. (2011) - Daubech et al. [4] have carried experiments with two cylindrical chambers having volume 1 m^3 and 10.5 m^3. They have used hydrogen as a fuel and varied its composition between 10% and 27%. The smaller chamber has a vent area of 0.15 m^2, while the larger enclosure is having a vent area of 2 m^2. Fuel air mixture is ignited near to the wall opposite to the vent, for both the geometries. P1 is found to be the dominant pressure for most of the cases.

3.0 ENGINEERING MODELS

3.1. EN 14994 Model – The EN 14994 model [6] is divided into two formulations, one for a compact enclosure (with $L/D \leq 2$) and the other for elongated enclosure (with $L/D > 2$). The gas explosion constant 'KG' is taken as 550 bar. The comparison of experimental data from Bauwens et al [1] is shown in Fig. 1(a). As evident, there are only two values of predicted overpressure for all the experiments. From the model formulation, we can infer that for the same fuel and same enclosure geometry EN 14994 considers dependence only on the vent area. So, the two values predicted correspond to the two vent sizes used by Bauwens et al. [1]. It must be noted that various physical properties may vary, even for the same fuel and same geometry, for example, with the change in equivalence ratio or change in ignition point. So the model should be able to incorporate these variations in order to give accurate predictions. Moreover, the calculated values are highly over-predicting peak pressure. This will give rise to very large vent sizes or very sturdy and costly enclosure designs.



(a) EN 14994 formulation

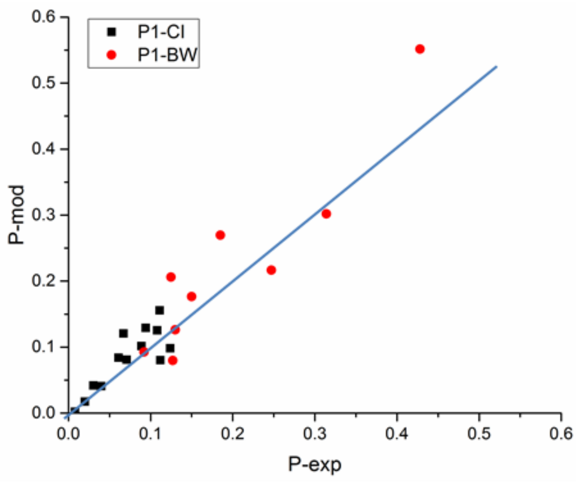
(b) NFPA 68 (2013) formulation

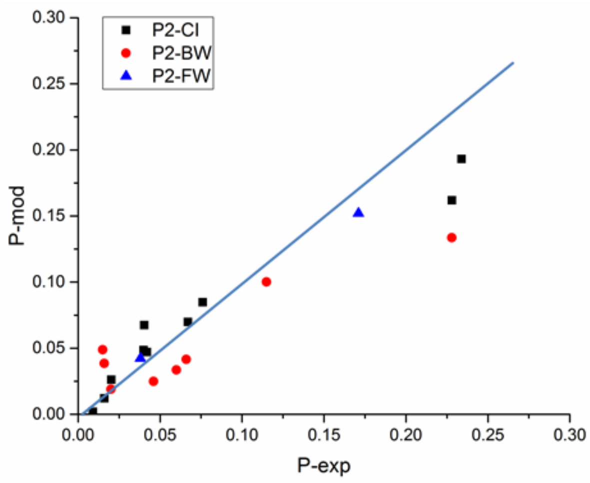
Figure 1. Comparison of the measured and calculated values of overpressure for Bauwens et al. [1] data using (a) EN 14994, and (b) NFPA 68 [4] formulations. P-mod denotes the modelled pressure while P-exp shows the experimentally measured pressure. Different symbols are used for different vent sizes in EN-14994 result.

3.2 NFPA68 (2013) model [7] - The National Fire Protection Association's (NFPA) standard on Explosion protection by deflagration venting (2013) model [7] considers mixture composition, dimensions of the enclosure and vent area. The comparison of predictions made by this model with the experimental results from Bauwens et al. [1] is shown in Fig. 1(b). As evident, NFPA model is consistently predicting higher values of overpressure as compared to the measurements. The enclosure based on this design will be capable to withstand higher overpressures than required, but it will also result in over-design and higher cost.

