AN INTER-COMPARISON EXERCISE ON ENGINEERING MODELS CAPABILITIES TO SIMULATE HYDROGEN VENTED EXPLOSIONS

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ABSTRACT

A benchmark exercise on vented explosion engineering model was carried out against the maximum overpressures (one or two peaks) of published experiments. The models evaluated are Bauwens et al. (2012-1 and 2012-2) [4, 7] models, Molkov Vent Sizing Technology 1999, 2001 and 2008 models [12, 13, 6]. The experiments in consideration are Pasman et al. experiments (1974) (30% H_2 - 1m3) [1], Bauwens et al. (2012) experiments (64m^3) [4], Daubech et al. (2011) experiments (10 to 30% H_2 - 1 and 10 m^3) [2] and Daubech et al. (2013) [5] experiments (4 m^3 – H_2 10 to 30%). On this basis, recommendations and limits of use of these models are proposed.

1.0 INTRODUCTION

Early (forklifts, backup or base load electricity production ...) and mature (cars, buses ...) hydrogen energy applications could be localised in confined zones (cabinet, cars, garage ...). Explosion venting is a protective measure preventing unacceptable explosion pressure build-up inside confined spaces leading to enclosure destruction and formation of flying fragments. In order to be effective the vent must be designed correctly to keep the explosion pressure below the failure pressure of the building structure.

Vented explosions have been investigated by many researchers. Unfortunately, experiments concerning hydrogen are very limited. In cylindrical conditions (1 to 10 m^3), Pasman et al. (1974) [1] and Daubech et al (2011) [2] have performed experiments with reactive mixtures. At large scale (120 m^3), Kumar experiments (1974) [3] have investigated lean mixtures with different ignition positions. The most reliable experimental data are coming from Bauwens et al. (2012) (64m^3) [4] and Daubech et al. (2013) [5] experiments (4 m^3) which have investigated a variety of hydrogen concentrations, ignition locations and also the presence of obstacles.

About models, it is now well known that NFPA 68 [11] correlation is not able to predict overpressure for hydrogen applications [2, 6, 7].

In vented explosions, a number of different factors (e.g. enclosure size and geometry, vent size, ignition location and obstacle configuration) can affect the pressure development of a propagating flame in a vented enclosure. Recently, Bauwens et al. [4] [8] and Chao et al. [9] have shown different pressure peaks during the vented explosion. When the flame front was observed in the high speed videos to reach the vent and ignite the vented-unburned mixture, the first peak (P_1) was observed in the pressure histories, indicating that P_1 was generated by an external explosion.

A second pressure peak (P_2) is observed as the flame approaches the walls. Based on frequency analyses of the pressure-transient data and of the chamber itself, it appears that this peak is controlled by resonant coupling between the flame and the acoustic modes generated by the geometry and the physical response of the enclosure. It is interesting to note that P_2 can be eliminated or reduced when the walls are lined with an acoustic-absorbing material or when obstacles are placed in the path of the propagating flame [10]. Although obstacles can significantly reduce P_2, they can also increase the maximum flame-surface area (as the flame stretches and folds around the obstacles), which generates a third-pressure peak (P_3) in addition to P_1 and to P_2 (if present). Moreover, obstacles can enhance P_1 due to an increased flame-surface area when the flame front reaches the vent and due to increased turbulence in the vented unburned mixture.

2.0 DATA DESCRIPTION

For this study, available in the literature hydrogen test data from intermediate (>1 m^3) to large scale room like enclosures (120 m^3) were considered. Table 3 summarizes the various data sources for the comparison.

In all experiments, the H_2 – air mixture is homogenous in the enclosure (no stratification or layer) and without initial turbulence.

