1. **Title**

The burning characteristics and flame evolution of hydrocarbon and hydrogen flash fires

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4. **Colloquium that describes the research topic**

Fire research

5. **Total length of paper and method of determination**

Method 1

6196words

6. **List word equivalent lengths for main text, nomenclature, references, each figure with caption, and each table determined according to the instructions that follow**

Text:3373words

References: 458 words

Figures total: 2366 words

Figure 1: 211 words; Figure 2: 644 words; Figure 3: 339 words; Figure 4:336 words;

Figure 5: 168 words; Figure 6: 308 words; Figure 7: 152 words; Figure 8: 156 words

Figure 9: 145 words

Abstract

A flash fire is a sudden, intense fire caused by ignition of a mixture of air and a dispersed flammable substance such as a solid (including dust), flammable or combustible liquid (such as an aerosol or fine mist), or a flammable gas. The present study aims to gain insight about the combustion processes and flame structure and dynamics associated with flash fires through computational fluid dynamics (CFD) based numerical studies using FireFOAM, the large eddy simulation based fire solver with the frame of open source CFD code OpenFOAM. It will focus on the initial transient development to gain insight about flash fire growth and the underlying combustion process. The scope of the study is, however, limited to flash fires formed following rapid release of relatively large quantities of flammable gas. The predicted flash fire diameter and the lifting height were found to be in reasonably good agreement with published experimental data. To gain further insight of the flash fire transient behaviour, the flame structures, temperature profiles and pressure fields have also been analysed. The predicted incident radiation at different locations is discussed in relation to the resulting thermal radiation hazards.

Keywords: *Flash fire; flame structure; incident radiation; FireFOAM.*

1 Introduction

A flash fire is a sudden, intense fire caused by ignition of a mixture of air and a dispersed flammable substance such as a solid (including dust), flammable or combustible liquid (such as an aerosol or fine mist), or flammable gas. On January 8, 2007, a hydrogen gas explosion occurred during a routine delivery of hydrogen when a relief device failed at the Muskingum River Plant, resulting in one fatality and injuries to ten as well as significant damage to several buildings [1]. With the anticipated upscaling of hydrogen energy applications, the storage and transport of hydrogen in liquid form will play an important role. The high density of hydrogen in its liquid phase makes fuelling stations that store liquid hydrogen economically favourable. Hydrogen is being developed as an electrical energy storage medium, i.e. it is produced, compressed or liquefied, cryogenically stored and then converted back to electrical energy or heat. However, leaks of liquid hydrogen evaporate very quickly due to the extremely low boiling point. Liquid hydrogen evaporates with a volume expansion of 1:848, posing significant risk as a highly flammable gas. Ignition of accidentally released pressurised liquid hydrogen into an open environment may result in jet or flash fires depending on the nozzle size, release direction, duration and ignition position. Combustion of a large amount of hydrogen fuel released in the atmosphere in a short duration may lead to a flash fire, which can emit a large amount of radiant energy during its lifetime [2], resulting in thermal hazards over an area several times greater than the size of the fire [2]. While some limited experimental investigations have been reported about hydrogen flash fires in terms of fire diameter, rising height, burning time and surface emissive power using small and medium scale testing facility [3–5], considerable knowledge gaps exist for hydrogen flash fires.

Due to the short duration and inherently transient nature associated with flash fires, it is difficult to gain insight about their internal structure during cloud formation and evolution through experimental investigations. A number of numerical simulations are available in the literature on the formation, evolution and combustion of vapour droplet clouds resulting from the release of hydrocarbon fuels to the open atmosphere [6–10]. These studies uncovered some characteristics of hydrocarbon flash fires, but relatively little can be found in the literature about hydrogen flash fires.

The present study aims to gain insight about the combustion processes, flame structure and dynamics associated with flash fires through computational fluid dynamics (CFD) based numerical studies. It will focus on the initial transient development to gain insight about flash fire growth and the underlying combustion process. The scope of the study is, however, limited to flash fires formed following rapid release of relatively large quantities of flammable gas.

