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A simple model for calculating peak pressure in vented explosions of hydrogen and hydrocarbons

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ABSTRACT

The authors presented a basic mathematical model for estimating peak overpressure attained in vented explosions of hydrogen in a previous study (Sinha et al. [1]). The model focussed on idealized cases of hydrogen, and was not applicable for realistic accidental scenarios like presence of obstacles, initial turbulent mixture, etc. In the present study, the underlying framework of the model is reformulated to overcome these limitations. The flame shape computations are simplified. A more accurate and simpler formulation for venting is also introduced. Further, by using simplifying assumptions and algebraic manipulations, the detailed model consisting of several equations is reduced to a single equation with only four parameters. Two of these parameters depend only on fuel properties and a standard table provided in the Appendix can be used. Therefore, to compute the overpressure, only the two parameters based on enclosure geometry need to be evaluated. This greatly simplifies the model and calculation effort. Also, since the focus of previous investigation was hydrogen, properties of hydrocarbon fuels, which are much more widely used, were not accounted for. The present model also accounts for thermophysical properties of hydrocarbons and provides table for fuel parameters to be used in the final equation for propane and methane. The model is also improved by addition of different sub-models to account for various realistic accidental scenarios. Moreover, no adjustable parameters are used; the same equation is used for all conditions and all gases. Predictions from this simplified model are compared with experimentally measured values of overpressure for hydrogen and hydrocarbons and found to be in good agreement. First the results from experiments focussing on idealized conditions of uniformly mixed fuel in an empty enclosure under quiescent conditions are considered. Further the model applicability is also tested for realistic conditions of accidental explosion consisting of obstacles inside the enclosure, non-uniform fuel distribution, initial turbulent mixture, etc. For all the cases tested, the new simple model is found to produce reasonably good predictions.

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Introduction

Storage and generation of flammable gases is often required in various industrial installations. Cooking or heating for household applications also depend on these gases which are either stored in compressed form or send through pipelines. The amount of gas present is often more than what is required to cause an explosion. Hence, it is critical to assess plant or building safety and ensure adequate precautionary measures and arrangements. Explosion venting is a simple and effective method to relive pressure in case of accidental explosion. Venting is provided by mounting vent panels on enclosure or building wall. These vent panels open while pressure is rising due to explosion, and reduce internal pressure by venting out a large amount of burnt and unburnt gases. For explosion venting to be an effective safety measure, it is important that the vent panel is carefully designed and given appropriate area. Design of vent panels is an intricate exercise which depends on enclosure geometry and combustion characteristics of the fuel. There are several studies on vented explosion using experimental, computational or empirical modelling approaches. Experimental investigations focus on measuring peak pressure in a configuration for a given fuel mixture and vent area. By varying the fuel composition and vent area, the optimum vent area for that configuration can be estimated. It is important to understand that experiments are expensive, dangerous, and require significant infrastructure and safety precautions to conduct experiments on a large-scale enclosure or building. Only a few organizations and groups have infrastructure to conduct large scale experiments. Considering the issues with experimental investigation, computational approach may seem suitable option, but modelling a flame of the size of a realistic enclosure is a daunting task. Accurately modelling processes involved in a vented explosion is a difficult task even for most advanced computational models available. In a recent blind prediction study (Skjold et al. [2,3]), computational studies are found to give errors of an order of magnitude higher than the measured pressure. Additionally, computational modelling involves significant computational costs and run-time owing to the large and complex geometries involved. Considering the above-mentioned challenges in experimental and computational investigations, Engineering Models (EMs) appear to be the preferred method for investigating vented explosions. EMs are fast and easy to use and can give a reasonably accurate prediction. EMs are generally formulated to predict the peak pressure for a given configuration. Additionally, required vent area can be calculated if the permissible pressure is known.

Previous studies on vented explosions focus mainly on "idealized" empty container with uniformly mixed fuels and no obstacles (Kumar [4], Daubech et al. [6]). The configurations proved to be useful for fundamental studies, but a practical industrial installation will have equipment, pipes, and other objects in flame path which will act as obstacle. Recent experiments (Bauwens et al. [7,8], Skjold et al. [9,10]) have demonstrated that the presence of obstacles will increase the peak pressure significantly. Hence, this configuration needs to be studied in more detail and focussed modelling efforts are required. In recent reviews on engineering models (Sinha et al. [1,11,12]), it has been pointed out that currently existing models are not equipped to handle realistic accidental scenarios and focussed modelling efforts are required for practical configuration like presence of obstacles, stratified fuel distribution, etc. Additionally, the statutory norms require a simple model that can be implemented and computed easily, without much effort and computational costs. Hence, an ideal model will have minimum number of equations and input parameters. Moreover, it is preferred that the model does not involve use of any tuneable constants. This is to ensure that the model results are consistent, and do not vary with the experience and skill of the end-user.

A basic mathematical model is proposed previously (Sinha et al. [1]). This model has been demonstrated to predict accurately for idealized cases of hydrogen explosions. This model is reformulated in the present study. The venting formulation is replaced by a much simpler method, and the flame area computations are also simplified. However, as the effort was to account for various physical processes present in vented explosions, the resulting model became quite complicated and required solving several equations with many input parameters. Hence, to increase the applicability of this model and to make it more suitable to be recommended for standards, the final model is simplified, and reduced to a single equation. Further improvement is also carried out by adding various sub-models to account for realistic accidental scenarios. Modelling details for the detailed model, further improvements and all simplifying assumptions for this model are explained in detail in subsequent sections.

Basic model description

The earlier development of the basic model is described elsewhere (Sinha et al. [1]). Here a brief summary of final equations is provided for completeness. The model considers four steps to describe the venting process:

1 Initial flame propagation inside the enclosure,
2 External cloud formation,
3 External explosion, and
4 Internal overpressure for maximum internal flame area.

The computation process can be described briefly as:

The flame propagation speed is estimated using the experimental measurements from Bauwens et al. [13–15]:

$$\frac{U}{U_0} = \left(\frac{R}{R_0}\right)^{\beta} \quad (1)$$

Where U is the flame propagation velocity at a distance R from the ignition location, and U_0 is the flame speed at critical radius R_0, and β is the fractal excess. Further, the external cloud radius (R_{cl}) is estimated using the vortex roll-up theory from Sullivan et al. [16]:

$$R_{cl} = \sqrt[3]{\frac{3\,\pi\,R_P^2\,L_P}{2.2\Lambda}} \quad (2)$$

Where R_P is the radius and L_P is the stroke length of equivalent piston, and Λ is the parameter for ring vorticity [1]. Further, pressure generated form the external explosion (p_{ex}) can be calculated using Taylor's spherical piston theory (Strehlow et al. [17]):

$$p_{ex} = 2\,\gamma_u\left(\sigma^2 - \sigma\right) M_P^2 \quad (3)$$

where γ_u is the ratio of specific heats of unburnt gases, σ is the expansion ratio, and M_P is the Mach number of the flame in external cloud. Finally, the internal overpressure (p) can be computed by using the orifice equation from Tamanini [18].

$$p = \left[\left(\frac{A_f U}{u_{cd}\,A_v}\right)^2 (p_{cr} - p_{ex})\right] + p_{ex} \quad (4)$$

Where A_f is the surface area of the flame, U is flame speed near the vent, A_v is the vent area, p_{cr} is the critical pressure and u_{cd} is the vent parameter defined in Ref. [18].