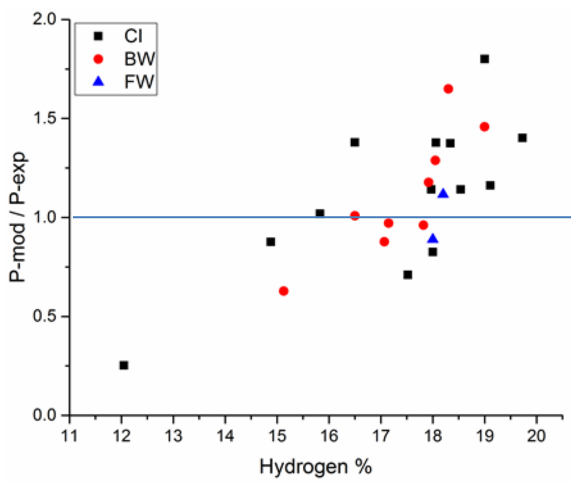
Both the EN 14994 and NFPA 68 formulations over-predict the pressure values and will recommend prohibitively larger vent sizes or enclosure strengths. Both the formulations are not discussed further. More details about these model predictions and comparison with other experimental studies can be found in our previous report [23]

3.3 Bauwens et al. model (2012) [1, 8-12, 25] – This is the only engineering model that considers multi-peak nature of overpressure in vented deflagrations. This model accounts for several physical properties of reactants and products into its formulation and predicts for pressure peaks caused by external explosion (P_{ext} or P1) and flame-acoustic interaction (P_{vib} or P2). This model calculates the maximum flame area in each configuration of ignition location, obstacles, etc. which gives the maximum pressure generated. Jallalis and Kudriakov [13] have also provided useful insights for this model. The model constants are taken as per FM Global model recommendations [25]. The values for physical properties are taken from Gaseq calculator [14]. The comparison with experimental values of P1 and P2 from Bauwens et al. [1] experiments are presented in Fig. 2





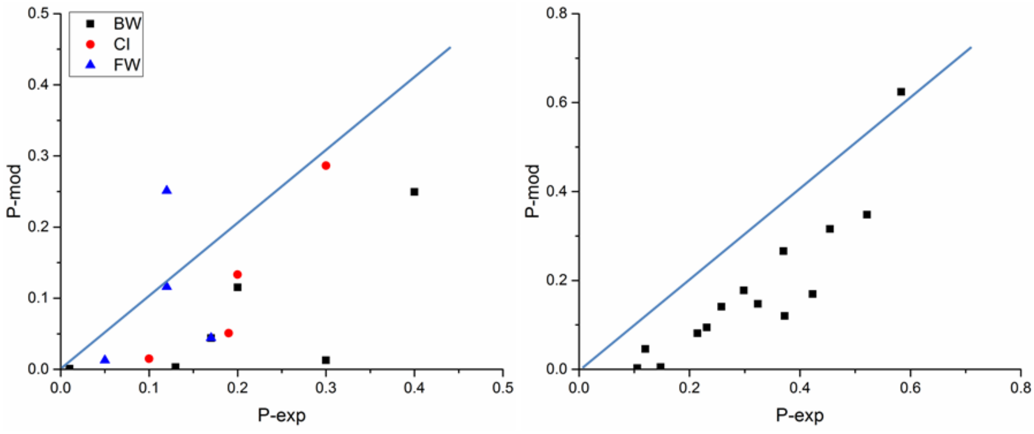
(a) Pext or P1 (b) Pvib or P2



(c) Ratio of predicted and measured pressure at various compositions

Figure 2. Comparison of the measured and calculated values of overpressure for Bauwens et al. [1] data using Bauwens et al [1] formulation. (a) Comparison of measured and predicted values of P1, (b) Comparison of measured and predicted values of P2. (c) Ratio of predicted and measured P1 values plotted with mixture composition. The symbols denote the central ignition (CI), back-wall ignition (BW), and obs is for obstacles.