2 Mathematical model

FireFOAM, the large eddy simulation (LES) based fire solver within the frame of OpenFOAM [11] is used. Detailed description about the methodology and solution strategy can be found in [11]. Briefly, the turbulent viscosity is calculated based on one eddy equation model with eddy coefficient of 0.07. The eddy dissipation concept is used for combustion assuming infinitely fast chemistry [12]. It is good approximation when the chemical kinetics is faster than the overall fine structure mixing. Transport equations were solved for species oxygen (O_2), water (H_2O), hydrogen (H_2), and nitrogen (N_2) to determine the gas compositions. The nitrogen mass fraction is calculated by the mass fraction of other species.

The finite volume discrete ordinates model (FVDOM) is employed to solve the radiative heat transfer equation (RTE). The accuracy can be increased by using a finer discretization. This framework allows for the incorporation of scattering, semi-transparent media, specular surfaces and wavelength-dependent transmission using banded-gray option and specific gas property models. The weighted sum of gray gases model is used in the present study to evaluate the absorption, emission coefficients [13,14]. This model is regarded as a reasonable compromise between the oversimplified grey gas model and narrow band type models. Soot model and scattering are also incorporated with radiation model for hydrocarbon flash fires.

The energy equation is solved for sensible enthalpy with due consideration for variations of enthalpies and heat capacities of individual species with temperature. The enthalpies of formation of various chemical species are calculated form JANAF thermochemical tables [15]. The CFD simulations were performed up to a physical time of 4 s with data being collected for every 0.1 μs following Courant–Friedrichs–Lewy (CFL) constraints.

3 Boundary and Initial Conditions

Figure 1 shows the three-dimensional rectangular domain selected to analyse the flash fire. The size of the domain was 16m × 16m × 20m based on preliminary calculations of the maximum diameter and the lifting height of the flash fire, which was determined with the help of mass based correlations for flash fire maximum diameter and lifting height in the literature [16]. The influence of boundaries on the evolution of flash fire was checked so that no significant velocities were formed at the boundaries. The sides and top of the domain were set as open atmosphere, in which free flow across the boundary of the domain was allowed. At y=0, the bottom plane (ground) of the domain was set as a wall with no-slip boundary condition.

The fuel inlet was circular and located at the centre of the bottom plane (XZ plane, y=0). The diameter was calculated for both cases following Makhviladze et al. [17]. Numerical predictions were conducted for flash fires from vertically released fuels. This configuration was chosen by taking into consideration of the measurements available in the tests of Hasegawa and Sato [19]. The fuel was injected in the vertical direction with a constant upward velocity for a calculated time span. As soon as the required fuel mass entered the computational domain, the inlet velocity was ramped down to zero.

Initially, the domain was filled with stagnant air at 300 K. The Computational grid was built based on the characteristic fire diameter [18]. In the characteristic fire diameter, $D^* = \left(\frac{\dot{Q}}{\rho_0 C p T_0 \sqrt{g}} \right)^{2/5}$, $\dot{Q}$ is the total heat release rate (HRR) of the fire. D^* is used to compare the optimum grid resolution with the ratio of characteristic fire diameter and the grid spacing $\left(D^*/\delta x \right)$. The grid size of $\left(D^*/\delta x \right) > 15$ is found adequate for the wide range of validation cases [18]. The grid spacing of 25 cm, $\left(D^*/\delta x \right) = 21.9$, is used in the simulation. This means that eddy of size above 25 cm has been resolved and turbulence at the scales below 25 cm is assumed to be isotropic and homogeneous.