Model simplification and generalization

The model presented in the previous section attempts to incorporate physical phenomenology. It was found to give accurate predictions for hydrogen explosions in previous studies (Sinha et al. [1], and Skjold et al. [3]). The major drawback of this model is that it has too many equations and input parameters. On a closer scrutiny, it appears that the model also computes many intermediate parameters. These intermediate parameters might be useful to gain physical insight, or analysing other aspects, but are not required to be computed explicitly for obtaining internal overpressure. The objective of the present endeavour is to simplify this model while retaining the same level of accuracy. The complexity can also be reduced by considering some simplifying assumptions, described in the subsequent section. The major areas of focus are:

1 External cloud radius
2 Flame surface area
3 Gas venting process.

External cloud radius (R_{Cl})

Computing R_{Cl} is a tedious task which requires several equations to be solved (Sinha et al. [1], Sinha and Wen [36]). In our previous work [36], it is shown that the cloud radius depends on ignition location. However, the difference in cloud radius for different ignition locations is not very large, as observed in Table 1:

Average R_{Cl} for a given enclosure is plotted with respect to enclosure volume, as shown in Fig. 1, where computations were made for the tests data in Refs. [2,5–7,24]. As evident, the

Table 1 – Average cloud radius (in m) for various ignition locations.

	CI	BWI
Bauwens et al. [7]	1.280	1.701
Kumar [4]	1.664	2.091

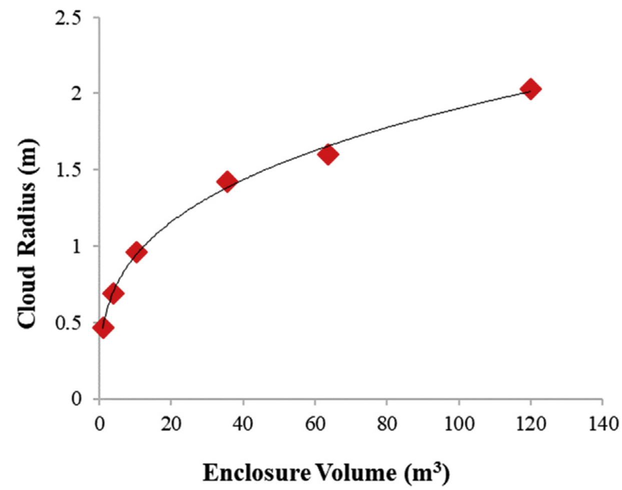

Fig. 1 – Average cloud radius for various enclosure volumes. Symbols show computed radius using Eq. (2). The curve is for the function $R_{Cl} = 0.5\,V^{0.3}$.

average cloud radius increases with enclosure volume and the relationship can be expressed as:

$$R_{Cl} = 0.5\,V^{0.3} \quad (5)$$

This is a major simplification for the model, as a large part of computational effort (see Sinha and Wen [36]) can now be saved using the approximation of Equation (5).

To further assess this simplified approach, cloud radius predictions using Eq. (5) are compared with the experimental measurements of Daubech et al. [24] and Proust and Leprette [25] in Table 2. As clear from this comparison, Eq. (5) provides a reasonably accurate predictions for cloud radius.

Flame surface area

The flame shape calculation is also cumbersome and can be simplified. It is a reasonably good approximation to express the flame surface as a percentage of total internal surface area of the enclosure (A_{in}). The flame surface area (A_f) is computed as:

$$A_f(BWI) = 0.5\,A_{in} \quad (6)$$

$$A_f(CI) = 0.25\,A_{in} \quad (7)$$

for back-wall and central ignition cases respectively. The enclosure internal area can be estimated as:

Table 2 – Comparison of measured cloud radius from Refs. [24,25] with calculated radius values using Eq. (5).

Fuel	Vol (m^3)	Measured cloud radius (m)	Calculated cloud radius (m)
Hydrogen [24]	4	0.70	0.76
Methane [25]	1	0.47	0.50
	10	1.10	1.00
	100	2.00	1.99

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$$A_{in} = 2(L \cdot B + B \cdot H + L \cdot H) \tag{8}$$

where L, B, and H are enclosure dimensions.

Gas venting process

Gas venting through the enclosure is described using Tamanini's equation [18] in the previous model [1]. This can be replaced by a simplified analysis as described in this section. The flow of gases escaping from the vent can be approximated by using Bernoulli's equation. The computation is made for time instant when the flame is approaching the vent. Considering two points X1 and X2 in the unburnt gases, just inside and outside the vent:

$$\frac{p_1}{\rho_u} + \frac{u_1^2}{2} = \frac{p_2}{\rho_u} + \frac{u_2^2}{2} \tag{9}$$

where subscript 1 is for the internal (X1) and 2 is for the external (X2) location, as shown in Fig. 2.

Now, the velocity u_1 can be approximated as:

$$u_1 = U_{Leff}\left(\frac{\sigma - 1}{\sigma}\right) \tag{10}$$

where is U_{Leff} is the flame-speed near the vent computed using Eq. (1), and σ is the expansion ratio for fuel. Similarly, u_2 can be expressed as:

$$u_2 = \left(\frac{A_f}{A_v}\right) U_{Leff}\left(\frac{\sigma - 1}{\sigma}\right) \tag{11}$$

Substituting Eqs. (10) and (11) in Eq. (9):

$$p_1 - p_2 = \left[\frac{\rho_u}{2 \cdot 10^5}\left\{U_{Leff}\left(\frac{\sigma - 1}{\sigma}\right)\right\}^2\left\{\left(\frac{A_f}{A_v}\right)^2 - 1\right\}\right] \tag{12}$$

This gives the pressure drop across the vent for the instance when the flame is approaching the vent. Expressing the variables in the Right-hand side (RHS) of Eq. (12) in S.I. units will produce pressure in N/m^2. To convert this pressure in *bar*, which is a general unit used in explosion literature, the RHS is divided by 10^5. It is reasonable to assume that the same pressure drop is maintained across the vent at the time of peak pressure. Now, for peak internal pressure, the maximum pressure produced by external explosion must be considered. Hence, from Eq. (3):

$$p_2 = p_{ex} = 2\,\gamma_u(\sigma^2 - \sigma)\,M_P^2 \tag{13}$$

Substituting the value of Mach number M_P:

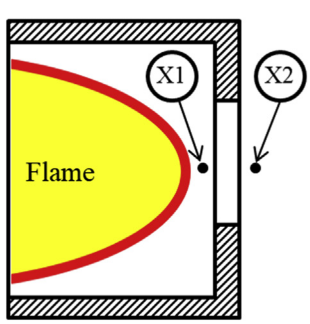

Fig. 2 – Locations of points X1 and X2.

