Numerical Modelling of Vented Lean Hydrogen–Air Deflagrations using HyFOAM

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Introduction

Hydrogen is being considered as a sustainable future energy carrier with least environmental impact in terms of combustion by-products. It has unique physical properties of very wide flammability range, between 4% to 75% by volume and high flame speeds, which are challenging factors in designing safe hydrogen installations. An accidental release in enclosures can easily result in the formation of flammable mixtures, which may upon ignition lead to fast turbulent deflagrations or even transition to detonation. Explosion venting is frequently used to mitigate explosions in industry, but it is not straightforward to design vent systems that will reduce the explosion pressure sufficiently to prevent collapse of structures and formation of projectiles. Validated predictive techniques will be of assistance to quantified analysis of possible accidental scenarios and designing effective mitigation measures such as vents. While explosion venting has been previous studied experimentally and numerically, relatively little information has been gathered about the configurations used in hydrogen energy applications and in the presence of obstacles; a viable predictive technique for such scenario is still lacking.

The use of standard 20 feet ISO shipping containers for self-contained portable hydrogen fuel cell power units is being widely considered. Fresh experiments for this configuration have been carried out by GexCon AS as part of the HySEA project supported by the Fuel Cells and Hydrogen 2 Joint Undertaking (FCH 2 JU) under the Horizon 2020 Framework Program for Research and Innovation. In the present study, numerical modelling and simulations have been conducted to aid our understanding of the vented gas explosion in these self-contained portable power units using HyFOAM, an in-house modified version of the open source Computational Fluid Dynamics (CFD) code OpenFOAM for vented hydrogen explosions. The convective and diffusive terms are discretised using Gaussian-Gamma bounded and Gaussian linear corrected numerical schemes with in OpenFOAM. The temporal terms are discretised using Euler implicit scheme making the solver second order accurate both in spatial and time coordinates.

Numerical Model

The turbulent deflagration is modelled using flame surface wrinkling model proposed by Weller et al.[3] in the large eddy simulation (LES) context. It assumes that combustion takes place in the flamelet regime in the relatively thin layers that separate regions of unburned and fully burned gases. The flame

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front locally propagates at unstretched laminar flame speed, and in the mean time stretched and strained by the turbulent flow field. The turbulence induced flame stretching increases flame surface area which results in an increase of the burning rate. The turbulent flame speed correlation and unstretched laminar flame speed correlation are important input parameters for this model. The volume fraction of the unburnt zone is denoted as regress variable (b), taking values b = 1 in fresh gases and b = 0 in fully burnt gas region. The thermophysical process of flame propagation is represented by the transport equation for the resolved part of regress variable given as:

$$\frac{\partial \overline{\rho}\tilde{b}}{\partial t} + \nabla.\left(\overline{\rho}\tilde{U}\tilde{b}\right) - \nabla.\left(\overline{\rho}\mu_{sgs}\nabla\tilde{b}\right) = -\overline{\rho}_u S_L \Xi \left|\nabla\tilde{b}\right| \tag{1}$$

where, Ξ is subgrid flame wrinkling, which can be regarded as the turbulent to laminar flame speed ratio and is formally related to the flame surface density by $\sum = \Xi|\nabla\overline{b}|$, ρ is the density, S_L is laminar flame speed and μ_{sgs} is the subgrid turbulent diffusion coefficient. Symbols with overbar ($\overline{\ }$) and tilde ($\tilde{\ }$) represents the filtered and the density weighted filtering operations respectively. The subscripts u indicates conditioning on the unburned gases region. The resolved unburned gas volume fraction $\overline{b}$ is related to $\tilde{b}$ through $\overline{\rho}_u\overline{b} = \overline{\rho}\tilde{b}$. The closure for the sub-grid wrinkling is provided by a balanced transport equation,

$$\frac{\partial \overline{\rho}\Xi_t}{\partial t} + \hat{U}_s \nabla\Xi_t = \overline{\rho} G \,\Xi_t - \overline{\rho} R(\Xi - 1) + \overline{\rho}\max\left[\left(\sigma_s - \sigma_t\right), 0\right] \Xi_t \tag{2}$$

where, $\hat{U}_s$ is the surface filtered local instantaneous velocity of the flame, which is modelled as

$$\hat{U}_s = \tilde{U} + \left(\frac{\overline{\rho}_u}{\overline{\rho}} - 1\right) S_L \Xi\, n_f - \frac{\nabla(\overline{\rho}\,\mu_{sgs}\nabla\tilde{b})}{\overline{\rho}\,|\nabla\tilde{b}|} n_f \tag{3}$$