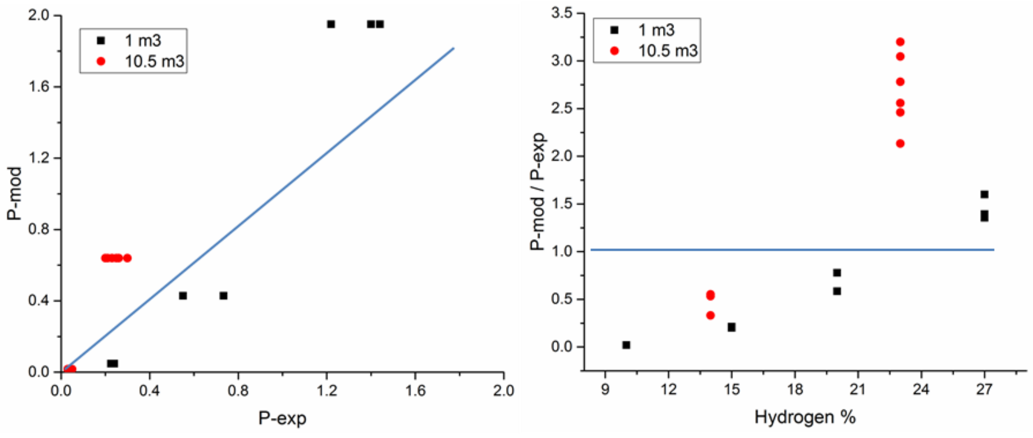
As shown, the model values match very closely with the measured values of P1, while the values of P2 are slightly over-predicted for higher experimental pressure values. Fig. 2(c) shows that the P1 values are predicted reasonably well for hydrogen concentration of 16% to 21%. Pressure values are under-predicted for leaner mixtures and over-predicted for richer mixtures.



(a) Kumar-2006 (K1) (b)Kumar-2009 (K2)

Figure 3. Comparison of the measured and calculated values of overpressure for (a) Kumar -2006 [2], and (b) Kumar-2009 [3] data using Bauwens et al. [1] formulations. For (a), symbols show cases with central ignition (CI), back-wall ignition (BW). For (b) symbols show different vent area in m^2.

Figure 3 shows the comparison of predictions by Bauwens et al. [1] model with the experiments of Kumar [2, 3]. K1 represent the data points from the 2006 study [2] while K2 is for the 2009 experiments [3]. The K1 data set shows some scatter in predicted value but most of the points are slightly under-predicted. For the data set K2, almost all data points are slightly under-predicted. Both the studies have been carried out in same enclosure using same fuel and similar operating conditions. Only difference between them is that the K1 experiments are done with quiescent conditions, while for K2, initial turbulence levels are enhanced using fans.

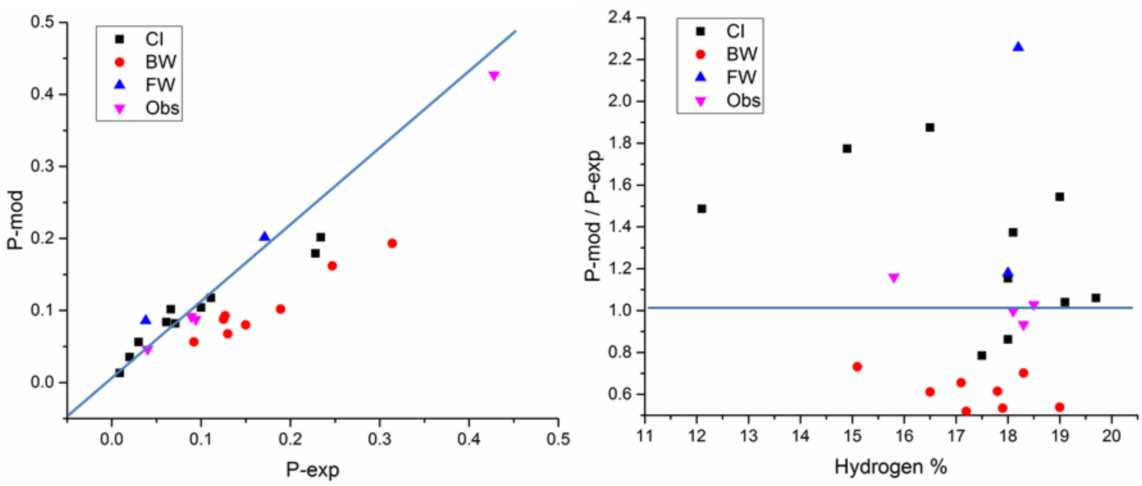


(a) (b)