Table 2. Summary of experimental test data with hydrogen (Cyl : Cylindrical / Par : Parallelepiped)

Test reference	Number of tests	Chamber Geometry	Chamber volume (m^3)	%(H_2)	Ignition locations	Vent area (m^2)	Pressure peaks
Pasman et al. [1]	2	Cyl	1	29.7	C	0.3 and 0.2	P_1
Kumar et al. [3]	9	Par	120	8 to 12%	BW, C, F	0.55	P_2
Daubech et al. [2]	6	Cyl	1 and 10.5	10 to 27%	BW	0.13 and 2	P_1
Bauwens et al. [4]	20 + 4 (obstacles)	Par	64	12.1 to 19.7	BW, F, C	2.7 and 5.4	P_1 & P_2
Daubech et al. [5]	10 + 9 (obstacles)	Par	4	10 to 29%	BW, F, C	0.25 and 0.49	P_1 & P_2

The first set of two experiments was performed by Pasman [1] in a 0.95 m^3 cylindrical vessel of 0.97 m diameter and 1.5 m length. A flange was located at the back of the vessel to accommodate a rupture membrane. The vent diameters were 0.62m (0.3 m^2) and 0.5m (0.2 m^2) with an opening pressure of 13.5 and 7.5 kPa respectively. The H_2/Air (29.6%) mixture was ignited in the centre of the vessel. Since Bauwens and al. model [4] does not take into account the vent presence, these experiments are modelled in this paper without considering the vent opening pressure. Due to the small size of the enclosure, the maximal overpressure is linked to the external overpressure (P_1).

The second set of experiments was performed by Kumar et al. [3] from AECL (Atomic Energy Canada Ltd) in a rectangular enclosure (L10*W4*H3m - 120m3) (called LSVCTF : Large-Scale Vented Combustion Test Facility) in the single chamber configuration. Lean hydrogen mixtures (8 to 12%) were tested with different vent areas. The influence of the ignition location was also investigated (central, near vent and far vent). In this article, only experiments with H_2 concentrations of 11 and 12% are taken into account. This allows avoiding buoyancy effects on flame propagation which are not considered in the models. On the other hand, there are some uncertainties on the laminar flame velocity for the very lean mixtures. For these experiments, the maximum reported overpressure is due to the flame – structures interaction P_2.

The third set of experiments was performed at INERIS research center [2] in two cylindrical chambers of 1 (length 1.4 m and internal diameter 0.94m) and 10.5 m^3 (length 5.5 m and internal diameter 1.6 m). The vents are respectively of 0.13 and 2 m^2. In all these experiments, the ignition point was at bottom of the cylinder (backwall). The hydrogen mixtures tested are between 10 and 27%. In this configuration, the maximal overpressure is P_1.

Unfortunately, for the Pasman, Kumar and Daubech [4] experiments, very limited information is available on peak dynamics (one or two) and on data filtering. For Bauwens and Daubech [5] experiments, the filtering parameters are known and for all the experiments, the P_1 and P_2 overpressure are reported in the publications.

The fourth set of experiments was performed in a 63.7m^3 chamber (4.6x4.6x3m) chamber with hydrogen/air mixtures from 12 to 20 %H_2 in a vent opening of 2.7 or 5.4m^2 located on one wall of the chamber. Three ignition points were used: the centre of the chamber (CI), the back wall (BW) and at front vent (FI). For some experiments, eight (in two rows of 4 obstacles) 40*40cm square obstacles (pillars) are present. The blockage ratio (BR) is 0.6 and the average numbers (N) of obstacles flame path are respectively of 2, 0.5 and 0 for back wall, central and front ignition.

The fifth set of experiments was performed by Daubech et al. (2013) in a transparent enclosure having overall dimensions of 2.0×2.0×1.0 m and an overall volume of 4 m^3. A square vent with two possible surface areas, either 0.49 or 0.25 m^2, was located on one of the chamber's vertical walls. The experimental setup is described in great details in the article also submitted to ICHS. The hydrogen-air mixture (from 10 to 27% H_2) was ignited at one of three following ignition locations: opposite the vent (backwall ignition), at the center of the chamber (center ignition), or at the center of the vent (front-wall ignition). Several tests were performed with obstacles (6 cylinders of diameter 0.2 m or 0.325 m) spanning the full width of the chamber and distributed in three or two rows. The area blockage ratio (BR) is 4.7% and 12,44% and N are the same as Bauwens and al. [4].

Experiments performed by Kumar et al. [15] in a spherical vessel with a duct (6.85 m3) and experiments of Groethe et al. [16] in a partially filled 78.5 m tunnel have been excluded to the comparison because there are very geometrically specific and un-adapted to models assumptions.