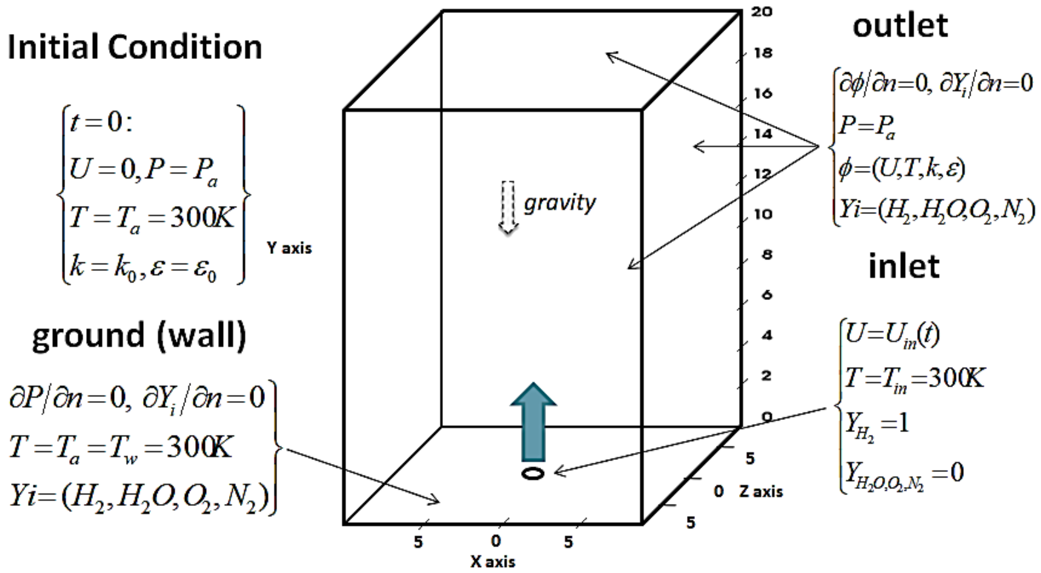

Fig. 1: The computational domain.

4 Results and discussion

As stated earlier, only flash fires resulting from the release of gaseous fuels were considered. Due to the lack of experimental measurements for hydrogen flash fires, validation was firstly performed using published test data for a propane flash fire resulted from vertical release in the atmosphere. The formation, evolution and combustion of flash fires resulting from highly volatile hydrocarbons do share considerable similarity with that of hydrogen flash fires despite the difference in combustion energy and products of combustion. Accidental release of hydrogen gas may form a liquid droplet spray due to depressurisation. As the latent heat of vaporization for hydrogen (0.449 kJ/kg) is small compared to the heat of combustion i.e. 141.58 kJ/kg, the heat required for the droplet spray to evaporate is small and the evaporation process is very short. The simulation here, which does not consider droplet spray and evaporation, should hence be a good representation of hydrogen flash fire resulting from the release of liquid hydrogen.

4.1 Hydrocarbon flash fire

The full scale tests of Hasegawa and Sato [19] for flashing releases of 5.85 kg propane in the vertical direction is considered. The computational setup mimics that of the experiment. The fuel cloud was ignited with a pilot flame positioned at 4m from the fuel injection orifice. As no precise data on the size of orifice was given [19], the inlet diameter was chosen to provide a ratio of 3 between the inlet diameter to the cubic root of initial gas volume ($\delta = d_{in} / V_0^{1/3}$), which corresponds to “cloud-like” release for a finite duration [20]. Smaller inlet diameter would lead to the formation of quasi-stationary jet. The injecting velocity of 60.6 m/s was set for a duration of 0.25 s [6] to form an enriched vapour cloud. Figure 2 shows the comparison between the experimentally observed and predicted flame envelope at two instant moments of 0.48 and 0.71s. The size of the burning cloud grows with time and forms a mushroom shape. As shown in Fig. 3.5 of Reference [19], the fuel was injected vertically at 60.6 m/s and the pilot flame was located 2.5 m above the fuel container opening and the depicted evolution of fireball formation was captured 4m above the ground where the glass vessel/ steel tank was kept (and not from the ground). In the numerical simulation, no pilot flame was used as ignition source. The combustion model was treated by the Eddy Dissipation concept, which calculates the rate of reaction based on turbulent mixing. This difference in the treatment of ignition would result in some differences in the detailed flame structure, but its influence in the global flame features such as flash fire diameter and lifting height are reasonably small. This is evidenced by the reasonably good agreement achieved on these two parameters. Indeed, reasonably good agreement is achieved between the predicted and measured diameter and lifting height. The predicted temperatures for the outer envelope of the fire are between 900 to 1500 K, while the temperatures in the stem are less than 800 K. This is attributed to the cooling of the flame at local areas due to thermal radiation. The existence of the stem is similar to experimental observations [20]. The predicted diameters and vertical flame extents are in reasonably good agreement with the measurements. In Fig.2c, contour lines for carbon dioxide (CO_2) are shown. A thin zone is clearly