Figure 4. Comparison of the measured and calculated values of overpressure for Daubech et al. [4] data using Bauwens et al. [1] formulations. (a) Predicted and measured pressure comparison. (b) Ratio of predicted and measured pressure plotted with hydrogen concentration. Symbols show different volumes of enclosures used in this study.

Figure 4 shows the comparison of predicted values using Bauwens et al. model [1] and experimental results of Daubech et al [4]. Both the enclosure geometries investigated are included in this comparison. It is evident form Fig. 4 that pressure is over-predicted for the larger (10.5 m^3) enclosure and is under-predicted for the smaller (1 m^3) vessel. One important difference between those two enclosures is that the aspect ratio of smaller enclosure is closer to 1 (L/D = 1.4), while for the larger enclosure, the aspect ratio is much higher (L/D = 3.3). The model calculates flame area assuming an ellipsoidal shape for the flame, but for a larger L/D enclosure, flame will not be ellipsoidal and the flame surface area will be much smaller than the values calculated using this model. A higher calculated flame area will result in over-prediction of pressure as evident in Fig. 4.

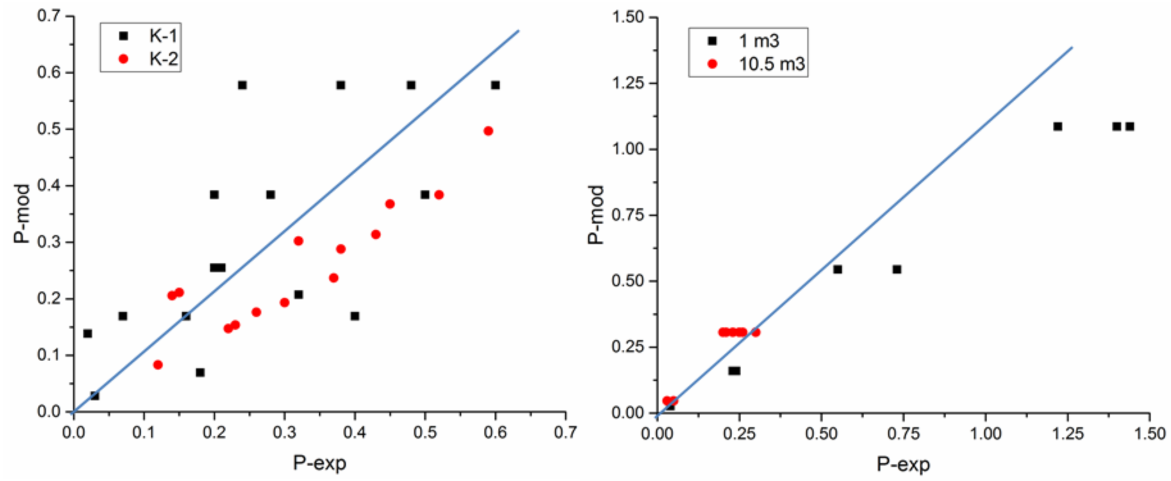
3.4 Molkov and Bragin model (2016) – Molkov and Bragin [15] have developed a vent sizing correlation based on the dependence of overpressure to the turbulent Bradley number. The model is being developed in several past studies [16-22], however, the latest formulation of the model [15] is discussed here. This model does not account for the multi-peak nature of vented deflagrations, but is based on the DOI formulation using the Bradley number for flame exiting through the vented area. Several factors like initial turbulence, aspect ratio of enclosure, turbulence generated by the leading flame front, etc. are taken into account. Predictions from this model will now be compared with the experimental data from various sources.



(a) (b)

Figure 5. Comparison of the measured and calculated values of overpressure for Bauwens et al. [1] data using Molkov and Bragin [15] formulations. (a) Predicted and measured pressure comparison. (b) Ratio of predicted and measured pressure plotted with hydrogen concentration. The symbols denote the central ignition (CI), back-wall ignition (BW), forward-wall ignition (FW), and obs is for obstacles.

