CFD simulation of hydrogen deflagration in a vented room

I C Tolias\textsuperscript{1,2}, A G Venetsanos\textsuperscript{1}, N C Markatos\textsuperscript{2} and C T Kiranoudis\textsuperscript{2}

\textsuperscript{1}Environmental Research Laboratory, National Center for Scientific Research Demokritos, Agia Paraskevi, 15310, Greece
\textsuperscript{2}National Technical University of Athens, School of Chemical Engineering, Heroon Polytechniou 9, Zografou, 15780, Greece

E-mail: tolias@ipta.demokritos.gr

Abstract. In the present work, CFD simulations of hydrogen deflagration in a real scale vented room are performed. Two ignition points were simulated: at the wall opposite to the vent (back ignition) and at the center of the chamber (center ignition). The overpressure time series and flame front velocities are compared with the experimental results. The combustion model is based on the turbulent flame speed concept. The turbulent flame speed is calculated based on a modification of Yakhot's equation, in order to account for all the main physical mechanisms which appear in hydrogen deflagrations. Special attention is given to the simulation of Rayleigh-Taylor instability. This instability occurs at the vent area and results in sudden explosion of the mixture that has been pushed outside the chamber at the initial stage of the explosion. The importance of this external explosion to the generated overpressures inside the chamber is highlighted. The agreement between experimental and computational results is satisfactory in both back ignition and center ignition cases.

1. Introduction

Hydrogen is a very promising alternative fuel which is expected to play a significant role in the near future. However, significant safety issues are associated with it. In the case of an accidental release, hydrogen mixes with air and can form a flammable mixture over a wide range of concentrations. An accidental release in a closed space can have catastrophic consequences in the case of an explosion. The confined space will lead to the development of much higher overpressure compared to a similar explosion in an open space. The venting of the hot products out of the closed space is the final protection measure in order to mitigate the damages of the explosion. Even thought there are guidelines for the minimum size of the vent for a given space, there are not reliable and commonly accepted \cite{1}. As a result experiments and simulations for confined hydrogen explosions have to be conducted, in order to gain a better insight on the phenomenon.

An experiment revealing the complexity of vented hydrogen explosions was carried out by Cooper et al. \cite{2}. Four characteristic overpressure peaks were identified: The first one took place because of the opening of the vent, the second one was caused by the external explosion of the fuel which has been pushed outside the room during the initial stages of the explosion, the third one by the reduction of the combustion rate when the flame touches the walls and the last one by the instabilities which enhance the combustion process because of flame-acoustic interaction. A recent analysis of the peak overpressures in vented explosion has been made by Chao et al. in \cite{3}, where the effects of fuel, enclosure size, ignition location, vent size and obstacles were examined. Special attention to external
explosion has been paid by several authors such as Harrison and Eyre (1987) [4], Jiang et al. (2005) [5], Ferrara et al. (2008) [6], and Proust and Leprette (2010) [7]. In the past years, the increase of computational power has rendered Computational Fluid Dynamics (CFD) as a very attractive methodology for risk assessment of hydrogen applications. Previous CFD studies about hydrogen deflagration in vented spaces have been performed by Baraldi et al. (2010) [8], Bauwens et al. (2011) [9] and Keenan et al. (2014) [10]. In [8] a comparison of CFD models has been made for hydrogen deflagration in a 0.95 m$^3$ vented vessel. In [9] and [10] hydrogen deflagration in a 64 m$^3$ room was simulated. In both works special attention to the modelling of the Rayleigh-Taylor instability was paid. The instability was modelled through an additional transport equation which takes into account the generation and the suppression rate of the instability.

2. Experiment overview
Experiments of hydrogen deflagration in real-scale vented room were performed by FM-Global [9]. The top view of the room with its dimensions can be seen in figure 1. The room has a volume of 64 m$^3$ (4.6 x 4.6 x 3.0 m) and a square vent of 5.4 m$^2$ is located at a vertical wall. The room is filled with homogeneous hydrogen-air mixture of 18% v/v. Two cases for the ignition position were studied: one at 0.25 m from the center of the wall opposite to the vent (back ignition) and one at the center of the room (central ignition). The pressure was measured at the center of the right wall (point P1 in figure 1). The experimental pressure was filtered with an 80 Hz low pass filter.