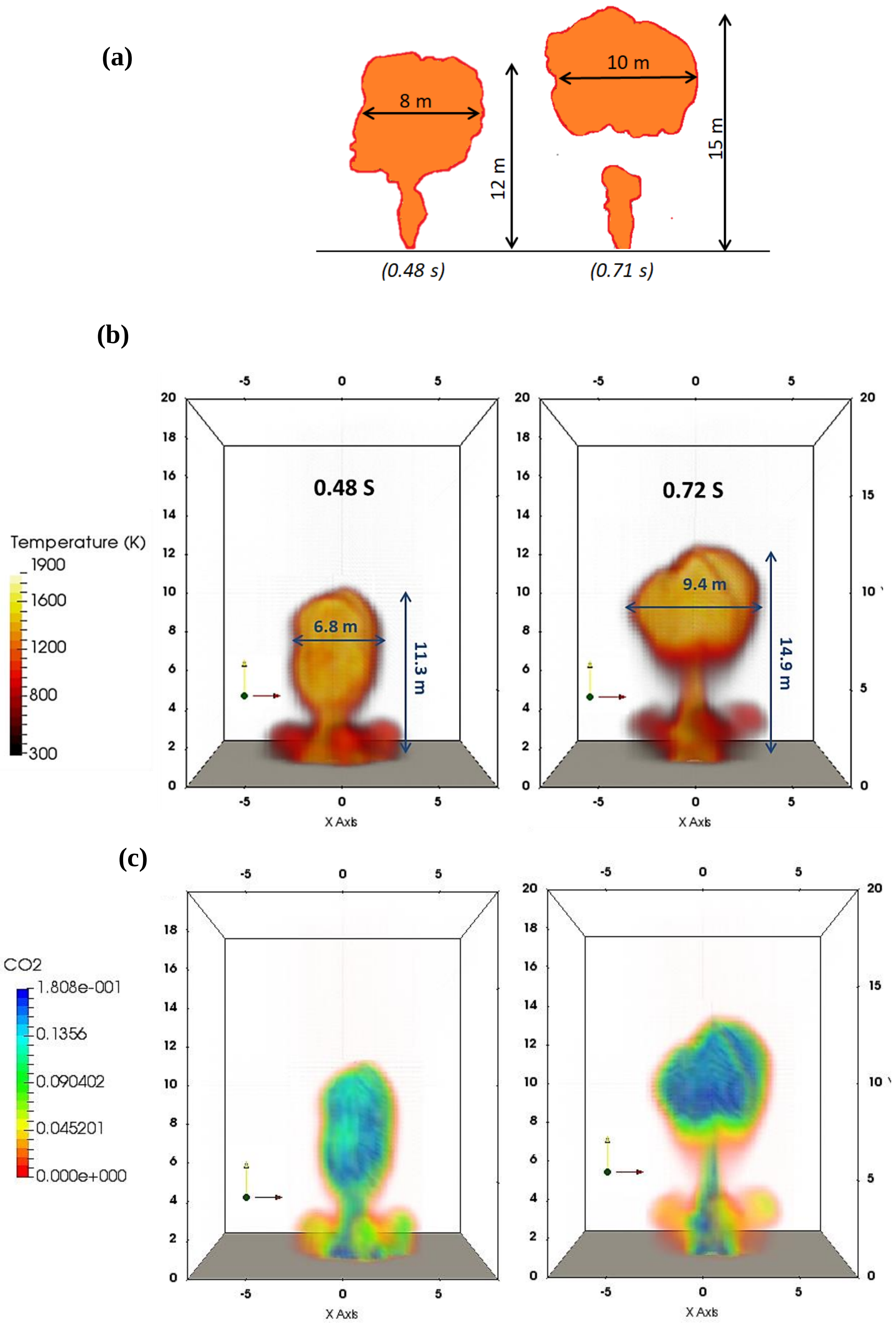

Fig. 2: Instantaneous flash fire shape resulting from combustion of 5.85 kg propane released vertically (a)Experiment [19] (b) Predicted temperature profiles (c) Predicted CO_2 mass fraction.

seen at the outer edge of the cloud where products of combustion disperse into the atmosphere. Temperatures are relatively low due to radiative heat loss to the surroundings.