Figure 5 shows the comparison with this model prediction with Bauwens et al. [1] data. The model gives reasonably good predictions for this set of experiments. The experiments with back wall ignition are slightly under-predicted, and central ignition cases are slightly over-predicted. This could be attributed to the model formulation where the ignition location is not considered and a sort of average behaviour is calculated. Overall, this model works reasonably well for this set of experiments. Further comparisons are made with experiments of Kumar [2, 3], and Daubech et al. [4] as shown in in Fig. 6. Both experiments of Kumar show reasonable match with the predictions. Although, Kumar's quiescent data [2] show some scatter and turbulent experiments [3] are mostly under-predicted; the predictions are within acceptable limits. Similar is the case for experiments from Daubech et al. [5]. The predictions compare reasonably well with the data sets but the cases with smaller enclosures are mostly under-predicted while the cases with larger enclosures are slightly over-predicted. These experiments cover a hydrogen concentration from 10% to 30%, and Molkov and Bragin formulation [15] appear to work well within this limit.



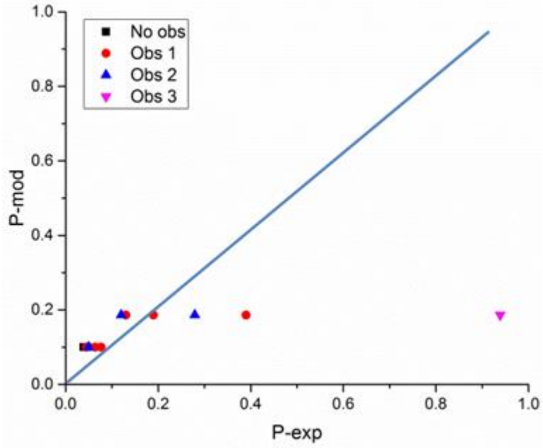
(a) (b)

Figure 6. Comparison of the measured and calculated values of overpressure for (a) Kumar [2, 3], and (b) Daubech et al. [5] data using Molkov and Bragin [15] formulations.

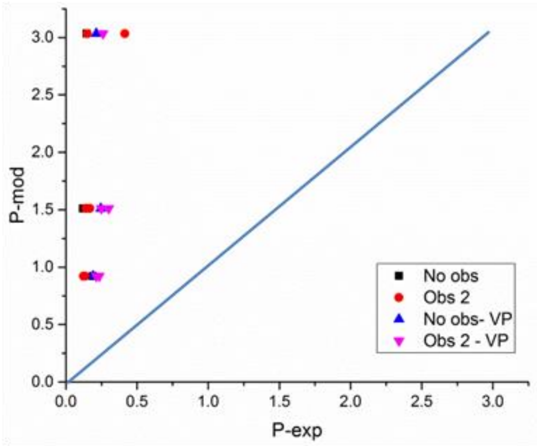
4.0 PREDICTION FOR 20 FEET ISO CONTAINER

As a part of HySEA project supported by Fuel Cells and Hydrogen Joint Undertaking, GexCon has carried out some experiments using hydrogen air mixtures. They have used standard 20 feet ISO shipping containers, for experiments ranging from 15% to 24% hydrogen concentrations. The experimental test matrix consists of tests without obstacles, and with using two obstacle configurations. The first obstacle configuration contains stacks of empty commercial bottles, and other obstacle configuration contains pipe rack and some smaller objects placed on it. More details about the experiments can be found at [24]. These set of experiments provide a good basis to evaluate the predictive capability of engineering models. Predictions from all the engineering models discussed previously are compared with the experimental results in Fig. 7.