3.0 MODELS DESCRIPTION

The most used methodology for vent sizing is NFPA68 [11]. It is now well known that this methodology is not adapted to hydrogen. Another commonly used vent sizing methodology is the "Innovative Vent Sizing Technology" developed by Molkov [12, 13, 6]. The third and most comprehensible methodology has been proposed by Bauwens et al [14, 7]. This methodology takes into account the different peak transients (P_1 and P_2), the ignition location and the presence of obstacles in the enclosure.

Very recently, Bauwens and al. have modified their model in order to take into account the initial turbulence before ignition [17].

Unfortunately, at present, the presence of a concentration gradient in the enclosure or presence of obstacles outside the enclosure nears the vent. Moreover, experiments with obstacles inside enclosure remain scarce.

3.1 Bauwens models

In recent studies, vented explosion under various experimental conditions were systematically investigated using multiple pressure and flame speed measurement associated to high speed videos. From these studies, three main pressure transients were identified, each of which could potentially produce the maximal overall peak overpressure depending of the experimental conditions. The three pressure peaks were associated with: the external explosion (P_{ext} or P_1) of the fresh gas expelled by the internal explosion, flame acoustic interactions as the flame approaches the chamber walls (P_{vib} or P_2) and an increase in flame surface area associated with the presence of obstacles (P_{obs}).

Bauwens et al. have published in 2012 [4, 7], a simple physics-based model which allows to estimate the magnitude of each pressure peak P_1 and P_2 (and another peak P_3 in case of obstruction). The Bauwens model takes into account the gaseous mixture composition, the enclosure size and geometry, the vent size, the ignition location and the obstacle configuration if present. A brief description of the model is given in this paper since it has been clearly described by Bauwens et al. [8] and Chao et al. [9].

For the P_1 maximal overpressure, to take into account the thermal diffuse effects, Bauwens et al. [4] have proposed that the initial flame velocity Su_0, could be dependent on the Lewis number of the mixture, L_e, following the expression: $Su_0 = 0.9\ L_e^{-1}\ S_L$, with S_L the laminar flame speed.

According to this model, the maximum peak pressures in vented explosion could be modeled with only two fitted constants, k_T for P_1 and Ξ_A for P_2.

For hydrogen, the constant k_T was adjusted ($k_T = 3.21\ m^{-1}$) by Chao et al. [9], taking into account a vented gas composed of 90% of products and 10% of reactants. In the present work, only products were considered in the vented gas. Products properties as temperature, molar mass, calorific capacity are calculated using the GASEQ equilibrium calculator software [14].

Then, a value of $k_T = 10.78\ m^{-1}$ was obtained with a new fitting performed on the Bauwens et al. (2012) experiments using a linear law giving an important weight to the higher pressure experimental data. With this fitted value, a good agreement was obtained and the absolute average deviation for P_1 is of 21% for the Bauwens et al. [4] experiments.

For the pressure peak P_2, the burning velocity increases due to flame-acoustic interactions and it is modeled with the expression: $Su = \Xi_A S_L$ where Ξ_A is a constant flame-wrinkling factor. Using the same methodology developed for k_T, the P_2 parameters Ξ_A is fitted to 3.17 which gives an average deviation of 34% for the Bauwens and al. [4] experiments. It should be noticed that the value is very similar to the one (3,2) reported by Chao et al. [9].

The model takes into account the obstacles. The only governing parameters are the area blockage ratio BR and the average number (N) of layer s of obstacles in the flame path.
For the discharge coefficient of the vent, a value of 0.6 has been fixed.

This model with these parameters ($k_T = 10.78\ m^{-1}$ and a constant $\Xi_A = 3.17$) is used in this paper and is named **Bauwens 2012-1 model**.

The figure 1 presents the parity plots obtained with these fittings against the Bauwens et al. experimental data for the peaks P_1 (left) and P_2 (right). General behavior of the present results is similar to the results of Bauwens, although there is some difference in numerical values. The difference may be due to difference in the values of k_T, laminar velocity and expansion ratio.