$$p_2 = \left[2\,\gamma_u(\sigma^2 - \sigma)\left(\frac{U_{Rcl}}{a_0}\right)^2\right] \tag{14}$$

where U_{Rcl} denotes flame propagation speed at the edge of external cloud computed using Eq. (1), and a_0 is the acoustic velocity in unburnt gases. From Eqs. (12) and (14):

$$p_1 = \left[\frac{\rho_u}{2 \cdot 10^5}\left\{U_{Leff}\left(\frac{\sigma - 1}{\sigma}\right)\right\}^2\left\{\left(\frac{A_f}{A_v}\right)^2 - 1\right\}\right] + \left[2\,\gamma_u(\sigma^2 - \sigma)\left(\frac{U_{Rcl}}{a_0}\right)^2\right] \tag{15}$$

Further simplification

Eq. (15) can be re-written as:

$$p_1 = \left[\frac{\rho_u}{2 \cdot 10^5}\left\{\frac{U_0}{R_0^\beta}\left(\frac{\sigma - 1}{\sigma}\right)\right\}^2\right]\left[\left(L_{eff}^{\beta 1}\right)^2\left\{\left(\frac{A_f}{A_v}\right)^2 - 1\right\}\right] + \left[\frac{2\,\gamma_u(\sigma^2 - \sigma)}{a_0^2}\left(\frac{U_0}{R_0^\beta}\right)^2\right]\left[R_{Cl}^{\beta 2}\right]^2 \tag{16}$$

This equation can also be expressed in simplified form:

$$p = (F1 \cdot G1) + (F2 \cdot G2) \tag{17}$$

where

$$F1 = \left[\frac{\rho_u}{2 \cdot 10^5}\left\{\frac{U_0}{R_0^\beta}\left(\frac{\sigma - 1}{\sigma}\right)\right\}^2\right], \tag{18}$$

$$F2 = \left[\frac{2\,\gamma_u(\sigma^2 - \sigma)}{a_0^2}\left(\frac{U_0}{R_0^\beta}\right)^2\right], \tag{19}$$

$$G1 = \left[\left(L_{eff}^{\beta 1}\right)^2\left\{\left(\frac{A_f}{A_v}\right)^2 - 1\right\}\right], \tag{20}$$

$$G2 = \left[R_{Cl}^{\beta 2}\right]^2. \tag{21}$$

Hence, the detailed model is simplified and reduced to a single equation – Equation (17) which predicts overpressure for vented explosions. Another major simplification is in the form of terms $F1$ and $F2$. A closer inspection reveals that these terms do not contain any geometrical parameters and are completely determined by the fuel properties. This is a major advantage, as these terms can be computed in advance and look-up tables can be created for future calculations. Tables containing $F1$ and $F2$ for hydrogen, methane and propane are given in Appendix. Moreover, the terms $G1$ and $G2$ can further be simplified as:

$$G1 = \begin{cases} \left[(L)^{2\beta 1}\left\{\left(\frac{0.50\,A_{in}}{A_v}\right)^2 - 1\right\}\right] & \text{for Back-wall ignition (BWI)} \\ \left[\left(\frac{L}{2}\right)^{2\beta 1}\left\{\left(\frac{0.25\,A_{in}}{A_v}\right)^2 - 1\right\}\right] & \text{for Central-ignition (CI)} \end{cases} \tag{22}$$

$$G2 = \left(0.5\,V^{0.3}\right)^{2\,\beta 2} \tag{23}$$

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Where L is the enclosure length in the flame propagation direction, A_{in} is the enclosure internal area, A_v is the vent area and V is the volume of the enclosure, β is the fractal excess, as shown in Equation (1), $\beta1$ and $\beta2$ are modified fractal excess parameters. Values of β, $\beta1$ and $\beta2$ for various fuels are given in Appendix. Hence, from the above discussion, it can be summarized that overpressure can be computed using the simplified equation (Equation (17)) using pre-tabulated values of $F1$ and $F2$, and only $G1$ and $G2$ need to be calculated, which are further simplified and expressed in terms of enclosure dimensions. This is a major simplification for the model, as a large part of calculation effort can now be saved. Steps required for overpressure calculations using the present simplified model are explained briefly in Appendix. Further validation of this simple model and additional sub-models for realistic conditions are given in Section Results.

Results

The present model and other models available in literature are used to predict maximum overpressure obtained for conditions investigated in experiments of Bauwens et al. [7]. Other models used are EN-14994 [19], NFPA-68 [20], Bauwens detailed model [21], Bauwens simplified model [22], and Molkov model [23]. Predictions from all these models are compared with experimental results in Fig. 3. As evident, the present model gives accurate or comparable predictions than other models. Another advantage is that the present model tends to over-predict within a reasonable limit, which is desirable, especially for formulating safety standards. This model is further tested for applicability in various conditions and realistic accidental scenarios. The experimental studies considered in this study are summarized in Table 3. Experimental investigations can be divided into various groups based on the configuration and consideration of realistic scenarios: (1) Idealized configuration, (2) Elongated enclosures, (3) Initial turbulent conditions, (4) Presence of obstacles, (5) Stratified mixture distribution and (6) Combination of realistic accidental conditions.

Idealized configuration

These are experiments with enclosure having standard geometrical shape, no obstacles, uniformly mixed fuel, and quiescent starting conditions. Results that fall into this category are obtained from the studies of Bauwens et al. [7], Daubech et al. [6,24] Proust and Leprette [25], Wang et al. [37], and Skjold et al. [9,10], for hydrogen. As the focus of this study was on lean mixtures for hydrogen, hence experiments with near stoichiometric composition (like Pasman et al. [38]) are not considered. For hydrocarbons like methane and propane, experiments from Bauwens et al. [8], Chao et al. [26], Harrison et al. [27], Bimson et al. [28], and Tomlin et al. [29] are referred. Experiments from Bimson et al. [28] are also used for Solvex validations. The enclosures used in idealized experiments have volume in the range 1 m^3 (Daubech et al. [24]) to 550 m^3 (Bimson et al. [28]). The predictions for these set of experiments are shown in Figs. 4 and 5. Predictions for enclosures with larger volumes are shown in Fig. 4 and for enclosures with smaller volume are shown in Fig. 5. As clear from these results, the present model gives considerably accurate predictions for a large range of conditions, different fuels and enclosure geometries.

