Modelling of Vented Explosion of Hydrogen-Air Mixtures

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ABSTRACT

The authors developed a new mathematical model for predicting overpressure in accidental explosions of hydrogen in previous studies (Sinha et al. [1, 2]). The model produced reasonably accurate predictions. However, it appeared to be too complicated for use in vent panel design. In the present study, the model has been simplified and reduced to a single equation with only four parameters. Two of these parameters are determined only from fuel properties and can be pre-tabulated. Hence, only two parameters based on geometry need to be calculated. These two geometric parameters have inputs related to enclosure dimensions, and are much easy to compute. Only one geometric parameter also includes the flame surface area and some effort is required to estimate it. The flame area computation is also reduced by taking simplifying assumptions for the flame shape. The major advantage of this model is that there are no adjustable parameters or tunable constants and the same equation is to be used for all conditions and geometries. This makes the model simple to use and unambiguous. Same model is also used for other fuels by considering their physical properties. The model results are compared with experimentally measured overpressures and a reasonable match is found.

KEYWORDS: Vented explosion, hydrogen deflagration, fire safety.

INTRODUCTION

Storing and production of combustible gases is a common practice in several industrial and household applications. The amount of gas is generally much more than what is required to form an explosive mixture and it is also not difficult to find sources of ignition in the near vicinity. Hence, storage and use of combustible gases is a potential hazard which has to be evaluated for safety. Major safety concern is the overpressures generated which could potentially damage building and weaken structural integrity of enclosures or equipment. Venting is the most commonly used and simplest method to protect buildings from accidental explosions. Vent panels are attached to enclosure walls which open at specified pressure, and relieve pressure by venting of gases. Vent area required for a given geometry and fuel can be estimating using engineering models. Engineering models are used to predict overpressure in a given configuration and also to compute vent size required for a permissible pressure limit. Several engineering models available for predicting overpressure in vented explosions of hydrocarbon fuels. However, hydrogen which is much prone to leakage, and has a higher burning velocity is scarcely been studied. Recent reviews demonstrate that the available engineering models for hydrogen are not adequate to account for realistic accidental scenarios (Sinha et al. [1, 2]). A major concern with the current standards (EN 14994 [11] and NFPA 68 [12]) is that they are very conservative, which makes them not suitable to be used for low-strength enclosures. The increasing use of hydrogen and its acceptability as a green fuel which could replace other more polluting gases in future calls for renewed efforts to investigate phenomenology of hydrogen explosion in detail and suggest recommendations for hydrogen safety. HySEA project is aimed to address this issue. As a part of this project detailed experiments are

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conducted on 20-foot ISO container using hydrogen (Skjold et al. [3, 4]). The present effort addresses the modelling aspects for hydrogen.

MODEL FORMULATION

The model is based on the physical description of the vented explosion and the objective is to identify each sub-process separately and incorporate their effect in the model. The phenomenology of vented explosion can be explained as following. First, due to leakage of fuel gases, a combustible mixture is formed inside an enclosure or a building. This mixture will get ignited once a source of ignition, such as an electrical circuit is found. The ignited flame is understood to expand spherically and move towards the vent opening. The vent is designed to open within a short time after ignition and to reduce pressure built-up by venting out unburnt gases. This strategy works well till the flame reaches the vent and pressure is substantially reduced by venting the unburnt gases. However, as soon as the burnt gases reach the vent area, they also ignite the vented unburnt gases and cause external explosion. This explosion hinders further venting, and contributes in pressure build-up inside the enclosure. At the same time, the inside flame area reaches its maximum and a pressure peak is attained. The present model attempts to account for this pressure peak. Interestingly, one more dominant pressure peak is observed due to flame-acoustic interactions (Bauwens et al. [5]). However, this peak is found in a few cases, and also suppressed in presence of realistic conditions like initial turbulence or obstacles. This peak is non-repeatable, too complex to model, and considering this peak will unnecessarily complicate the model.