The velocity vectors in Fig. 3 illustrates the burning cloud being detached from the ground and form a mushroom shape under the influence of vortices accompanying the flash fire. During the combined momentum and buoyancy-driven upward lift, cold air is drawn from the bottom of the flash fire, resulting in the stem like structure. The flame is affected by multiple vortices causing its distortion and breakdown in Fig.3. The mushroom shape of the burning cloud is attributed to the combined effects of buoyancy and viscus forces. and pressure gradients which promotes baroclinic torque ($\nabla\rho \times \nabla p$) and generates vorticities due to Richtmyer Meshkov (RM) instability.

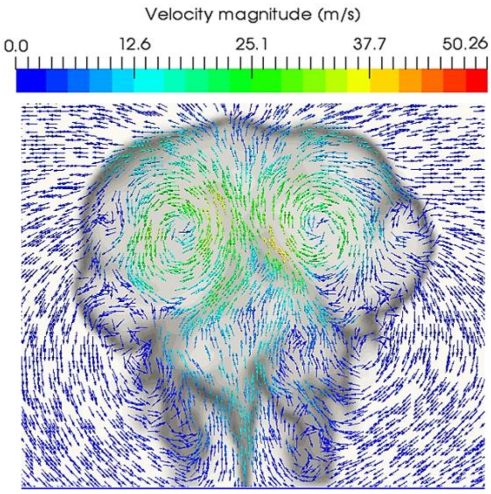

Fig. 3: Velocity vector plot showing multiple vortices.

4.2 Hydrogen flash fire

Numerical simulations are performed for hydrogen flash fires with a vertical inlet velocity of 60.6 m/s and a release rate of 5.8 kg. Figure 4 illustrates the flash fire evolution with the predicted temperature contours. The average diameter during this evolution is found to be 7.73 m. Once the fireball grows to its maximum size of 9.39 m (at 1.0 s), it starts to disperse into the atmosphere (1.5

and 2.0 s). The stem of the rising cloud remains attached to its base during the entire lifecycle. Like the hydrocarbon flash fire, the stem cools down earlier than the burning cloud. At the outer surface, air is impulsively accelerated due to volumetric expansion of the flash fire, resulting in Rayleigh–Taylor instabilities. The vortices near the edge of the cloud suck air into the core regions creating a mixing of fuel and oxidizer (see Fig. 4b) which greatly enhances the burning, promoting self-sustaining turbulent combustion. Once the fuel has burnt out, the temperature starts to decrease and the combustion products start dispersing into the atmosphere. This is thought to be the reason why flash fires become more translucent after burning as shown in the last frame of Fig. 4a.

Figure 5 shows the predicted HRR profiles. The HRR quickly reaches its maximum and then delay gradually. The transient behaviour of the turbulent combustion process is also reflected in the fluctuation of the predicted HRRs. The span of the fluctuation starts to reduce steadily from about 0.3 s. From around 1 s, the HRR starts to decay rapidly and there is significantly much less fluctuation in the predicted HRR. The predicted HRR become almost zero from about 1.1 s. Comparing this with Fig. 4, it is observed that after 1.0 s, the temperature of the surface falls down from almost 1800 K to 1300 K. This may be due to the limited amount of fuel available to feed the flash fire. The time of 1.1 s probably marks around the end of the combustion process, which is then followed by the upwards motion of the hot plume. Although the flash fire only lasted a relatively very short duration, the increased harm caused by the intense, short duration radiation is also of important safety concern [22].