Elongated enclosures

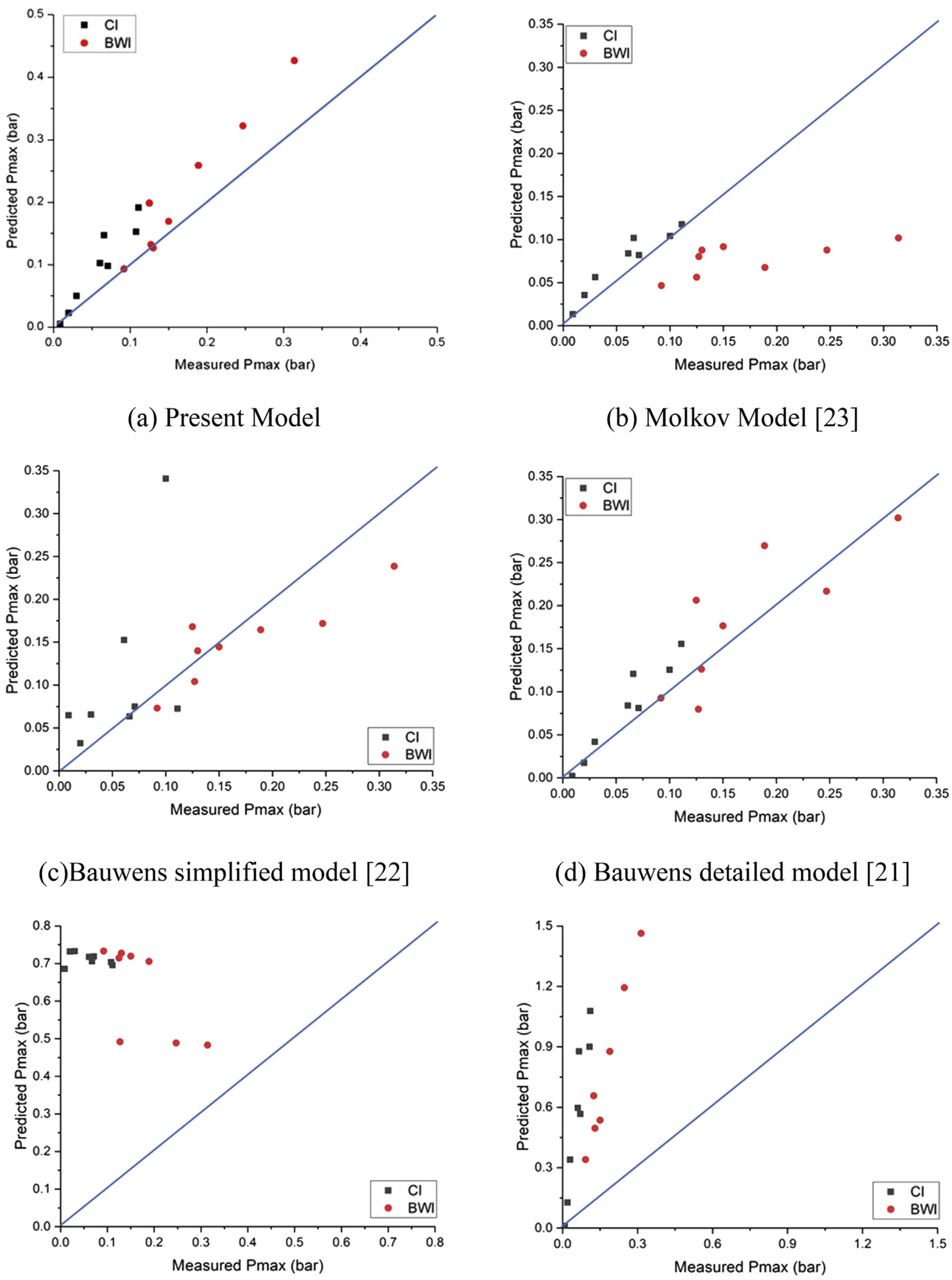
These sets of experiments are undertaken in idealized conditions using an enclosure whose aspect ratio (L/D) is larger than 2.5. The studies that are considered for this section include the studies of Kumar [5] and Daubech et al. [6]. The flame reaches to the side walls much before it reaches the vent. Hence, flame near the ignition region at back-wall is expected to burn out till the forward moving flame reaches the vent. Using flame area equation for a compact enclosure is expected to give higher flame areas than available. So, realistic estimate of the actual flame area is required for this set of experiments. It is assumed that for this configuration, the actual flame area for back-wall ignition is half of what is obtained from Eq. (6), and other equations remain unchanged. The predictions compared with experimental measured values are shown in Fig. 6. It is observed that a good agreement is obtained with the experimental measurements and predicted values. Daubech et al. [6] carried out experiments for only two fuel concentration using their 10.5 m^3 enclosure. Hence, their results show variation in experimental repeatability. However, the model produces same output for the same fuel concentration in same configuration. Hence, same prediction is obtained for different experiments which is observed in Fig. 6(a). As evident, the present model produces accurate predictions for enclosures with $L/D \leq 4$. Larger L/D ratios will be for pipes or ducts. For longer pipes, especially with obstacles, there is additional risk of Deflagration to Detonation Transition (DDT) which is beyond the scope of this model. Hence, it is recommended to use this model for enclosures with $L/D \leq 4$.

Initial turbulent conditions

These set of experiments deal with experiments where the initial fuel mixture is made turbulent, usually by running a set of fans inside the enclosure before ignition. This condition is closer to realistic accidents, as it is expected that any fuel leakage will generate turbulence. The major effect of turbulence is observed in increase of flame speed. This effect is accounted for by modifying the flame speed parameter $\beta1$. The objective is to obtain a simple model with reasonably good predictions. It is also desirable to obtain conservative estimates of peak pressure. Hence, turbulence intensity is not accounted for and a conservative value of $\beta1$ is chosen. The recommended values of $\beta1$ are given in Table A3. Predictions using this modified $\beta1$ for experiments of Bauwens et al. [29], Kumar [5] and Daubech et al. [30] are shown in Fig. 7. As observed, a close approximation is obtained with this approach.

Presence of obstacles

Enclosures in industrial installations are highly likely to have various equipment and machinery which will act as obstacles



(a) Present Model

(b) Molkov Model [23]

(c)Bauwens simplified model [22]

(d) Bauwens detailed model [21]

(e) EN-14994 [19]

(f)NFPA-68 [20]

Fig. 3 – Comparison of prediction from various models for experiments of Bauwens et al. [7].

in flame-path. Similarly, explosions in a household building will also have furniture and other objects which act as obstacle. Hence, this set of experiments represents a closer scenario that is observed in actual accidents. The experimental results from Bauwens et al. [7,8], Chao et al. [26], Bimson et al. [28], Skjold et al. [9,10], Tomlin et al. [31], and Diakow et al. [32] are considered for this study. Obstacle can be treated as a bluff body in flame path. Flow past an obstacle

Table 3 – Experimental investigations considered for the present study.

		Fuel	Vol (m^3)	Fuel Composition (%)	Remarks
1	Daubech et al. [6]	Hydrogen	1	10–20	Idealized
2	Skjold et al. [9,10,35]	Hydrogen	35.7	15–21	Idealized
3	Wang et al. [37]	Hydrogen	1	14, 25	Idealized
4	Kumar [4]	Hydrogen	120	9–12	High L/D
5	Daubech et al. [6]	Hydrogen	10.5	14, 23	High L/D
6	Bauwens et al. [7]	Hydrogen	63.7	12–20	Obstacles
7	Daubech et al. [24]	Hydrogen	4	10–25	Idealized
8	Bauwens et al. [36]	Hydrogen	63.7	12–15	Initial turbulence
9	Kumar [5]	Hydrogen	120	8–11	Initial turbulence
10	Daubech et al. [30]	Hydrogen	4	10–21	Initial Turbulence
11	Schiavetti et al. [34]	Hydrogen	1.14	8–20	Stratified
12	Skjold [9,10]	Hydrogen	35.7	18–24	Obstacles, Stratified, Initial turbulence
13	Chao et al. [26]	Methane	63.7	Stoichiometric	Obstacles
14	Bauwens et al. [8]	Propane	63.7	Stoichiometric	Obstacles
15	Chao et al. [26]	Propane	2.42	Stoichiometric	Idealized
16	Bimson et al. [28]	Methane	550	Stoichiometric	Obstacles
17	Bimson et al. [28]	Propane	550	Stoichiometric	Obstacles
18	Bimson et al. [28]	Methane	2.5	Stoichiometric	Obstacles
19	Bimson et al. [28]	Propane	2.5	Stoichiometric	Obstacles
20	Harrison et al. [27]	Natural Gas	30	Stoichiometric	Idealized
21	Harrison et al. [27]	Propane	30	Stoichiometric	Idealized
22	Diakow et al. [32]	Propane	391.5	Stoichiometric	Obstacles
23	Tomlin et al. [31]	Natural Gas	182	Stoichiometric	Obstacles