The direction of flame propagation is represented by $n_f = \nabla\tilde{b}/|\nabla\tilde{b}|$, σ_S and σ_t are the surface filtered resolved strain-rates relating to the surface filtered local instantaneous velocity of the flame ($\hat{U}_s$) and surface filtered effective flame velocity of the flame surface ($\hat{U}_t$) modelled as

$$\sigma_t = \nabla(\tilde{U} + S_L\Xi_t\, n_f) - n_f[\nabla(\tilde{U} + S_L\Xi_t\, n_f)]n_f$$

$$\sigma_s = \frac{\nabla\tilde{U} - n_f\,(\nabla\tilde{U})\,n_f}{\Xi_t} + \frac{(\Xi_t + 1)[\nabla\,(S_L\, n_f) - n_f[\nabla(S_L\, n_f)\; n_f]}{2\,\Xi_t} \tag{4}$$

The terms $G\Xi_t$ and $R(\Xi_t - 1)$ in Eq. 2 are sub-grid turbulence generation and removal rate, with G and R as rate coefficients requiring modelling,

$$G = R\frac{\Xi_{eq} - 1}{\Xi_{eq}} \quad \text{and} \quad R = \frac{0.28}{\tau_\eta}\frac{\Xi^*_{eq}}{\Xi^*_{eq} - 1},$$

$$\Xi^*_{eq} = 1 + \frac{0.46}{Le}\, Re_t^{0.25}\left(\frac{\hat{u}}{S_{Lo}}\right)^{0.3} \text{and } \Xi_{eq} = 1 + 2(1-b)(\Xi^*_{eq} - 1) \tag{5}$$

where, τ_n is the Kolmogorov time scale, $\hat{u}$ is the sub grid turbulence intensity and Re_t is the turbulent Reynolds number.

The Lewis number effects are widely acknowledged to be important in the lean hydrogen-air combustion processes [1,2]. The wrinkling of the flame increases with the decrease of the Lewis number, which is also accompanied by the broadening of the flame brush. The Darrieus–Landau and thermodiffusive instabilities also affect the flame propagation in lean mixtures. Turbulent flame speed increases with decreasing Lewis number of the deficient reactant, this effect is especially profound for lean hydrogen mixtures, which are typical in facilities which use venting as a measure for explosion mitigation. The incorporation of the Lewis number (Le) effect is hence important for numerical modelling of the vented hydrogen explosion scenario. In HyFOAM, this is accounted for in Eq.5 by taking into account the Lewis number (Le) effects in the turbulent flame speed correlation using the algebraic reaction rate closure proposed by Muppala et al. [4], which has been successfully applied to both pure and mixed fuels involving different Lewis numbers [2,5-6] in both RANS and LES simulations. Its predictions for the turbulent flame speed (S_T) for equivalence ratio between and inclusive of 0.4 and 0.8 along with Goulier et al [8] correlation are compared with the experimental measurements of Kitagawa et al. [7] in Figure 1. The predicted S_T trends are consistent with the measurements.

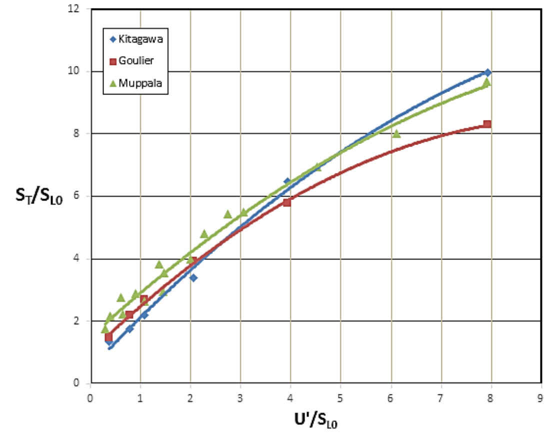


Figure 1. Comparison of the turbulent flame speed correlation of Goulier et al. [8], Muppala et al.[4] with the experimental data of Kitagawa et al. [7] (Green line – Muppala, Red – Goulier, blue – Kitagawa)

The flame wrinkling due to the Darreius-landau instability is modelled as algebraic expression based on Bauwens et al. [9] as,

$$\Xi_{DL} = \max\left[1, \alpha_1 \left(\frac{\Delta}{\lambda_c}\right)^{1/3}\right] \tag{6}$$

Where, λ_c is the cut off wavelength of unstable scales and $\propto_1$ is a coefficient to account for uncertainty in λ_1. The values used in these constants are based on experimental findings of Bauwens et al. [9].