Detailed model description

The model description with detailed derivation is presented elsewhere (Sinha et al. [2]). Here a brief description of the complete model is presented. First the flame is assumed to expand spherically from point of ignition. The flame-speed and associated time-scale computations can be done using the measured flame speed by Bauwens et al. [6]. The flame speed is given by

$$\frac{U_f}{U_0} = \left(\frac{R}{R_0}\right)^{\beta}, \tag{1}$$

where U_f is the flame speed at radius R, U_0 is the critical velocity at critical radius R_0 and β is the fractal excess [6]. This flame-speed relation is used to determine the flame speed at a known distance form the ignition point. This relation is also used to estimate the flame arrival time to the vent. Further, the maximum flame area of the internal flame is expressed as a percentage of internal flame area. The flame surface area (A_f) is computed as

$$A_f(\mathrm{BWI}) = 0.5\, A_{in} \tag{2}$$

$$A_f(\mathrm{CI}) = 0.25\, A_{in} \tag{3}$$

for back-wall and central ignition cases respectively, where A_{in} is the internal surface area of the enclosure. The peak pressure computed using Bernoulli's equation in the flow exiting from the vent. The peak pressure is given as

$$p = \left[\frac{\rho_u}{2 \cdot 10^5}\left\{U_{Leff}\left(\frac{\sigma - 1}{\sigma}\right)\right\}^2 \left\{\left(\frac{A_f}{A_v}\right)^2 - 1\right\}\right] + p_{ext}\ , \tag{4}$$

where p is the internal peak pressure, A_v is the vent area, A_f is the internal flame surface area given by Eqs. (2) or (3), U_f is the flame speed evaluated using Eq. (1). The external pressure can be estimated by using Taylor's spherical piston analogy [7]

$$p_{ext} = 2\,\gamma_u \left(1 - \frac{1}{\sigma}\right) \sigma^2\, M_P^2 \ , \tag{5}$$

where γ_u is the ratio of specific heats of unburnt gaseous fuels, σ is the expansion ratio, and M_P is the Mach number of expanding flame-front at cloud boundary. The external cloud radius is computed using vortex ring theory by Sullivan et al. [8].

Model simplification

It is observed that computing the cloud radius is the most cumbersome step of the detailed model. Further, considering the average cloud radius for each geometry, it was observed that the cloud radius can be approximated as

$$R_{Cl} \approx 0.5V^{0.3}, \tag{6}$$

where V is the enclosure volume. Using this approximation and combining other equations, the internal pressure can be expressed as

$$p = \left[\frac{\rho_u}{2 \cdot 10^5}\left\{\frac{U_0}{R_0^{\beta}}\left(\frac{\sigma - 1}{\sigma}\right)\right\}^2\right]\left[\left(L_{eff}^{\beta 1}\right)^2\left\{\left(\frac{A_f}{A_v}\right)^2 - 1\right\}\right] + \left[\frac{2\,\gamma_u(\sigma^2 - \sigma)}{a_0^2}\left(\frac{U_0}{R_0^{\beta}}\right)^2\right]\left[R_{Cl}^{\beta 2}\right]^2. \tag{7}$$

This can further be simplified in this form

$$\boldsymbol{p} = (\boldsymbol{F1} \cdot \boldsymbol{G1}) + (\boldsymbol{F2} \cdot \boldsymbol{G2}). \tag{8}$$

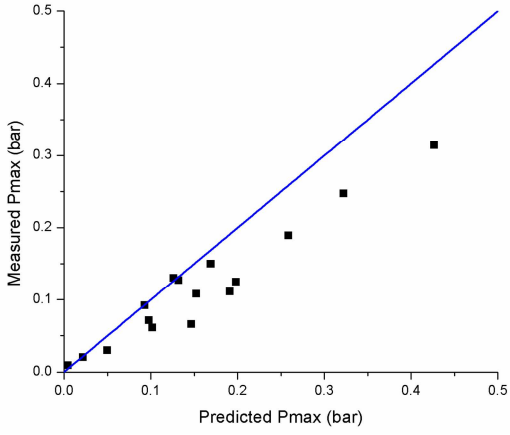
It is to be noted that the factors *F1* and *F2* are determined by fuel properties alone and hence can be computed in advance for various fuel concentrations and pre-tabulated. Sample table is also presented in the appendix. Further G1 and G2 are dependent on enclosure geometry and can be easily calculated. Hence, Eq. (8) is the final form of simplified equation which is to be used for various fuels and enclosure configurations.