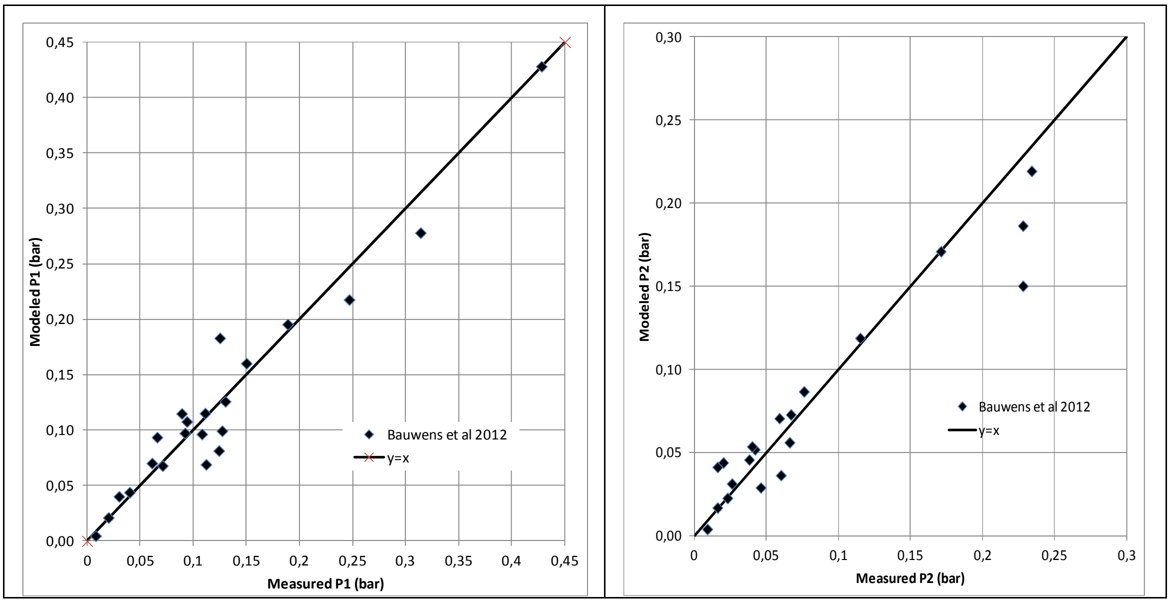

Figure 1. Comparison between measured and modeled peak internal pressure P1 and P2 for Bauwens et al. [4] experimental data

Very recently, Bauwens and al. [7] have proposed improvement in the model. The last version of the model accounts the vent opening pressure and deployment kinetic. Unfortunately, to our knowledge, except Pasman and al. experiments, there is no available experimental data in this configuration with hydrogen.

Some modifications have been also proposed to take into consideration to improve the model for smaller vent sizes in asymptotically approaching a constant volume explosion pressure P_{cv}, when the surface area approaches zero and to take into account the effects of enclosure aspect ratio on the P_2 peak using Ξ_A corrected with the aspect ratio. This model is named **Bauwens 2012-2 model** in this article.

3.2 “Innovative Vent Sizing Technology” VST [12, 13, 6]

The VST models (published in 1999, 2001 and 2008) have been already described in the literature. This methodology computes a deflagration-outflow interaction number (DOI or χ/μ) and correlates the overpressure with a turbulent Bradley number.

The main empirical formulas and tuning parameters are briefly described in this article.

$$\frac{\chi}{\mu_{app}} = \alpha \left[\frac{(1+e.V^{g})(1+0.5Br^{\beta})}{1+\pi_{v}} \right]^{0.4}$$	With V : enclosure volume (m^3) π_v : vent overpressure activation Br : Bradley Number

The constants (α, β, e, g) of this formula have been modified in the different versions of the model (table 2).

Table 2. Parameters in Molkov models

	Molkov 1999 [12]	Molkov 2001 [13]	Molkov 2008 [6]
α	0.9	1	1
β	1	0.8	0.8
e	10	10	2
g	0.33	0.33	0.94

The overpressure formulas have been also modified in the 1999 and 2001 version.

Table 2. Equations in Molkov models (Br_t : turbulent Bradley Number)

Molkov 1999 [12]	If $Br_t > 1$	$\pi_{red} = Br_t^{-2.4}$
	If $Br_t < 1$	$\pi_{red} = 7 - 6.Br_t^{0.5}$
Molkov 2001 [13] and 2008 [6]	If $Br_t > 2$	$\pi_{red} = 5{,}65.Br_t^{-2.5}$
	If $Br_t < 2$	$\pi_{red} = 7{,}9 - 5{,}8Br_t^{0.25}$

The three versions of this model are compared in this paper.