The unstrained laminar flame speed ($S_{L,0}$) for lean hydrogen-air mixture is adopted based on numerical study carried out by Verhelst [10] for evaluating S_L at a given equivalence ratio ($\phi = 1/\lambda$) and reference condition expressed as power law function of elevated temperature and pressure,

$$S_L = S_{L0}(\lambda, P)\left(\frac{T_u}{T_{u0}}\right)^{\propto(\lambda,\ P)} \tag{7}$$

$$S_{L0} = 499.63 - 308.60\lambda + 48.887\lambda^2 - 76.238P + 4.825P^2 + 45.813\lambda P - 2.926\lambda P^2 - 7.163\lambda^2 P + 0.436\lambda^2 P^2$$

$$\alpha(\lambda, P) = 1.85175 - 0.70875\lambda + 0.50171\lambda^2 - 0.19366P + 0.0067834P^2 + 0.27495\lambda P - 0.0088924\lambda P^2 - 0.052058\lambda^2 P + 0.00146015\lambda^2 P^2$$

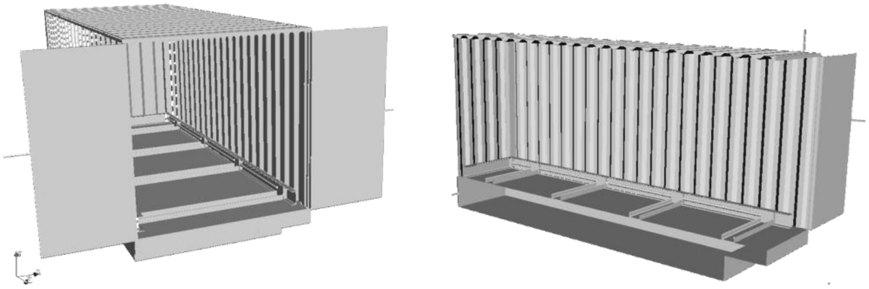
where S_L in cm/s , P is pressure in bar and T_u the unburnt gas temperature in K. The above correlation is valid for the equivalence ratios (ϕ) between 0.33 and 0.47 (lean mixtures), pressures range of 1bar ≤ P ≤ 8.5 bar and temperature range of 300 K ≤ T ≤ 800 K, with reference state T_{u0} = 300 K. The flame wrinkling factor in eq. 1 is given as

$$\Xi = \Xi_t * \Xi_{DL} \tag{8}$$

Equations (1)-(8) complete the combustion model in HyFOAM for lean hydrogen-air mixtures.

Experiments considered

The standard 20-ft ISO container of 20’ × 8’× 8’.6” was used in the experiments carried out by GexCON AS [11]. The container was positioned 0.36 m above ground level on H-beams. The pressure sensors are positioned in the U-beams frame (200 mm × 75 mm placed on floor) along the side walls of the container as shown in Figure 2. Within the container the pressure sensors were placed symmetrically at distances 0.86 m (P1-P2), 2.45 m (P3-P4), 4.0 m (P5-P5) and 5.56 m (P7-P8) from the backend wall. Outside the open doors of the container, the pressure probes were placed at elevation of 1.65m and at 5 m (P9), 10 m (P10) and 15 m (P11) from the open end along the centreline. The series of experiments were conducted for different hydrogen concentrations, both with and without any obstacles inside the container. As the first step of validation for HyFOAM, the present study considered the case with no internal obstacles and the doors were fully open with 15% hydrogen concentration by volume. The mixture was ignited by an electric inductive spark at the centre of the back end wall at the mid height of the container.



(a) Isometric view (b) Cut section along the centreline

Figure 2. The standard 20-ft ISO container with frame to hold the pressure sensors in the experiments.