![Figure 1. Top view of the experimental facility.](image)

3. Mathematical methodology

3.1. Governing equations
For the CFD simulations the ADREA_HF code was used [11]. The model used solves the space-averaged Navier-Stokes equations along with the energy equation and the conservation equation of each of the mass fraction of the species that take part in the combustion process. Turbulence is modelled using the RNG LES. The set of main equations that was used are presented in [12].

The implemented in ADREA_HF code combustion model [12], originally proposed in [13, 14], is based on turbulent flame speed concept. In the utilized model, the calculation of the turbulent flame speed is based on Yakhot’s equation for premixed turbulent combustion [15]:

$$S_t = \Xi_A \cdot \Xi_{ip} \cdot \Xi_f \cdot \Xi_{RT} \cdot S_u \cdot \exp \left( \frac{u'}{S_t} \right)^2$$  \hspace{1cm} (1)

where $S_u$ is the laminar burning velocity (constant, equal to 0.64 m/s in our simulations) and $u'$ the subgrid scale velocity. Yakhot’s equation has been derived based on the renormalization group theory.
and at its original form does not include the $\Xi$ factors. These factors have been included in the equation in order to take into account the mechanisms which can increase the turbulence burning velocity in deflagrations.

One mechanism which leads to an acceleration of the flame front, is the turbulence generated by the flame front itself. As described in [16], the source of this turbulence is the thermal expansion of the combustion products. The upper limit for a flame wrinkling factor due to the turbulence generated by the flame front itself can be estimated by the equation $\Xi^\text{max} = (E - 1)/\sqrt{3}$ where $E$ is the expansion coefficient. The wrinkling factor, $\Xi_k$, gradually increases from the value of one at the ignition point to the maximum value of $\Xi^\text{max}$ at the critical radius where the turbulence is fully developed. This critical radius is approximately equal to $R_0 = 1.0 - 1.2 \text{ m}$ for near stoichiometric hydrogen-air mixtures. The formula that was used for the wrinkling factor which takes under consideration these parameters is:

$$
\Xi_k = 1 + \left( \psi \cdot \Xi^\text{max}_k - 1 \right) \cdot \left[ 1 - \exp\left( -R/R_0 \right) \right]
$$

(2)

where $R$ is the distance from the ignition point and $\psi$ is a model constant which represents the level at which the maximum value $\Xi^\text{max}_k$ is reached ($0 \leq \psi \leq 1$). This constant is suggested to be equal to 0.5 for near stoichiometric mixtures and equal to 1 for lean hydrogen-air mixtures. In the present study we set $R_0 = 1.0$, $E = 5.2$ and $\psi = 0.90$.

Another mechanism which leads to acceleration of the flame front is the preferential diffusion which causes an increment of the burning velocity. Based on the work of Zimont and Lipatnikov [17], a correction factor $\Xi_\varphi$ for the laminar burning velocity can be calculated for a given mixture composition. Based on [17], the value of this factor for 18% hydrogen-air mixture composition should be 2.08. This value is very close to the value 1.96 of the ratio of the initial flame speed measured in the experiment to the theoretical flame speed [9]. The value of 1.96 for $\Xi_\varphi$ was chosen in the present simulations.

The fractal structure of the flame front increases flame surface and thus flame speed. The $f$ coefficient takes under account this phenomenon. Details about this coefficient can be found in [18].

As the combustion develops inside the enclosure, unburned mixture is pushed outside through the vent. When the flame reaches the vent, this mixture will start burning leading to the external explosion. This explosion seems to have much more strength than combustion models predict. The main reasons that have been proposed for that behavior are: 1) the creation of extensive turbulence in the area outside the vent, because of the jet-like flow and 2) the development of Rayleigh-Taylor instability due to the acceleration of the less dense products through the vent to the more dense unburned mixture. Both reasons potentially lead to an augmentation of the reaction rate which leads to a violent external explosion. Thus, the models should be improved. In this respect a $\Xi_{RT}$ factor has been added to the combustion model in order to reproduce the reaction rate enhancement due to the Rayleigh-Taylor (RT) instability. Its value is constant at the area immediately outside the vent where the RT instability develops and equal to one elsewhere. A similar modelling approach has been used in a large scale vented methane explosion in [19].