creates a recirculation wake region in downstream direction. This recirculation region has high shear at its boundary, and it impedes flame moving towards the obstacle in downstream direction. Bluff-body stabilized combustors utilize this recirculation region to stabilize or hold the flame. In case of vented explosion, the additional flame wrapped around the obstacle provides increased flame-surface area and hence results in increase in overpressure. The surface area of the flame around an obstacle can be equated to the recirculation region formed by the obstacle. This recirculation length (L_{rec}) can be approximated as (Minguez et al. [33]):

$$L_{rec} = 0.6\, L_{obs} \tag{24}$$

where L_{obs} is the characteristic length scale of the obstacle. The flame area around the obstacle can be estimated as:

$$A_{obs} = (P_{obs} + 2\, L_{rec}\,)\; H_{obs} \tag{25}$$

where A_{obs} is the area of flame wrapped around obstacle, P_{obs} is the obstacle perimeter, and H_{obs} is the obstacle height. Combining Eqs. (24) and (25):

$$A_{obs} = (P_{obs} + 1.2\, L_{obs}\,)\; H_{obs} \tag{26}$$

This additional area (A_{obs}) must be added to flame surface area (A_f), as computed in Eq. (6) or Eq. (7). Moreover, configuration with obstacles can also be classified as low or highly congested. Configurations with obstacles in one or two rows in the flame path can be classified as low congestion. However, for cases with greater number of rows, the congestion is high, which promotes interaction of wakes from different rows of obstacles and consequently the pressure is much higher than lower congestion cases. Another possible effect of higher congestion is that the repeated rows of obstacles keep the turbulence levels higher throughout the flame path and prevent any re-laminarization effects. Hence, the flame speed also increases, and resulting overpressure is much higher. This increase in flame speed can be accounted for by modifying β1, as shown in Table A3. Predictions for cases with obstacles are shown in Fig. 8. As evident, a good match is noticeable for most experiments. The deviations are also slightly over-predicted values, which makes this model safer to use.

Stratified mixture distribution

This configuration can be understood to mimic the accidents caused by gas leakage. As leakage of fuel gases produces an explosive mixture quickly, it doesn't get enough time to mix uniformly, and the mixture remains in stratified configuration by the time it gets ignited. Experimental results from Schiavetti et al. [34] are used for this study. For hydrogen, the stratification is always vertical, and the topmost layer is most reactive. For a vertically oriented enclosure, as used in Ref. [34], it is understood that the peak pressure is caused by the most reactive layer situated at the top. Hence, this configuration can be modelled assuming the most reactive concentration to be the equivalent concentration; and using the model equations from section 3. Comparison of predictions and experimental measurements for this class of experiments are shown in Fig. 9.

Combination of realistic accidental conditions

All previously discussed conditions represent idealized investigations on actual accidental scenarios, with each subsection focussing on one scenario alone. Real accidents will involve a combination of two or more scenarios presented in previous sub-sections. To assess significance of each configuration, they are investigated separately. But to

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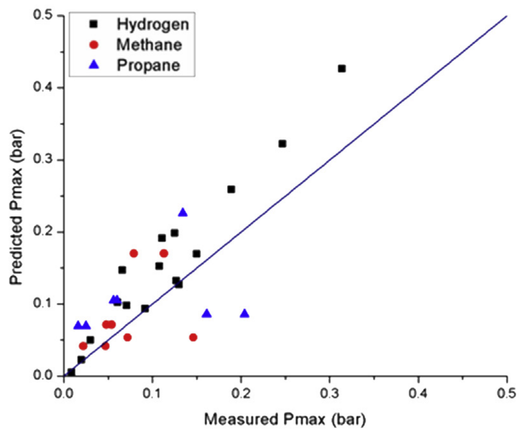
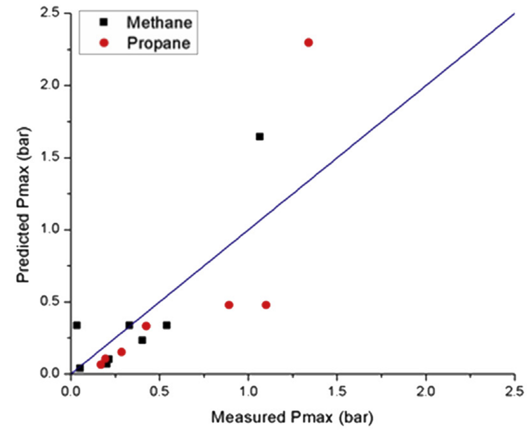
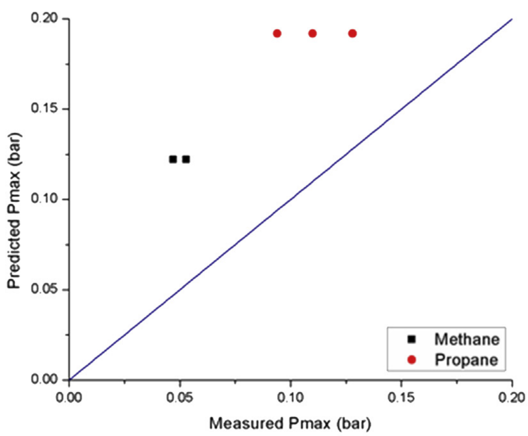


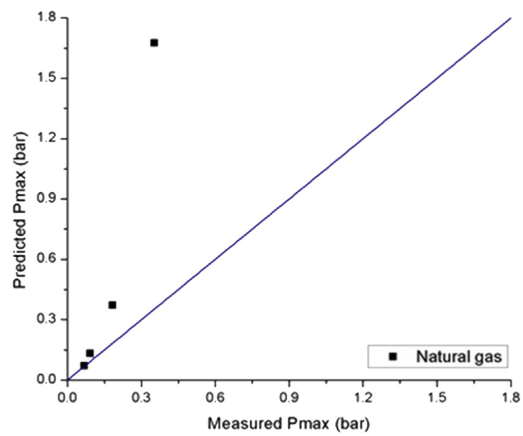
(a) Bauwens et al. – 63.7 m^3 [7, 8, 26]



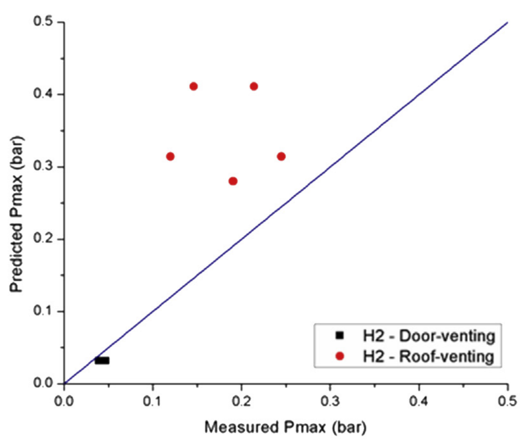
(b) Harrison et al. – 30 m^3 [27]