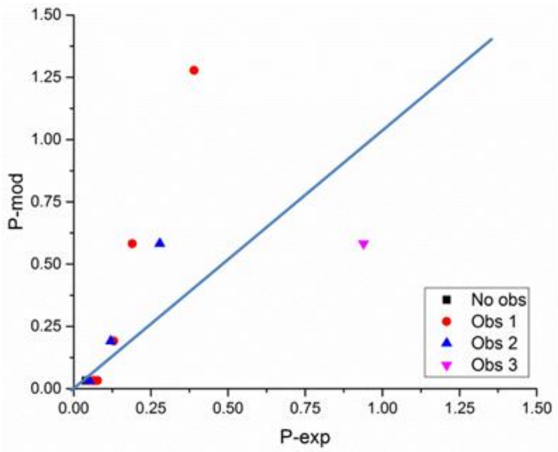
EN 14994 model show some scatter for the door-venting cases, some cases are also under-predicted. On the other hand- the cases with venting from the roof are highly over-predicted. Predictions from NFPA model also show a similar trend. The roof-venting cases are all over-predicted, while the door-venting cases have higher predictions as compared to the EN 14994 results. Molkov and Bragin model appears to work well for most of the experiments where venting was through the door. It was found to under-predict only one data point which corresponds to a relative high hydrogen concentration of 24%. Other data points are predicted reasonably close to the actual data. It must be noted that as there are no guidelines for calculating the coefficient for obstacles (ΞO), the best fit value is used here (ΞO=1.2) following testing with different values. For venting through roof, this model shows a large scatter but the predicted values are reasonably close to the experimental results again using tuned best fit value for ΞO. Bauwens et al. model also show some scatter for the door-venting cases but the predictions are reasonably close to the experimental values, especially for cases with lower over-pressure. For cases with venting through the roof, Bauwens et al. model shows significant over-prediction for all the data points. This set of experiments by GexCon provides a standard data set for vented deflagration in practical geometry; and can be further utilized to improve the existing models and to validate new modeling efforts.