4.0 MODELS EXPERIMENTS COMPARISON

Bauwens 2012-1

The figure 2 shows the comparison between the experiments of table 1 with the Bauwens 2012-1 model. For all experiments, the calculated maximum pressure of the two peaks has been retained.

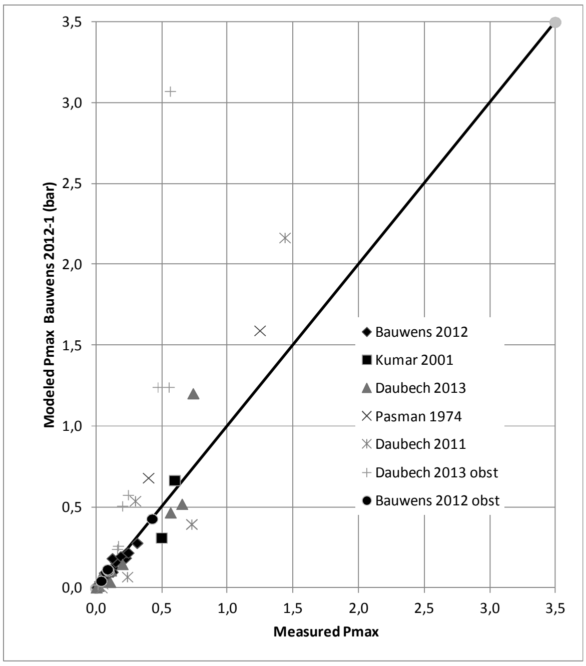

Figure 2: Comparison between measured and Bauwens et al. (2012-1)

The plot shows that the model agrees well across the full range of experimental data.
The larger discrepancies are for the more reactive cases with H_2 concentration more than 20% of hydrogen which is outside the initial range of validation of the model. In presence of obstacles, for concentrations higher than 18%, the agreement is not as good as in the case of lower hydrogen concentrations.

It should also be noticed that the assumption for back wall ignition considering that the flame area is a half of an ellipsoid area with a length twice of enclosure length and width and height equal to those of enclosure is questionable for the case of experiments with a 5.5 m long cylinder (10,5 m^3).

Except for some Bauwens trials (with central ignition), Pasman and Kumar experiments, the maximum overpressure is always due to the external explosion P_1.

Because Daubech and al. (2013) experiments are recent and well instrumented (two peaks are measured), we shall pay a special attention to these results. The figure 3 and 4 shows the comparison of the model with the experimental data.