(c) Bimson – 550 m^3 [28]

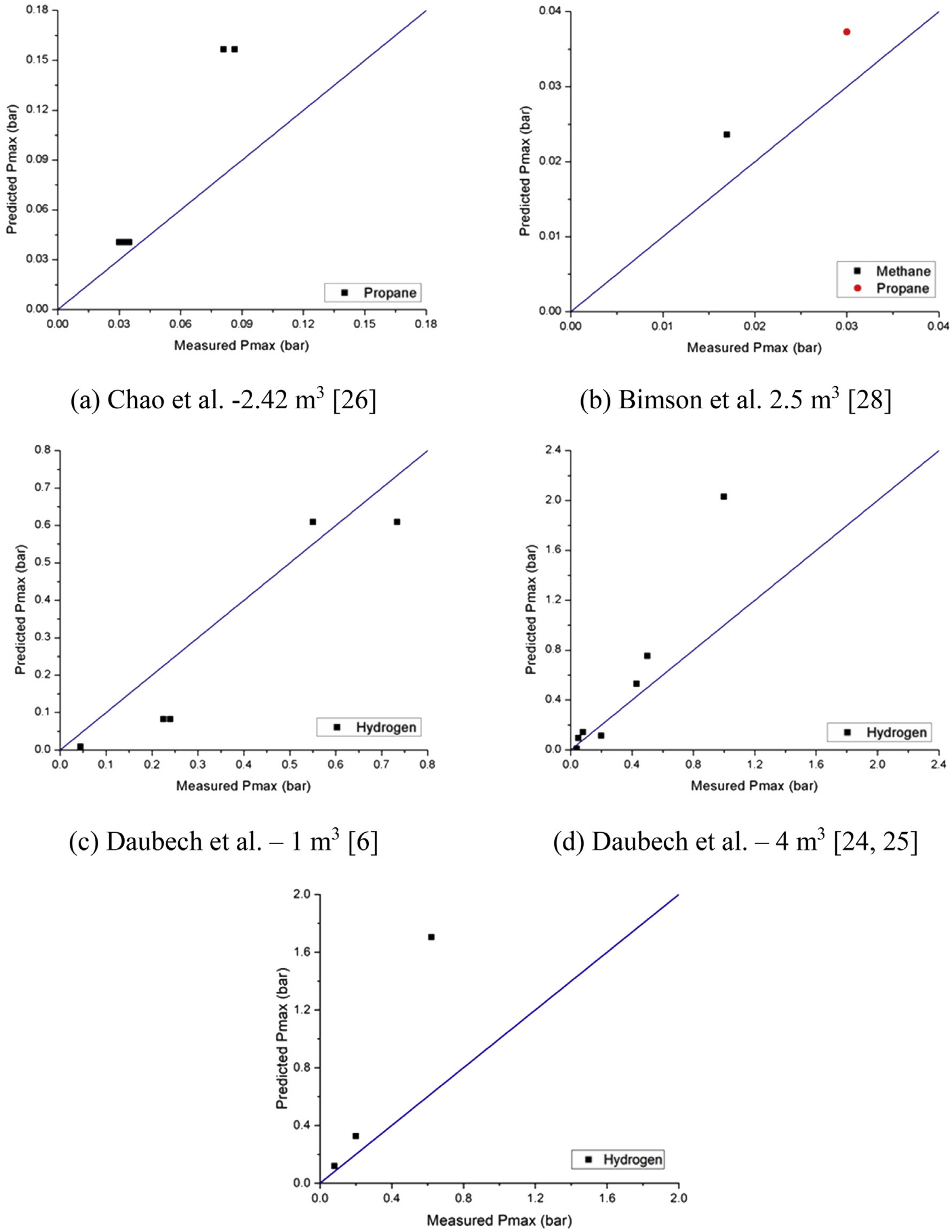


(d) Tomlin et al. – 182 m^3 [31]



(e) Skjold et al. – 35.7 m^3 [9, 10]

Fig. 4 – Comparison of model predictions with experimental results for idealized configurations of large enclosures.



(a) Chao et al. -2.42 m^3 [26]

(b) Bimson et al. 2.5 m^3 [28]

(c) Daubech et al. – 1 m^3 [6]

(d) Daubech et al. – 4 m^3 [24, 25]

(e) Wang et al. – 1 m^3 [37]

Fig. 5 – Comparison of model predictions with experimental results for idealized configurations of small enclosures.

represent actual accidents closely, combinations of these scenarios need to be considered. Unfortunately, there is a dearth of experimental data on these realistic scenarios. Recent experimental investigation under HySEA project attempt to address this issue (Skjold et al. [35]). They have considered a combination of stratified fuel, obstacles, and initial turbulent mixture. Predictions for these experiments are compared with experimental values in Fig. 10. It is observed that predictions from the present model are reasonably accurate for these realistic accidental cases, which further demonstrates the applicability of this simplified model.

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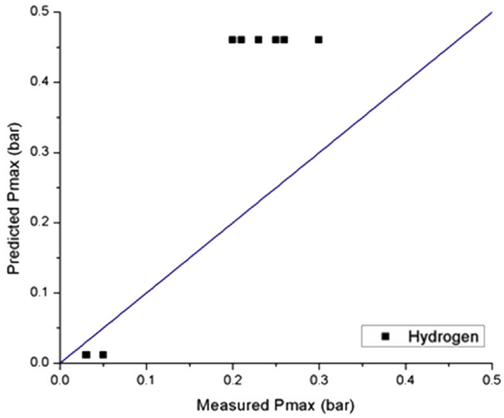
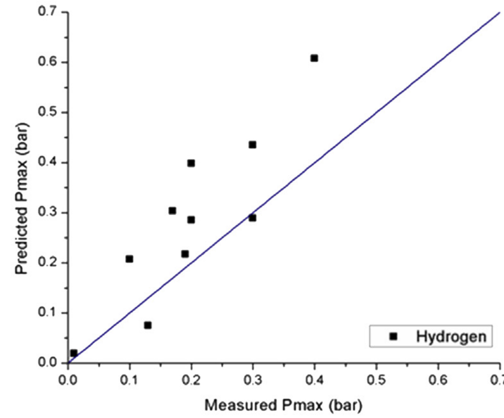
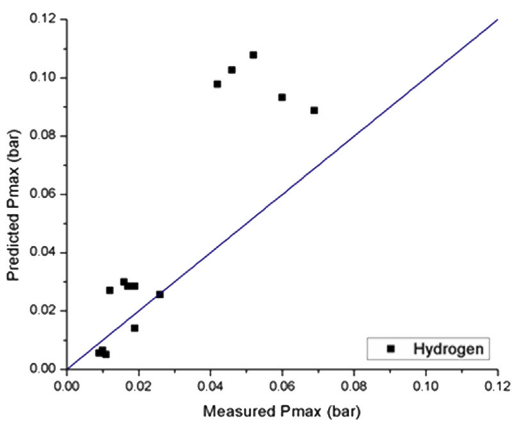