Computational details

The computational domain mimics the experimental setup shown in Figure 2 and the container walls are assumed to be rigid. An hybrid hexagon-tetrahedral computational mesh was generated for the container geometry using the ‘snappyHexMesh’ utility in OpenFOAM. The mesh distribution in the computation domain is shown in Figure 2. The volume enclosing the chamber is 30.0 × 15.0 × 35 m and meshed to capture the venting of the burnt gas, the external explosions and to reduce the effect of boundary conditions on the numerical predictions. A cell size of 1.5 cm was used in the ignition region, 3 cm inside the chamber and in the area immediately outside the chamber to resolve the external explosion. A total of 3.5 M grid cells were used.

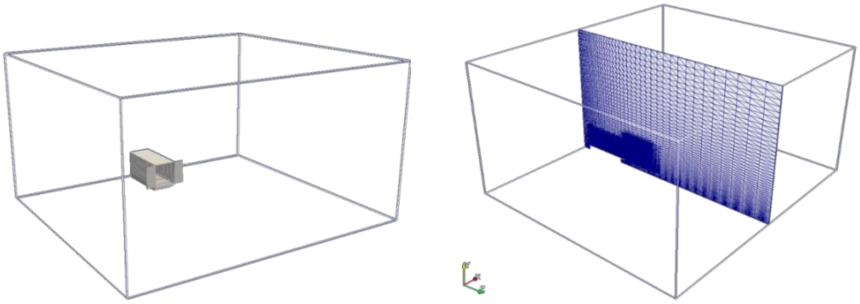
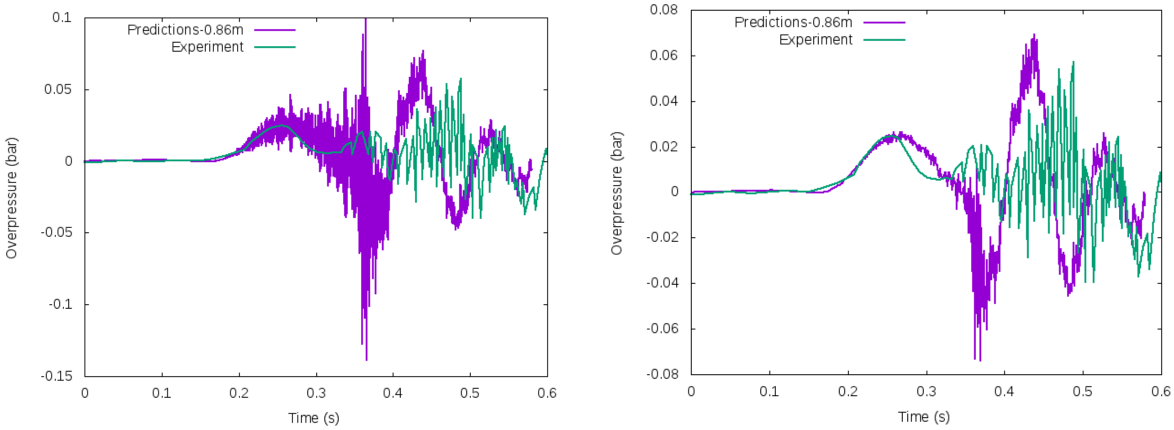


Figure 3. The computational domain and mesh distribution in a vertical plane.

The boundary conditions applied to the geometry were non-slip, adiabatic walls for the chamber walls and the ground as a conservative approximation. The 'totalPressure' and 'pressureInletOutletVelocity' boundary conditions were used for pressure and velocity respectively at the open boundaries. The 'totalPressure' boundary pressure is evaluated by subtracting the dynamic pressure from the total pressure value specified and the 'pressureInletOutletVelocity' assigns a velocity based on the flux in the patch-normal direction. This combination of pressure and velocity boundary conditions allows for the flow reversal at the open boundary patch. An open vent was used in the simulations with premixed fuel mixture initialized in the chamber volume. The random velocity field of the turbulent root mean square velocity u'= 0.1 m/s was initialized in the entire domain considering a low initial turbulence with in the domain. The mixture concentration of 15% hydrogen in air has approximately 0.42 equivalence ratio, the unstretched laminar flame speed is around 0.35 m/s, Lewis number 0.42 and mixture fraction 0.0122.