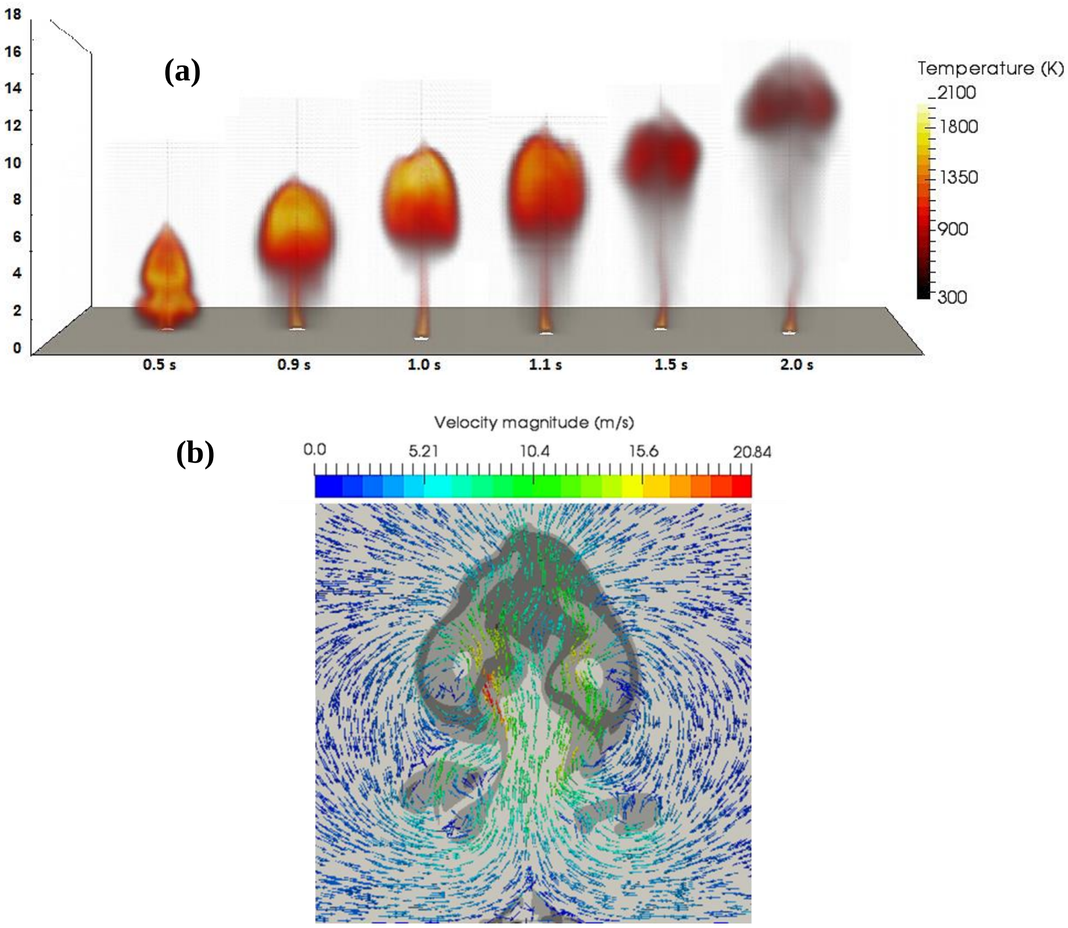

Fig. 4: Evolution of flash fire during occasioned from combustion of 5.6 kg of Hydrogen (a) Temperature surfaces (b) Velocity vector plot

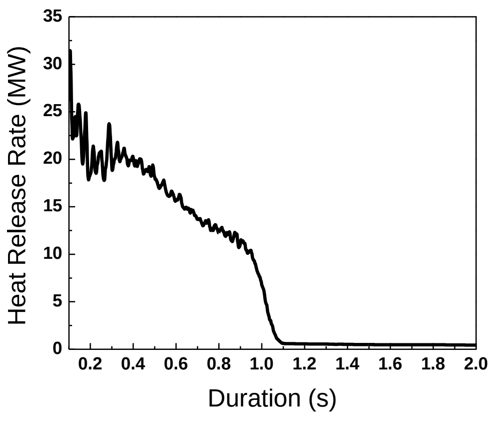

Fig. 5: The predicted heat release rate (HRR) during the evolution of the flash fire.

a) Mass fraction and temperature

To illustrate the internal structure of the flash fire, Figure 6a shows the instantaneous mass fraction of fuel (H_2), oxidizer (O_2) and water vapour (H_2O) along the centreline on XY plane at y=1.5 m z=0 m. It is seen that the fuel burns mainly at its outer surface and the combustion process is diffusive. The outer boundary of the diffusion flame shape is defined at the point where the fuel disappears. Complete combustion of the fuel was achieved due to the availability of ample oxygen from the surrounding air. The products diffuse in the atmosphere, resulting in the flash fire disappearing upwards in the atmosphere.

Figure 6b shows the temperature profile and local heat generated at the outer surface. The temperature at the outer surface decreases rapidly due to radiative heat loss to the surroundings.