(a) Daubech et al. [6]

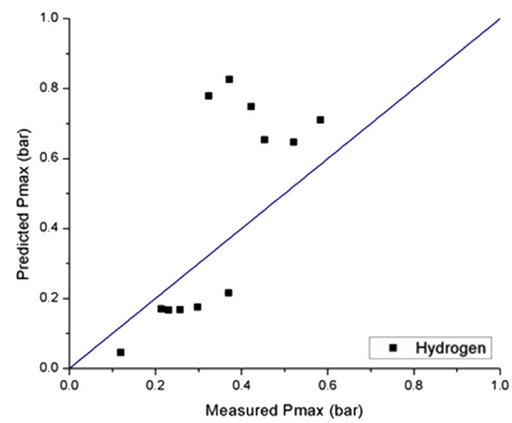


(b) Kumar [4]

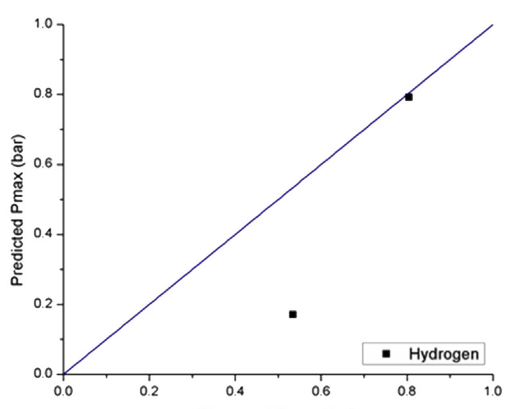
Fig. 6 – Comparison of predictions with experimental results for cases with high aspect ratios.



(a) Bauwens et al. [29]



(b) Kumar [5]



(c) Daubech et al. [30]

Fig. 7 – Comparison of predictions with experimental results for cases with initial turbulent mixture.

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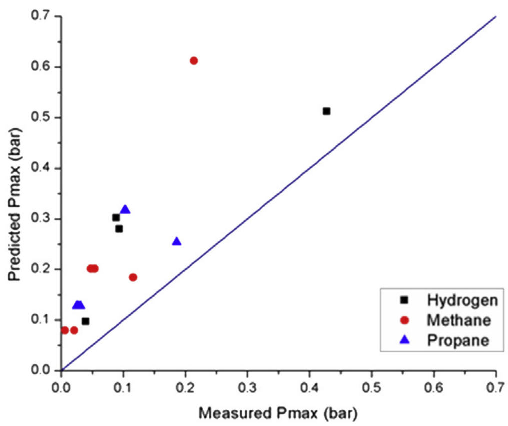
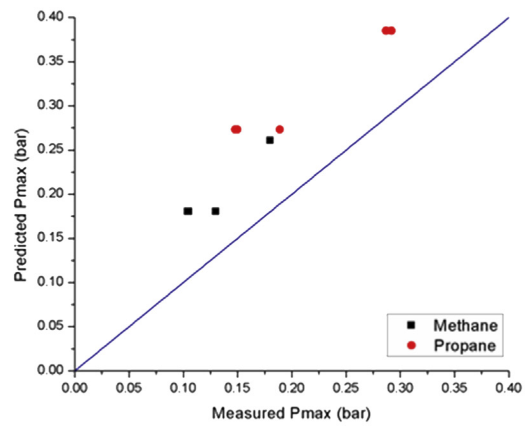
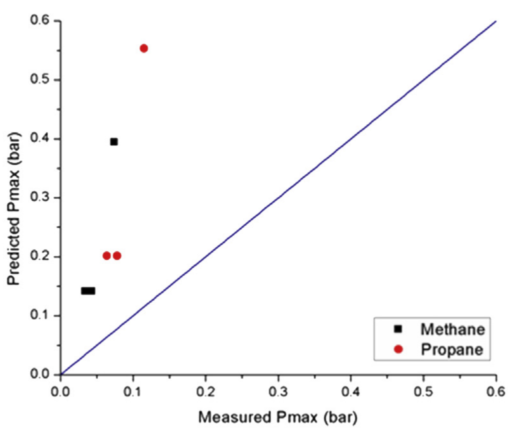


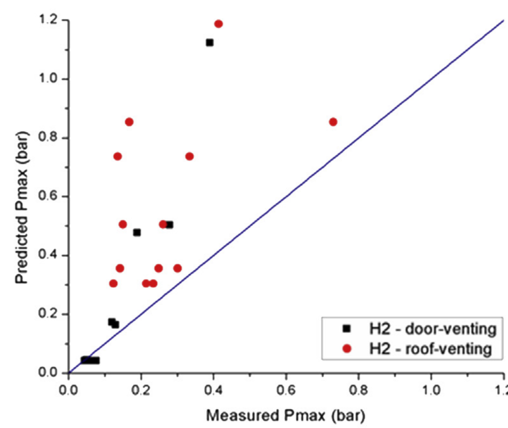
(a) Bauwens et al. [7, 8, 26]



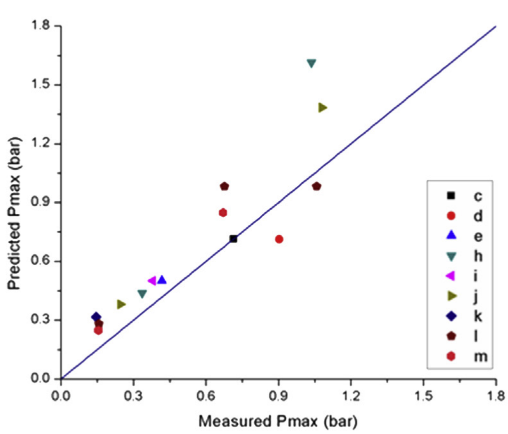
(b) Bimson – 550 m^3 [28]



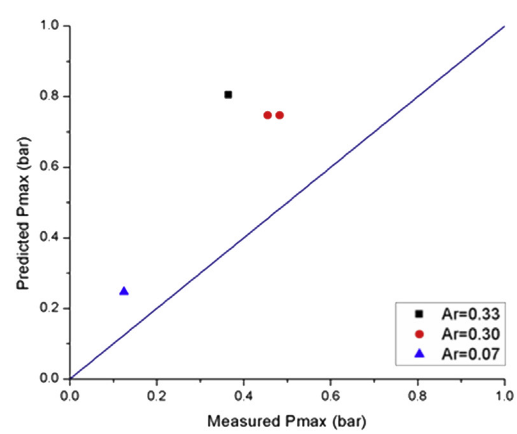
(c) Bimson -2.5 m^3 [28]



(d) Skjold et al [9, 10]



(e) Tomlin et al. [31] - different obstacle configurations are shown in symbols



(f) Diakow et al. [32] – different area ratio cases are shown in different symbols

Fig. 8 – Comparison of predictions with experimental results for cases with obstacles.