RESULTS AND DISCUSSION

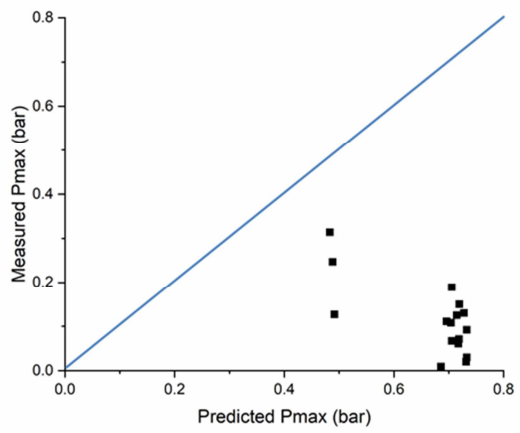
The simplified model is used for further predictions. First the results from this model are generated for standard data sets for experiments of Bauwens et al. [9]. Predictions for these experiments are also made using other models from Bauwens et al. [5], Molkov and Bragin [10], and standards – EN 14994 [11], NFPA 68 [12]. All these predictions are compared in Fig. 1. As evident, the standards are mostly over-predicting. The detailed models from [5] and [10] are giving better predictions than the standards but are cumbersome to use. The present simplified model which is much simpler to implement is also giving more accurate or comparable predictions as compared to these detailed models.

Further, the present model is also tested for different configurations and fuels. Experimental studies from Skjold et al. [3-4], Daubech et al. [13], Bauwens et al. [5], Chao et al. [14], Harrison et al. [15] are used for comparison. These experiments comprise of data using hydrogen, methane and propane. The comparison is shown in Fig. 2. As evident, the present model is showing a reasonably good match for different fuels. The comparison shown in Fig. 2 is for studies carried out using large containers. Further comparisons are also made for relatively smaller enclosures used by Chao et al. [14] and Bimson et al. [16]. These comparisons are shown in Fig. 3. The large enclosure results from Bimson et al. [16] are also shown in this Figure. It appears that the present model is working well for different enclosures and fuels. Form the presented comparison; it might appear that the model is giving more accurate results for hydrogen and much scatter for methane and propane. It is important to note that while tests with hydrogen are carried out for different concentrations, the tests

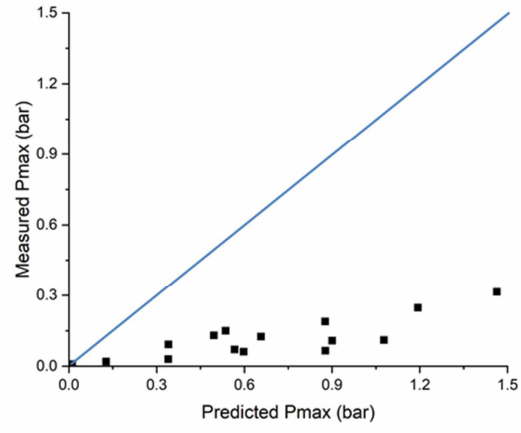
with methane and propane are mostly done for the stoichiometric mixtures. So, the apparent scatter in hydrocarbon results is mainly due to scatter in experimental data for the same conditions.



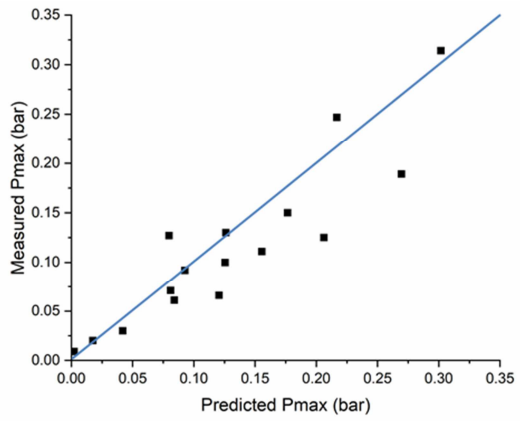
(a) Present model.



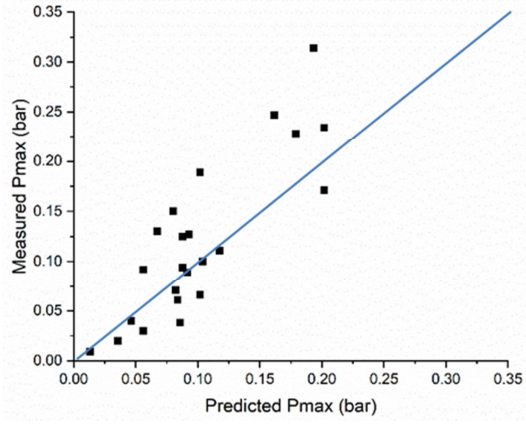
(b) EN 14994 [11].