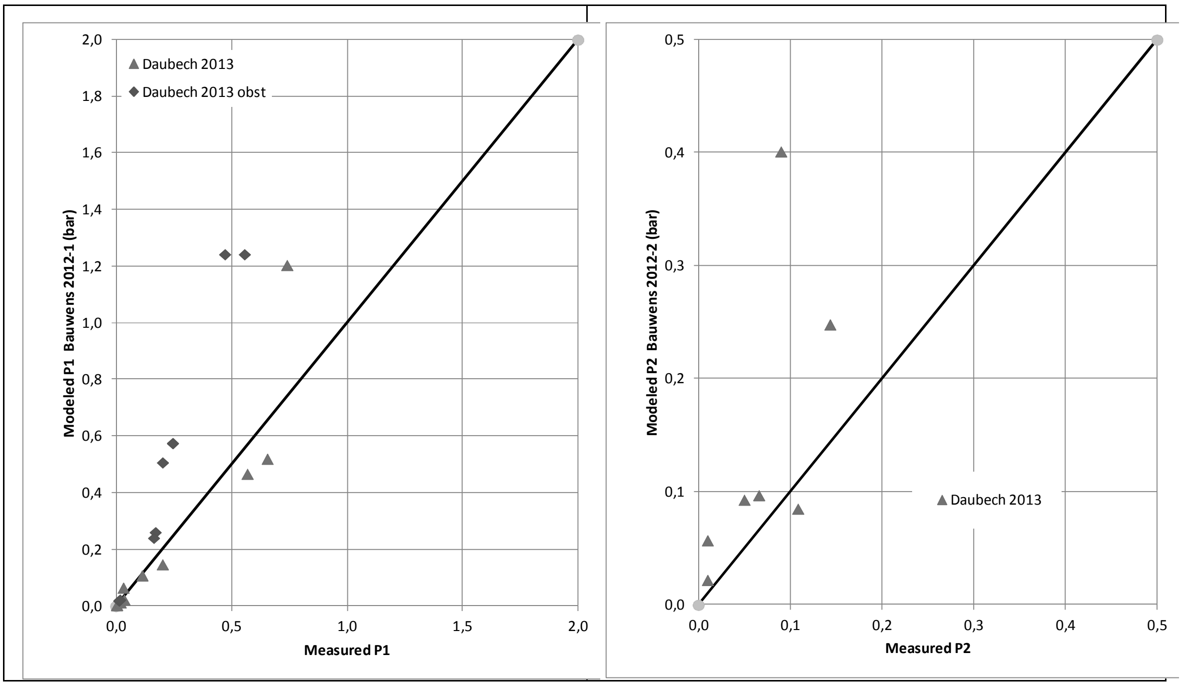

Figure 3 : Comparison between measured (Daubech et al. 2013) and Bauwens et al. (2012-1) model for P_1 and P_2

As shown of figure 3 (left), the agreement is globally acceptable for P_1. For the more reactive trials in presence of obstacles, the model overpredicts the overpressure. For P_2, the agreement is also good. For an unknown reason, a point is totally outside of the correlation (24,8% H_2, Av = 0,49 m^2, no obstacles) with a calculated overpressure of more than 0,4 bar compared to a measurement only of 0,02 bar.

Bauwens 2012-2

For enclosure without mechanical vent, the last version of the Bauwens and al model has been modified in order to take into account the enclosure aspect ratio for the flame acoustic parameter Ξ_A . A formula used to calculate the overpressure has been also modified to limit the value to the adiabatic constant volume overpressure for the smallest vents.

The figure 4 shows the comparison between Bauwens 2012-2 model results against experimental data.

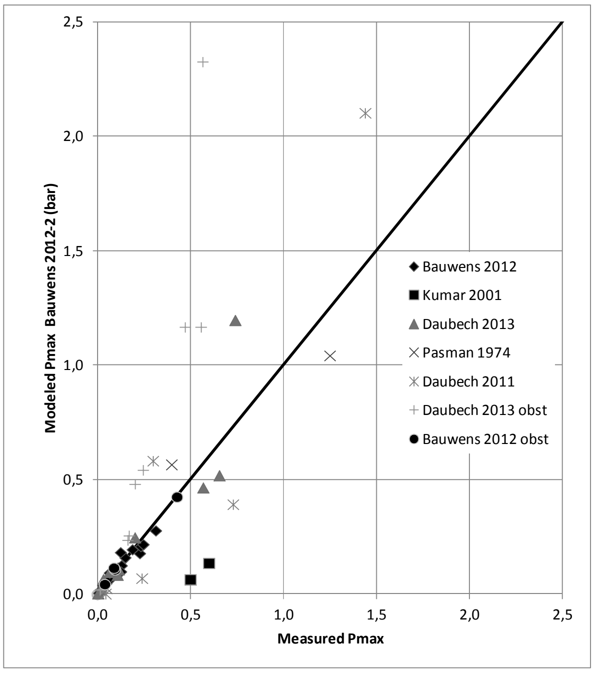

Figure 3: Comparison between measured (all points) and Bauwens et al. (2012-2) model for P_1 and P_2

Globally, the Bauwens 2012-2 model gives better results than the Bauwens 2012-1 model. The highest overestimated overpressures are well lowered by the new equation taking into account the constant volume explosion pressure. Concerning Kumar et al. experiments, the high aspect ratio of the enclosure (AR = 10/3) decreases widely the modified flame-wrinkling factor Ξ_A and leads to very low overpredicted overpressures.

Molkov et al. VST models 1999, 2001 and 2008

The figures 4, 5 and 6 presents the comparison of the maximal overpressure against calculated overpressures with the 1999, 2000 and 2008 version of the Molkov et al. VST model.

Due to the fact that the VST models do not take into account obstacles, experiments with obstruction were excluded from this comparison. Concerning ignition location, only the locations leading to the highest overpressures are considered (mainly back wall ignition).

The 1999 VST model globally gives a global good agreement. The main discrepancies are for the Kumar (120 m^3) lean experiments for which the maximum overpressure is the flame acoustic peak which is not considered in the model. Unlike the Bauwens model, for the highest hydrogen concentration (and then overpressure), the VST99 model gives reasonable results.