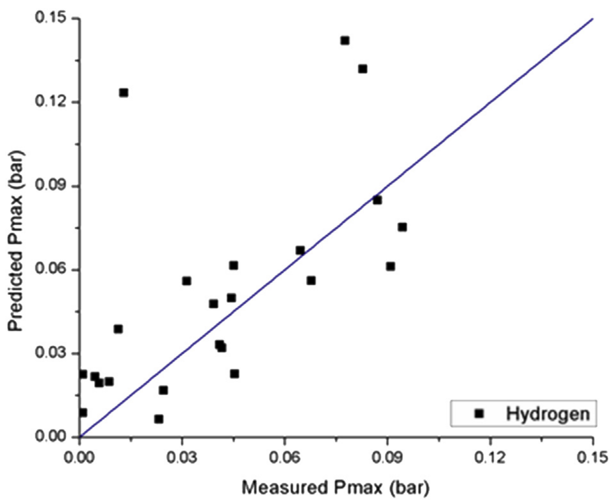


Fig. 9 – Comparison of predictions with experimental results for cases with stratified fuel distribution from Schiavetti et al. [34].

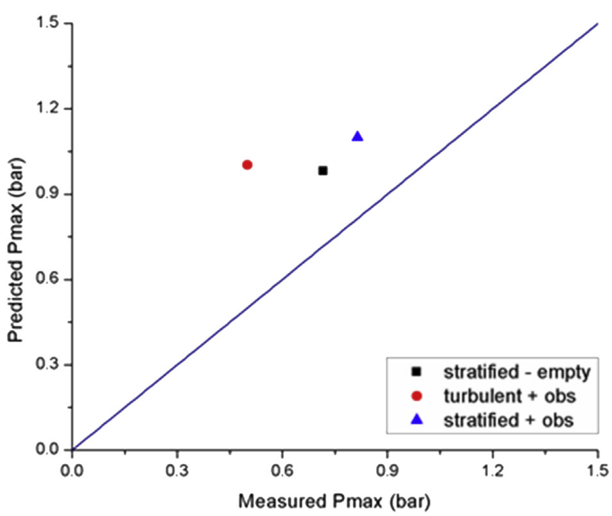


Fig. 10 – Comparison of predictions for cases with realistic scenarios from Skjold et al. [35].

Conclusions

This paper presents a simplified model to predict overpressure in vented explosions for various gases. The final model has one equation with four parameters. Two of these parameters only depend on the fuel properties and hence can be pre-tabulated (See Appendix). The other two parameters are simple functions of enclosure and obstacle geometry, which are relatively easy to compute. The new model is much simpler than other models in literature and existing standards. Moreover, predictions from this model are found to be either more accurate than or comparable with other existing models. A large set of experimental results have been used to assess the applicability of the new model. These include realistic conditions which involve obstacles, initial turbulence and mixture stratification. The model predictions were found to match well with the available measurements. Although the test data considered in this study comprise of results for hydrogen, methane and propane, the model can also be used for other gases by re-evaluating the two fuel parameters F1 and F2 from their physical properties.

Acknowledgements

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Appendix

Steps for computing Internal Overpressure.

1. Computer flame surface area (A_f) using Eq. (E.1)

$$A_f = \begin{cases} 0.50\ A_{in} & \textit{for ignition at the back} - \textit{wall}\ (\mathrm{BWI}) \\ 0.25\ A_{in} & \textit{for ignition at the centre of the enclosure}\ (\mathrm{CI}) \end{cases} \tag{E.1}$$

where A_{in} is the total internal surface area of the enclosure:

$$A_{in} = 2\cdot(L\cdot B + B\cdot H + H\cdot L)$$

Table A1 – F1 and F2 values for various hydrogen concentrations. Here E refers to the power of 10.

H2%	F1	F2
10	1.7761E-05	1.0417E-03
11	2.3292E-05	1.5248E-03
12	3.5502E-05	2.5724E-03
13	5.7926E-05	4.6089E-03
14	9.5632E-05	8.2934E-03
15	1.5514E-04	1.4562E-02
16	2.4434E-04	2.4661E-02
17	3.7235E-04	4.0159E-02
18	5.4944E-04	6.2953E-02
19	7.8694E-04	9.5249E-02
20	1.0971E-03	1.3953E-01
21	1.4929E-03	1.9849E-01
22	1.9884E-03	2.7497E-01
23	2.5978E-03	3.7187E-01
24	3.3362E-03	4.9201E-01
25	4.2191E-03	6.3805E-01
26	5.2621E-03	8.1227E-01
27	6.4812E-03	1.0165E+00
28	7.8921E-03	1.2520E+00
29	9.5108E-03	1.5189E+00
30	1.1353E-02	1.8169E+00

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Table A2 – F1 and F2 values for stoichiometric mixture of methane and propane.

	F1	F2
Methane	8.9585E-05	2.1652E-02
Propane	1.2468E-04	3.6814E-02

Table A3 – Value of β1 and β2 used for various configurations. Please note that as natural gas consists primarily of methane, we have assumed natural gas to have the same properties as methane, and F1 and F2 of Methane are used for Natural gas cases.

	Hydrogen		Methane		Propane	
	β1	β2	β1	β2	β1	β2
Ideal	0.243	0.243	0.5	0.5	0.5	0.5
obstacle-low congestion	0.243	0.243	0.5	0.5	0.5	0.5
obstacle-high congestion	–	–	0.9	0.5	0.9	0.5
Initial turbulence	0.5	0.243	–	–	–	–

2. Compute external cloud radius using Eq. (E.2)

$$R_{Cl} = 0.5V^{0.3} \tag{E.2}$$

where V is the volume of the enclosure.

3. Compute $G1$ and $G2$ using Eq. (E.3) and (E.4). Select $\beta 1$ and $\beta 2$ from table A3.

$$G1 = \left[\left(L_{eff}^{\beta 1}\right)^2 \left\{\left(\frac{A_f}{A_v}\right)^2 - 1\right\}\right], \tag{E.3}$$

$$G2 = \left[R_{Cl}^{\beta 2}\right]^2. \tag{E.4}$$

Where L_{eff} is can be defined as:

$$L_{eff} = \begin{cases} L & \textit{for ignition at the back} - \textit{wall (BWI)} \\ 0.5\,L & \textit{for ignition at the centre of the enclosure (CI)} \end{cases}$$

4. Compute internal overpressure using Eq. (E.5). Select F1 and F2 from table A1 for hydrogen and table A2 for methane and propane.

$$p = (F1 \cdot G1) + (F2 \cdot G2) \tag{E.5}$$

Sub-Models for Realistic Accidental Scenarios:

(i) **For obstacles** -Use Eq. (E.6) to compute additional flame surface area.

$$A_{obs} = (P_{obs} + 1.2\,L_{obs}\,)\;H_{obs} \tag{E.6}$$

Where P_{obs} is the perimeter of obstacle, L_{obs} is the length scale of obstacles (diameter for cylindrical and edge for square obstacle), and H_{obs} is the height of the obstacle. Add this additional flame area to the area computed in Eq. (E.1). Rest of the equations remains the same.

(ii) **For stratified mixture-** Use the maximum fuel concentration to select values from table A1 and A2. Rest of the equations remains unchanged.

(iii) **For elongated enclosures-** For elongated enclosures, the flame area is computed as:

$$A_f = 0.25\,A_{in} \tag{E.7}$$

(iv) **For initial turbulent mixture-** Select $\beta 1$ and $\beta 2$ values from Appendix for initial turbulent conditions. Rest of the equations remain unchanged.

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