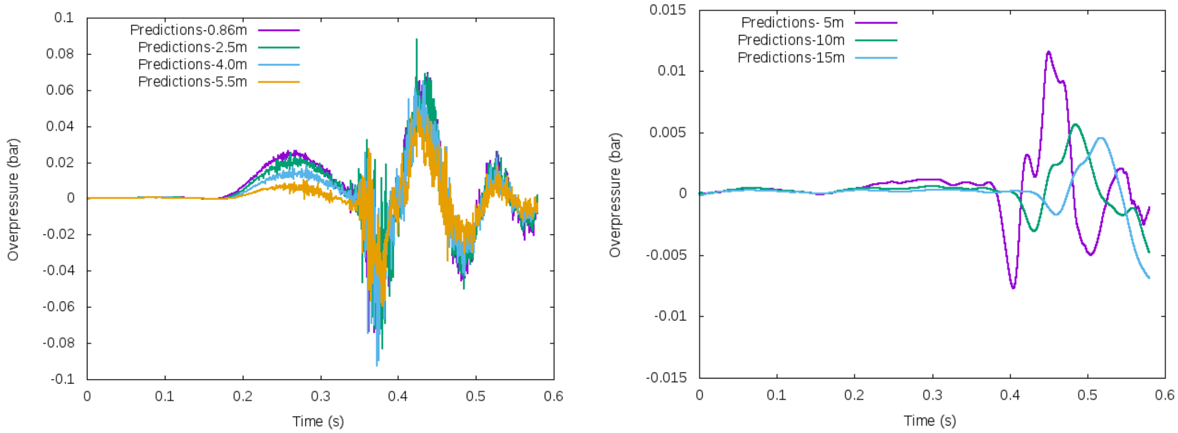
Results and discussion

The predictions are compared with the experimental measurements in Figure 4 for the peak overpressure at P1 location (at the moment only this experimental pressure trace curve is available with the authors to publish). The predicted overpressure trace curves for the pressure probe located within the container are shown in Figure 5(a) and outside in-front of the open container in Figure 5(b) after time averaging the curves for 5 ms, for showing the gross trend of the pressure-time curves.



(a) Instantaneous pressure profile (b) Time averaged profile for 5 ms

Figure 4. Comparison of the predicted and measured pressure trace curve for P1 pressure probe.



(a) (b)

Figure 5. The predicted pressure trace curves time averaged over 5 ms for other locations: (a) inside the container, (b) outside and in front of the open container door.

The second peak in the pressure trace curves in the container is much more oscillatory due to the presence of Helmholtz oscillation generated by venting of the bulk of the hot gases. It should be noted that the frequency of the oscillations observed in experiments were also affected by the structural vibrations of the container walls, which are not included in numerical simulations using the rigid wall assumption. In the experiments the container walls bulged and contracted during the positive and negative phase of the generated overpressures, this could be the reason for absence of strong negative pressure phase in the experiments as observed in the numerical simulations. Figure 5 (b) also shows that the vented explosion of 15% volumetric concentration of hydrogen in the container produced an overpressures greater than 9.8 kPa roughly up to 5 m from the container open end. Considering that 9.8 kPa overpressure is the human tolerable limit, such information is important in defining the safety distances around the hydrogen process installations.

Concluding remarks

HyFOAM has been developed on the basis of the open source CFD code OpenFOAM for vented hydrogen explosions. The flame surface wrinkling turbulent combustion model is improved with turbulent flame speed correlation accounting Lewis number effect and Darreius-landau instabilities along with suitable unstretched laminar flame speed correlation for modelling vented lean hydrogen gas explosion. As the first step of validation, predictions have been conducted for the lean hydrogen-air vented deflagration tests in an ISO container without obstacles. The predicted pressure trace curve at the peak pressure location is found to be in reasonably good agreement with the experimental data. The results have demonstrated the potential of the present numerical modelling for simulating lean hydrogen-air mixtures deflagrations in vented explosions scenarios.

Acknowledgement

The HySEA project is supported by the Fuel Cells and Hydrogen 2 Joint Undertaking (FCH 2 JU) under the Horizon 2020 Framework Program for Research and Innovation.

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