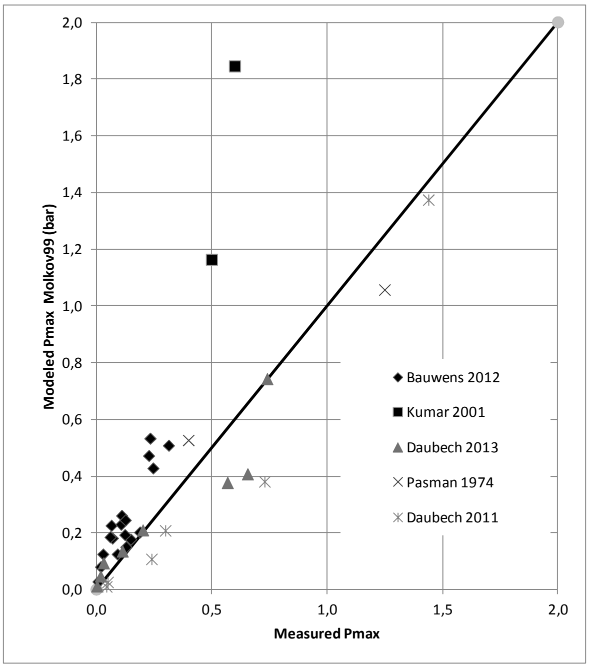

Figure 5 : Comparison between measured and Molkov VST model 1999

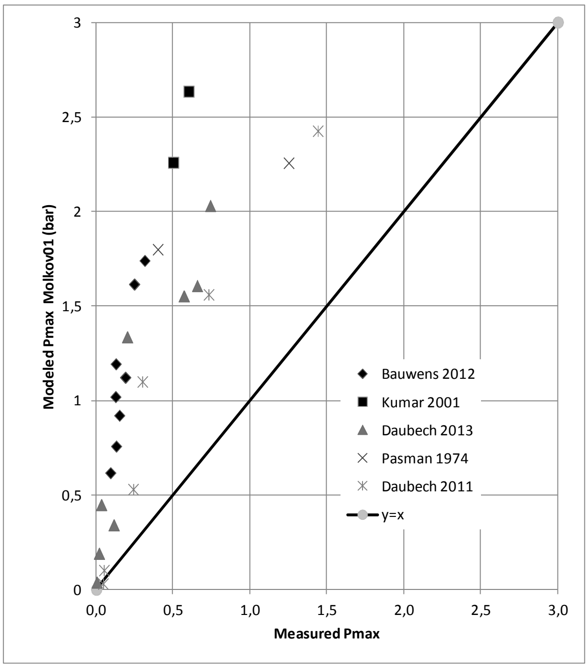

Figure 6 : Comparison between measured and Molkov VST model 2001

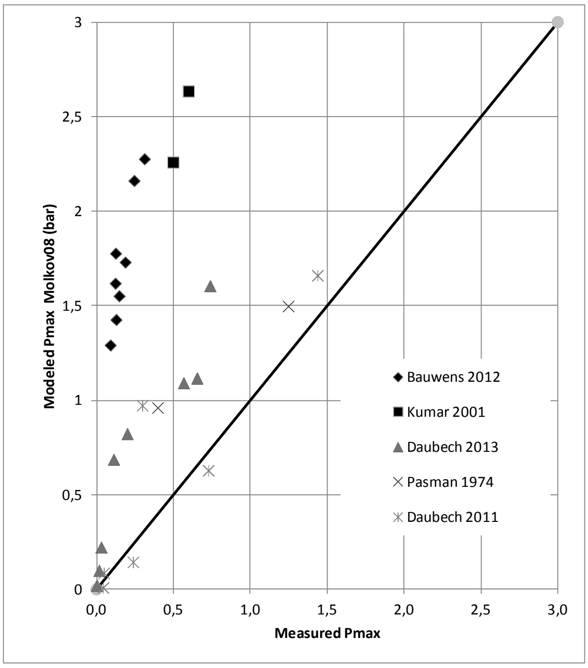

Figure 7 : Comparison between measured and Molkov VST model 2008

The recent versions (2001 and 2008) of the Molkov model give overconservative results. The modelled overpressure is largely overpredicted for almost all cases. A large part of this overestimation is because the authors were intentionally modified the correlation to produce conservative results [18]. It could be also due to the fitting of parameters against experiments in unusual geometrical situations (Kumar et al. [15] spherical vessel with a duct or Groethe et al. [16] partially filled tunnel).