3.2. Numerical details

ADREA-HF uses the finite volume method on a staggered Cartesian grid. For the discretization of the convective terms in the momentum equations a second order accurate bounded central scheme was used while in the conservation equations of species and energy a second order accurate bounded linear upwind scheme. For the time advancement, the second order accurate Crank-Nicolson numerical scheme was chosen. The time step is automatically adapted according to prescribed error bands and the desired Courant–Friedrichs–Lewy (CFL) number which maximum value was set equal to 0.8.
The computational domain was extended in all directions outside the room in order to minimize the effect of the implied boundary conditions. Its total size was 42.3 x 60.0 x 30.0 m. A more extended domain was examined and showed zero impact on the results. The total number of active computational cells was approximately 707,000. The length of the computational cells was almost uniform and equal to 0.1 m inside the room and at the area outside the vent. In all exit planes (lateral, front, back and top) the non-reflecting type boundary condition for the normal velocities was chosen, while for the parallel to the exit planes’ velocity components, zero-gradient boundary condition was applied. As initial conditions, a stagnant flow field with no turbulence was specified.

4. Results and discussion

In figure 2 the pressure inside and outside the room with and without the inclusion of RT instability modelling for the back ignition case is shown. The outside pressure was monitored at the distance of 1.2 m from the center of the vent. No experimental data are available for the outside pressure. We observe that external explosion strongly affects the pressure inside the room. The enhancement of the combustion rate at the area outside the vent, which was modelled with \( \Xi_{RT} \) factor, leads to the increase of the external pressure. This results also in the increase of the internal pressure, due to the suppression of the venting process. Modelling of the RT instability is crucial for the accurate prediction of the maximum overpressure inside the enclosure. When \( \Xi_{RT} = 1.0 \) (no RT modelling) the external pressure is lower and the combustion model fails to reproduce the maximum pressure value inside the room. In figure 2 the experimental and simulated flame speed velocity normalized by the laminar flame speed (which is equal to \( E \cdot S_{u} = 3.3 \) m/s) are also shown. The agreement up to a distance of 3.6 m from the ignition point is excellent. After that point we observe that the predicted flame speed is higher than the experimental.

![Figure 2](image)

Figure 2. Pressure inside and outside the room for two different values of \( \Xi_{RT} \) (left) and flame velocity normalized by laminar flame speed (right) for back ignition case.

Figure 3 shows the hydrogen mass fraction (the grid that was used is also presented), the flow velocity and the subgrid scale velocity for back ignition at t=0.222 sec. We can clearly see the unburned mixture that has been pushed outside the vent. The mixing with the ambient air is very low. This behavior has been observed also in a smaller scale experiment in [7]. The unburned mixture starts burning as the flame front exits the vent. Velocity contours reveal the increase of the flow speed after the vent and the strong turbulence that the flame front experience. Consequently, a violent external explosion occurs.

In figure 4, the pressure inside and outside the room, with and without the inclusion of RT instability modelling for the central ignition case is shown. We observe that very good agreement with the experimental pressure was achieved by using the same value of the \( \Xi_{RT} \) factor (equal to 1.9) as in the back ignition case. This is an important finding because it implies that the enhancement of the combustion rate outside the vent weakly depends on the ignition position. Different ignition point
implies different flow characteristics. Figure 5 shows the hydrogen mass fraction, the flow velocity and the subgrid scale velocity at the time of the external explosion. Comparing with the case of back ignition (figure 3), we notice that the value of velocity (both resolved and sub grid scale) is smaller. The smaller value is justified by the fact that for the central ignition case the flame does not have the time to accelerate much and it reaches the vent with a smaller velocity, because it is closer to it compared to the back ignition case. Even though velocity differs significantly, the $\Xi_{RT}$ value equal to 1.9 gives very good results for both cases. This leads to the conclusion that simple models and correlations for the external explosion may exist. Of course, simulations of more experiments need to be carried out.

![Figure 3](image)

**Figure 3.** Hydrogen mass fraction (left), velocity (middle) and subgrid scale velocity (right) contours at $t=0.222$ seconds (back ignition).