(c) NFPA 68 [12].

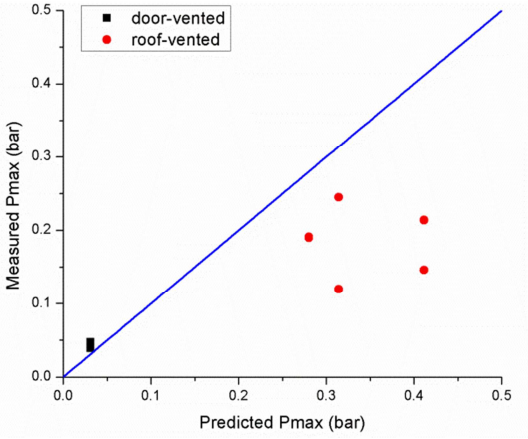


(d) Bauwens model [4].

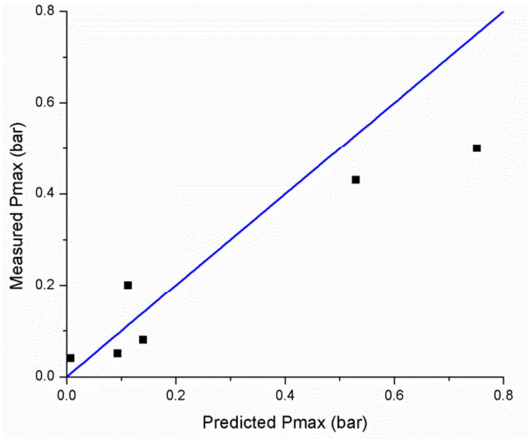


(e) Molkov model [10].

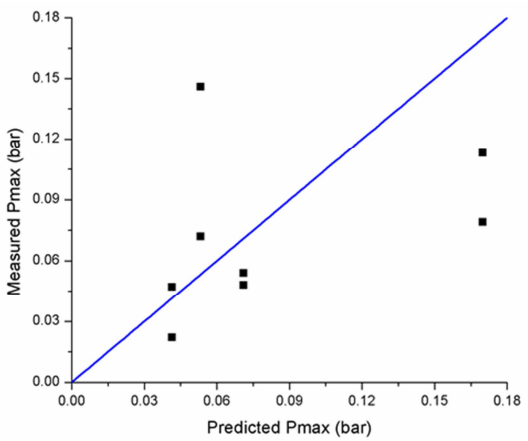
Fig. 1. Model predictions for results from Bauwens et al. [11].



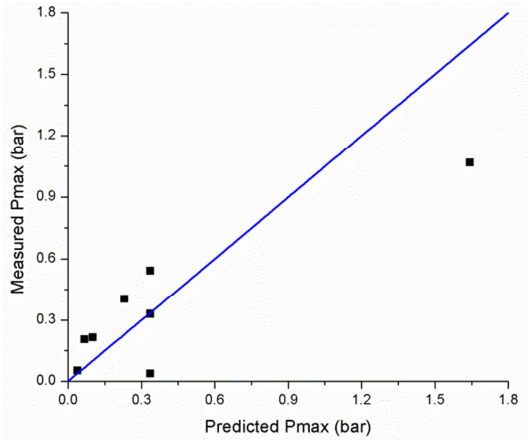
(a) Hydrogen – Skjold et al. [3-4].



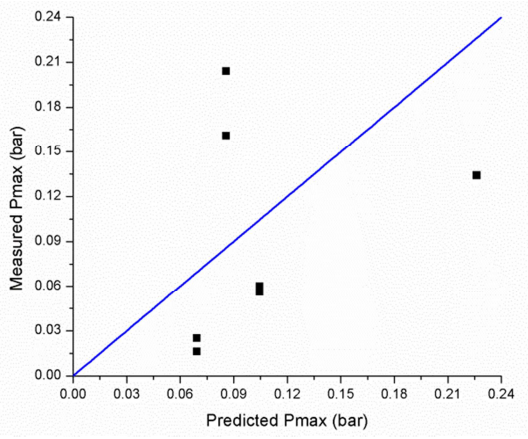
(b) Hydrogen – Daubech et al. [13].