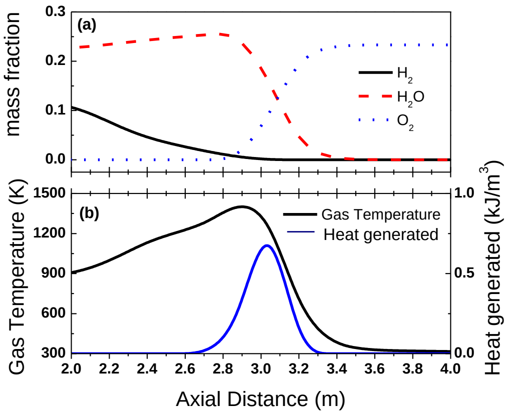

Fig. 6: Radial distribution of (a) Mass fraction of fuel, oxidizer and products (b) Temperature and heat generated.

b) Equivalence ratio and gas temperature

Figure 7 shows the variation of gas temperature within the burning cloud with fuel mass fraction and equivalence ratio. The diffusion flame temperatures depend only on the fuel/oxidizer combination. Due to availability of excess air and mixing by initial momentum, the flash fire mostly burns as lean mixture (Fig. 7a). Temperature variation is plotted along X-axis passing through Y=1.5 m at Z=0 at physical time of 0.8 sec in the Fig.7b. It is found that near stoichiometric ratio (ϕ=1, where $\phi = {8Y_{H_2}}/{Y_{O_2}}$, Y_{H_2} and Y_{O_2} are the fuel and oxidizer mass fractions [21]), the temperature reaches its maximum. Detailed analysis of the output fire for the predicted HRR also indicate that the inner portion of the fire has lower HRR due to limited availability of oxidant. This explains the surface dominating combustion phenomena for flash fires.

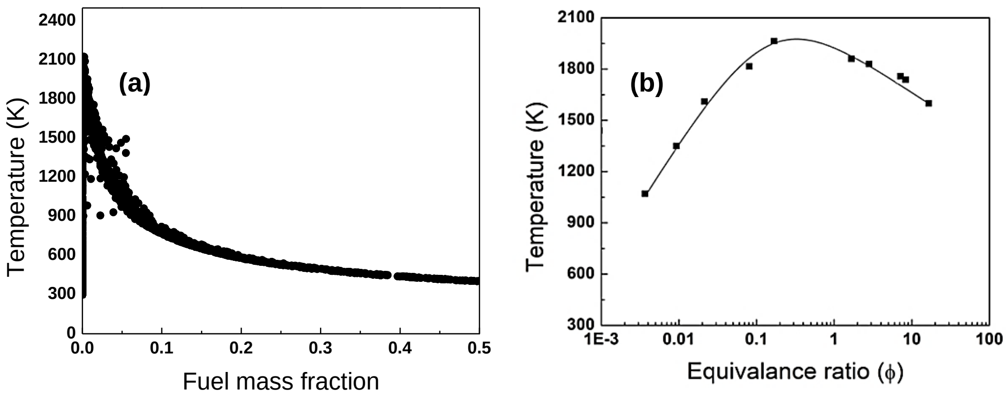

Fig. 7: Temperature variation with (a) fuel mass fraction and (b) equivalence ratio.

c) Incident radiation

Figure 8 depicts the time averaged incident radiative flux (for physical time of 4 s) on the ground level at x=0, 2, 4, 6 and 8 m. The predictions for both hydrogen and propane flash fires, which resulted from the same amount of fuel mass injection, are presented. At the centre (x=0 m), the averaged incident radiation fluxes are very similar. The incident heat flux from the hydrogen flash fire decays much more quickly than the propane fire. This is because the flash fire remains attached to the stem for longer duration in the later and the overall vertical extent of the propane flash fire is also larger. As evidenced in Fig. 2, the vertical extent of the propane fire already reached 14.9 m while it is attached to the stem and the cloud is still burning while the hydrogen flash fire only reached a maximum vertical extent of around 9.39 m when the combustion process almost completed. The differences might also be partly due to the absence of carbon and the presence of heat-absorbing water vapour in the hydrogen flash fire. Further away from the centre (x= 6 m and 8 m), the two fires have very similar radiative heat flux at ground level and much lower than the core region. This indicates that the thermal radiation hazards from flash fires mainly reside within the flame envelope and decay rapidly outside it. From the safety perspective, this would imply that flash fires pose significant risk to those in the immediate vicinity of the flammable gas release and within the flame envelope, but less so for those who are further away.