In figure 4 the overpressure with $\Xi_{RT} = 1.0$ model is also shown. As in the previous case, the external pressure is lower compared to the $\Xi_{RT} = 1.9$ case. This leads to the underestimation of the maximum pressure value inside the room. In the same figure the experimental and simulated flame speed velocity normalized by laminar flame speed are presented. The agreement up to a distance of 2.5 m from the ignition point is satisfactory. After that point some discrepancies between the experimental and the predicted flame speed are observed.

In figure 4 we observe also that a second peak exists in the experimental pressure which the numerical model fails to predict. This peak is related to the combustion of the unburned fuel that has been trapped inside the enclosure. Structural response of the room, which interacts with the acoustics, and flame-acoustic interaction enhance the combustion process at this stage giving rise to strong pressure oscillations. A modelling approach of this phenomenon needs to be developed for the accurate prediction of this second pressure peak.

![Figure 4](image)

**Figure 4.** Pressure inside and outside the room for two different values of $\Xi_{RT}$ (left) and flame velocity normalized by laminar flame speed (right) for central ignition case.
5. Conclusions

Hydrogen deflagration in a real scale vented room was simulated. Two cases were examined, a back ignition and a central ignition case. A multi-phenomenon combustion model was used which takes into account the main mechanisms of the deflagration process such as turbulence, turbulence generated by the flame front, preferential diffusion and fractal geometry. A simple extension of this model is proposed in order to take into account the enhancement of the combustion rate at the area outside the vent, due to the Rayleigh-Taylor instability. The model revealed very good agreement with the experimental results. The maximum pressure inside the room was predicted accurately only by the modified model. Despite the different flow characteristics between the two cases, the same value of the $\Xi_{RT}$ factor (equal to 1.9) was found to be appropriate for both cases. This shows that simple models and correlations regarding this factor may be derived.

Acknowledgments

This work has been supported by the project Hylndoor (“Pre-normative research on safe indoor use of fuel cells and hydrogen systems”, Grant agreement no: 278534). The first author would also like to acknowledge the “IKY Fellowships of Excellence for Postgraduate Studies in Greece - Siemens Program” for the financial support.

References

[1] Bauwens C R and Dorofeev S B 2013 5th Int. Conference on Hydrogen Safety Brussels
[2] Cooper M G, Fairweather M and Tite J P 1986 Combust. Flame 65 1–14
[3] Chao J, Bauwens C R and Dorofeev S B 2011 Proc. Combust. Inst. 33 2367–74
[4] Harrison A J and Eyre J A 1987 Combust. Sci. Technol. 52 91–106
[5] Jiang X, Fan B, Ye J and G. Dong 2005 J. Loss Prev. Process Ind. 18 21–6
[6] Ferrara G et al. 2008 J. Hazard. Mater. 155 358–68
[7] Proust C and Leprette E 2010 Process Saf. Prog. 29 231–5
[8] Baraldi D et al. 2010 Int. J. Hydrogen Energy 35 12381–90
[9] Bauwens C R, Chaffee J and Dorofeev S B 2011 Int. J. Hydrogen Energy 36 2329–36
[10] Keenan J J, Makarov D V and Molkov V V 2014 Int. J. Hydrogen Energy 39 20467–73
[11] Venetsanos A G, Papanikolaou E and Bartzis J G 2010 Int. J. Hydrogen Energy 35 3908–18
[12] Talias I C, Venetsanos A G, Markatos N and Kiranoudis C T 2014 Int. J. Hydrogen Energy 39 20538–46
[13] Molkov V, Makarov D and Schneider H 2006 J. Phys. D. Appl. Phys 39 4366–76
[14] Molkov V, Verbecke F and Makarov D 2008 Combust. Sci. Technol. 180 796–808
[15] Yakhot V 1988 Combust. Sci. Technol. 60 191–214
[16] Karlovitz B, Denniston D W and Wells F E 1951 J. Chem. Phys. 19 541
[17] Zimont V and Lipatnikov A 1995 Chem. Phys. Rep 14 993–1025
[18] Molkov V V 2012 Fundamentals of Hydrogen Safety Engineering www.bookboon.com
[19] Molkov V, Makarov D and Puttock J 2006 J. Loss Prev. Process Ind. 19 121–9