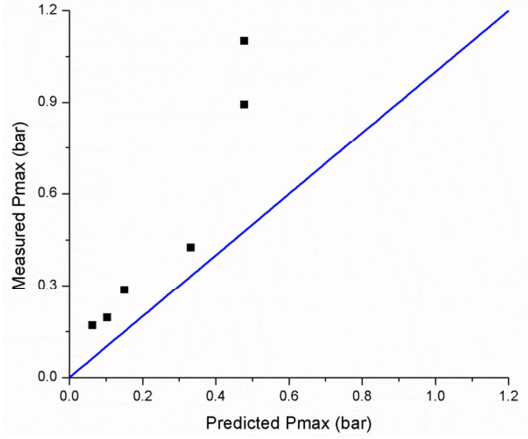
(c) Methane – Chao et al. [14].



(d) Methane – Harrison et al. [15].

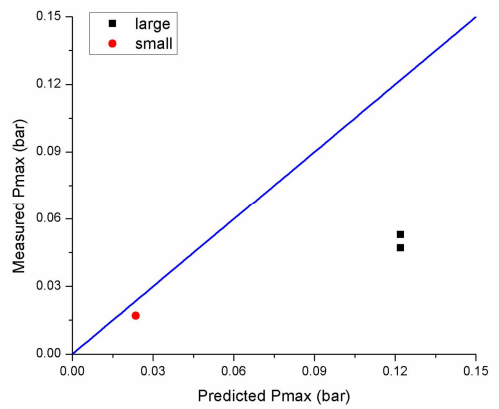


(e) Propane – Bauwens et al. [5].

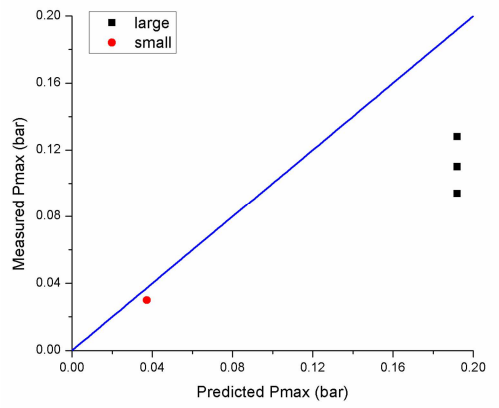


(f) Propane – Harrison et al. [15].

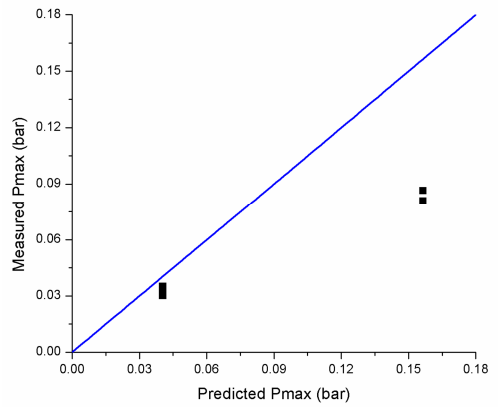
Fig. 2. Comparison of predictions from the present model with data for large-scale enclosures.



(a) Methane – Bimson et al. [16].



(b) Propane – Bimson et al. [16].



(c) Propane – Chao et al. [14].

Fig. 3. Comparison of predictions from the present model with data for smaller enclosures.

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APPENDDIX

Table A1. F1 and F2 values for various hydrogen concentrations

H2 %	F1	F2
10	1.78E-05	1.04E-03
11	2.33E-05	1.52E-03
12	3.55E-05	2.57E-03
13	5.79E-05	4.61E-03
14	9.56E-05	8.29E-03
15	1.55E-04	1.46E-02
16	2.44E-04	2.47E-02
17	3.72E-04	4.02E-02
18	5.49E-04	6.30E-02
19	7.87E-04	9.52E-02
20	1.10E-03	1.40E-01
21	1.49E-03	1.98E-01
22	1.99E-03	2.75E-01
23	2.60E-03	3.72E-01
24	3.34E-03	4.92E-01
25	4.22E-03	6.38E-01

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

	F1	F2
Methane	8.96E-05	2.17E-02
Propane	1.25E-04	3.68E-02