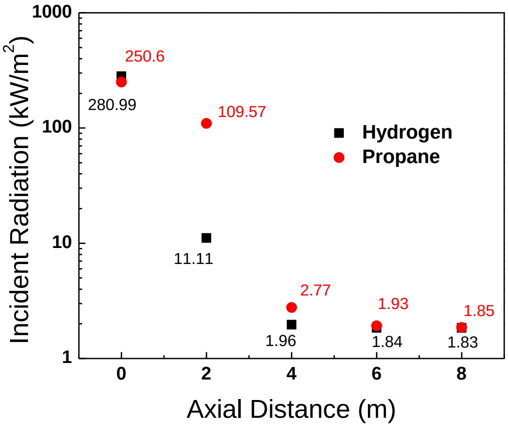

Fig. 8: Average radiative flux calculated at the locations on ground.

d) Overpressure

The variation of overpressure with time on the ground at different distances from the release point are plotted in the Fig.9. The predicted values are in line with those estimated by the semi-empirical equations in the Process Safety Guide [23]. The maximum overpressure at 2 m away is found to be 11.01 kPa, lasting only briefly for 0.01 sec. In general, unconfined fires do not reach sufficient flame speed to generate blast overpressure. Similar findings were also reported in some previous experimental studies [24].

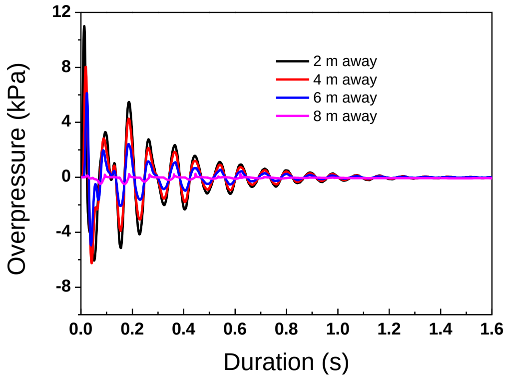

Fig. 9: The predicted overpressure on the ground at different distances from the release point.

5. Conclusion

Flash fires of propane and hydrogen formed from vertically released fuel within a very short duration have been numerically simulated using FireFOAM. For the propane flash fire, the predicted flash fire diameter and the lifting height were found to be in reasonably good agreement with the published experimental data [19]. The predictions for both fires have been analysed in detail to gain insight about the combustion characteristics, flame evolution and thermal radiation hazards from flash fire. The main findings are:

- Flash fires from propane and hydrogen show similarity in their formation and evolution, involving intense burning within a very short duration but the increased harm caused by intense, short duration radiation is also of important safety concern.
- Flash fires resulting from vertical release of flammable gases exhibit mushroom shape with the bulk of the flame envelope being supported by the stem. Once the fuel is fully consumed, the hot plume quickly detaches from the stem and rise into the atmosphere.
- In both flash fires, the stem cools down earlier than the main flame envelope.
- The flame is affected by multiple vortices causing its distortion and breakdown. The mushroom shape of the burning cloud is due to the combined effects of buoyancy and viscus forces.
- Due to availability of excess air and mixing by initial momentum, the flash fire mostly burns as lean mixture.
- At the outer surface, air is impulsively accelerated due to volumetric expansion of the flash fire, resulting in Rayleigh–Taylor instabilities. The vortices near the edge of the cloud suck air into the core regions creating a mixing of fuel and oxidizer (see Fig. 4b) which greatly enhances the burning, promoting self-sustaining turbulent combustion.
- The temperature at the outer surface of the flame envelope decreases rapidly due to radiative heat loss to the surroundings.

- Thermal radiation hazards from flash fires mainly reside within the flame envelope and decay rapidly outside it. From the safety perspective, this would imply that flash fires pose significant risk to those in the immediate vicinity of the flammable gas release and within the flame envelope, but less so for those who are further away.

Acknowledgement

The authors are grateful to EPSRC (grant number: EP/R029369/1) and ARCHER for financial and computational support as a part of their funding to the UK Consortium on Turbulent Reacting Flows (www.ukctrf.com).

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