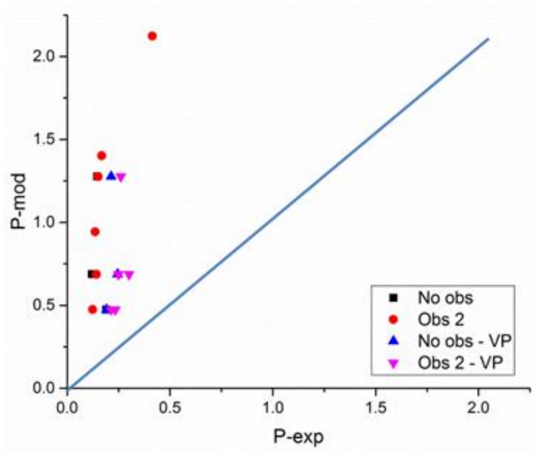
(a) door-venting –EN14994 model



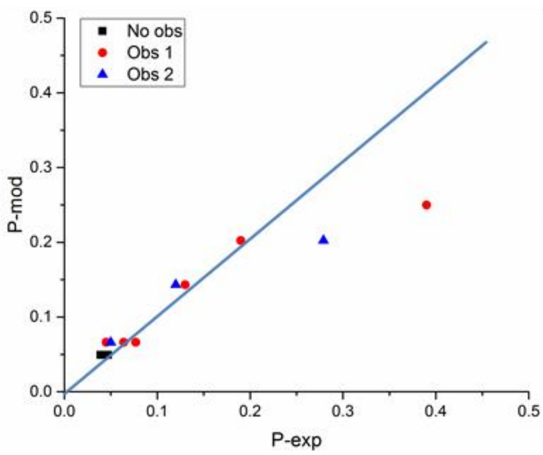
(b) roof-venting-EN14994 model



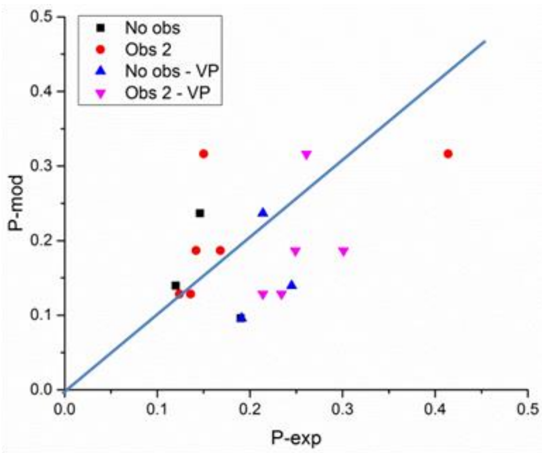
(c) door-venting-NFPA model



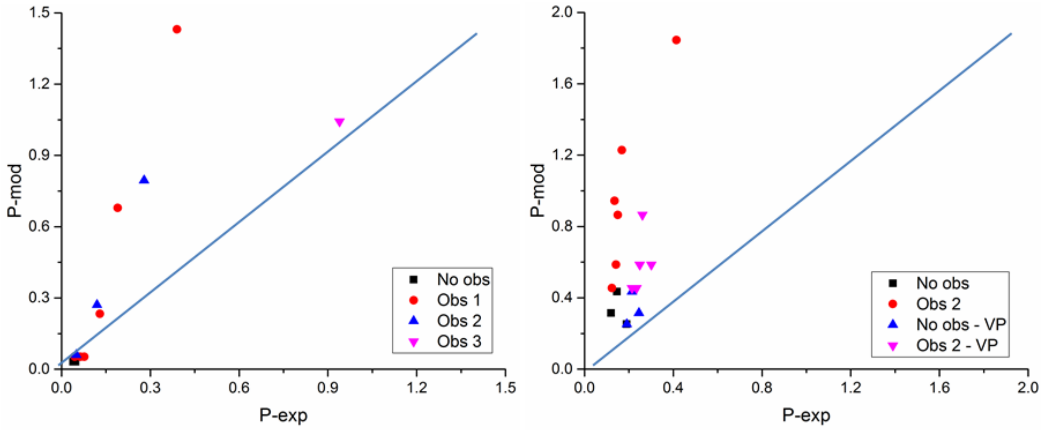
(d) roof-venting-NFPA model



(e) door-venting-Molkov model



(f) roof-venting- Molkov model



(g) door-venting-Bauwens model (h) roof-venting- Bauwens model

Figure 7. Comparison of the measured and calculated values of overpressure for 20 feet ISO container data for cases having door-venting and roof-venting using EN-14994 (a-b), NFPA, (c-d) Molkov and Bragin model (e-f), Bauwens er al. model (g-h). Some cases with vent panel are also discussed (VP)

6.0 CONCLUSIONS

This paper presents a review of experimental studies relevant to vented deflagration of lean hydrogen mixtures. Engineering models available to predict overpressure values are also reviewed and discussed. It is observed that the standards (EN 14994, NFPA 68) give very high prediction for overpressure. Their use could result in designs which are practically not feasible. Other models including that of Bauwens et al. [1] and Molkov and Bragin [15] have been firstly compared with published experimental data and found to give reasonable predictions. Bauwens et al. [1] model does not contain any coefficient which needs tuning and it has achieved reasonably good agreement with the published data, but it appears to have issues for experiments with initial induced turbulence and enclosures with large aspect ratio like ISO containers. Molkov and Bragin model [15] compare well with most of the published experimental studies without obstacles, but it does not consider ignition location. This affected the overpressure values. In addition as no guidelines are given to set the coefficient ΞO for obstacles in the model, ΞO needs to be adjusted for different experiments and the predictions here were based on the best fit following testing of different ΞO values. Both the models of Bauwens et al. [1] and Molkov and Bragin have only been previously tested with a limited set of data involving obstacles. The present paper attempts to address this issue by comparing their predictions with the recent GexCon tests using a 20 feet ISO container [24], where the effect of obstacles was systematically investigated. The comparison has highlighted the need to further improve these models for different venting arrangement.

Furthermore, the accuracy of the predictions are also to some extent hindered by the lack of experiments for lean hydrogen combustion, where even fundamental quantities like the laminar flame speed has not been accurately measured and there is a large scatter in the experimental data available. This uncertainty can be addressed by conducting more fundamental experiments and creating a universally acceptable database for physical properties to be used in engineering models. The existing discrepancy of data can create issues in the predictions of overpressure. For example, in Kumar's [3] experiments, a non-monotonous behaviour is observed near the hydrogen concentration of 10%. The database available should be able to capture this type of behavior for accurate predictions.

Acknowledgements

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