5.0 CONCLUSIONS

A comparison of the recent published engineering vented explosion models predictions with the available experiments with hydrogen has been performed. The models proposed by Bauwens in 2012 [4, 7] are in good agreement with experimental data for hydrogen concentrations below 20% and for enclosure with small aspect ratios. The initial 1999 Molkov et al. model [12] is less predictive but gives reasonable results. For concentration between 20 and 30% of hydrogen, its use seems to be even preferable. However, it should be used with care because at these concentrations in large volumes and particularly in presence of obstacles, a deflagration to detonation transition could not be ignored. The recent versions of Molkov et al. model [13, 6] largely overpredict the overpressure and should be used with care. Some improvements should be realized in the future in order to take into account hydrogen distribution (stratification and layers) in the enclosure

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REFERENCES

1. Pasman H.J., Groothuisen Th.M., Gooijer P.H. Design of Pressure Relief Vents, in “Loss Prevention and Safety Promotion in the Process Industries”, Ed. Buschman C.H., Elsevier, New-York, 1974, pp.185-189.

2. Daubech J, Proust C; Leprette E., Jamois D. Dynamics of vented hydrogen-air deflagrations ; ICHS4 ; San Francisco September 2011

3. Kumar R. Vented combustion of hydrogen-air mixtures in a large rectangular volume. AIAA conference (2001).

4. C.R. Bauwens, J. Chao, S.B. Dorofeev Effect of hydrogen concentration on vented explosion overpressures from lean hydrogen–air deflagrations International Journal of Hydrogen Energy, Volume 37, Issue 22, November 2012, Pages 17599-17605

5. Daubech et al. 2013 Paper presented at ICHS 2013 Brussels

6. Molkov V., Verbecke F, Saffers, J.B. Uniform hydrogen air deflagration in vented enclosures and tunnels : predictive capabilities of engineering correlations and LES - Seventh ISHPMIE – 2008 - St. Petersburg

7. C. Regis BAUWENS, Jenny CHAO and Sergey B. DOROFEEV Evaluation of a multi peak explosion vent sizing methodology IX ISHPMIE - International Symposium on Hazard, Prevention and Mitigation of Industrial Explosions – July 2012 - Cracow, Poland

8. Bauwens C; Chafee J ; Dorofeev S. Effects of ignition, vent size and obstacles on vented explosion overpressures in propane – air mixtures. Combustion Science and Technology 182: 1915 – 1932 – 2010.

9. Chao J; Bauwens C ; Dorofeev S. An analysis of peak overpressures in vented gaseous explosions. Proceedings of the combustion institute 2010.

10. F. Tamanini and J.L. Chaffee, Turbulent Vented Gas Explosions with and Without Acoustic Waves, Symposium (International) on Combustion, The Combustion Institute, Pittsburgh, 1992, 1845-1851.

11. NFPA 68 Guide for Venting of Deflagrations. National Fire Protection Association, Quincy, MA, USA, 1998.

12. V.V. Molkov, R. Dobashi, M. Suzuki, T. Hirano, Modelling of vented hydrogen-air deflagrations and correlations for vent sizing, J Loss Prev Process Ind 12 (1999)

13. Molkov V. Unified correlations for vent sizing of enclosures at atmospheric and elevated pressures - Journal of Loss Prevention in the Process Industries, Volume 14, Issue 6, November 2001, Pages 567-574

14. http://www.c.morley.dsl.pipex.com/

15. Kumar R., Dewit W., & Greig D. (1989). Vented explosion of hydrogen-air mixtures in a large volume. Combustion Science and Technology, 66, 251-266

16. M. Groethe, E. Merilo, J. Colton, S. Chiba, Y. Sato, H. Iwabuchi Large-scale hydrogen deflagrations and detonations International Journal of Hydrogen Energy, Volume 32, Issue 13, September 2007, Pages 2125-2133

17. Bauwens, C.R., and Dorofeev, S.B Effect of Initial Turbulence on Vented Explosion Overpressures .7th International Seminar on Fire and Explosion Hazards 5–10 May 2013 Providence, United States.

18. V. Molkov, personal communication