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## Boiling Liquid Expanding Vapour Explosion (BLEVE) of peroxy-fuels: Experiments and Computational Fluid Dynamics (CFD) simulation

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### Abstract

Fire and explosion hazards associated with storage and transportation of flammable materials have been a matter of great interest in the recent times. BLEVE is a scenario that occurs when a closed fuel container is subjected to heat for a longer duration. Such events are disastrous to human beings and assets both. In the past there have been numerous studies on BLEVEs and fireballs of hydrocarbon fuels, e.g. kerosene, gasoline, LPG, LNG and others. Though, the fireballs of peroxy-fuels are not looked into detail as such. This article tries to overcome this lack of knowledge. Both, experimental investigation and CFD simulations are performed to measure and predict the fireball characteristics of a peroxy-fuel. Due to thermal decomposition in the liquid phase and active oxygen content a peroxy-fuel fireball burns at a very fast rate and emit higher thermal radiation whereas exhibits smaller diameter and elevation compared to hydrocarbons. That eventually leads to consideration of larger safety distances from them which are also verified by CFD results.

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### 1. Introduction

The regulations for safe storage and transportation of flammable materials depend on the analysis of potential scenarios e.g. dispersion, fire and explosion and their corresponding consequences. BLEVEs are such seen scenarios when closed containers of flammable materials (liquids and liquefied gases) are subjected to heat for sufficiently longer duration [1,2]. Fireballs are the consequences of BLEVEs which pose thermal radiation as well as explosion hazards to the people and assets both. In the past there have been numerous investigations performed on the thermal radiation hazards of hydrocarbon fireballs e.g. of kerosene, diesel, gasoline, LNG (Liquefied Natural Gas), propane and others [1-8]. The following parameters describe typical characteristics of a fireball: total mass of fuel ( $M$ ), diameter ( $d$ ), elevation ( $H$ ), burn time ( $t_b$ ) and irradiance ( $E$ ). Previously, there have been several models developed which work successfully for hydrocarbons. All these models consider the fireball characteristics (from a fixed location) to be a function of fuel mass  $M$  and can be written as follows:

$$d, H, t_b, E = A(M)^B \quad (1)$$

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where A and B are the constants or coefficients depending on particular fuel and its properties. For hydrocarbon fuels a range for these constants have already been developed whereas for peroxy-fuels there is a lack of measured data to deduce these values. In the past the authors group has investigated pool fires of peroxy-fuels and found considerable different characteristics [9-18]. With an aim to extend the present knowledge on potential hazards of peroxy-fuels BLEVE and fireball investigations are carried out in this work.

## 2. Experiments

The experimental set-up is shown in Fig. 1. An IBC (a composite Intermediate Bulk Container for liquids with a rigid plastics inner receptacle and a steel outer grid, Type 31HA1 [19]) of capacity of 1000 liters was filled with 900 liters of a peroxy-fuel containing 70 % tert-butyl hydroperoxide, di-tert-butyl peroxide and water. Since this peroxy-fuel has an SADT (Self-Accelerating Decomposition Temperature) [10, 14] of 80°C the heating was done beyond the same. Heat resistant oil was supplied through insulated stainless steel tubes and the peroxy-fuel was heated with a rate of 0.8 K/min.

After about 10 hrs a substance temperature of 89 °C was reached. The peroxy-fuel starts to decompose releasing gaseous products and, finally, one hour later an explosion occurs connected with bursting of the IBC and formation of a fireball. Heat flux sensors and video cameras were used to measure the thermal radiation, fireball diameter and elevation, respectively [20].



Figure 1. Typical IBC (1000 l capacity) and set-up for performing the test

The evolution of fireball with time after the explosion is shown in Fig. 2. The measured average diameter and elevation using the video images were 28 m and 35 m, respectively, which were however over predicted by the usually used equations [4] for liquid hydrocarbons. Since peroxy-fuel vapors receive additional heat from decomposition and get some oxidizer from the molecule itself they burn faster. As a result fireball was not risen to the similar elevation like hydrocarbons and exhibited smaller overall diameter. Due to the fast combustion and relatively smaller soot production peroxy-fuels show higher flame temperatures and thermal radiation than hydrocarbons. The measured thermal radiation at 100 m from the IBC was 4 kW/m<sup>2</sup> whereas at 225 m it was 0.8 kW/m<sup>2</sup>.

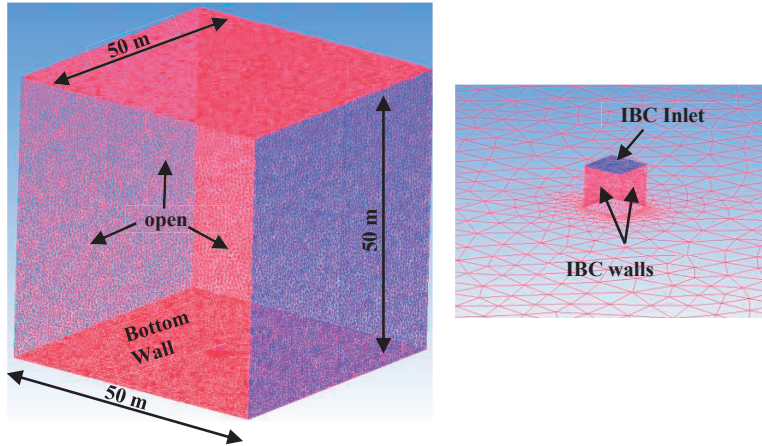


Figure 2. Time-dependent evolution of the fireball after the explosion.

Thus, the minimum thermal safety distance (for people) for them should not be less than 200 m. The explosion stretches the IBC steel grid so heavily that the type plate mounted on the grid blew up and was found 30 m away [20]. The explosion source overpressure was not measured directly. Though from the presented results the conservatively estimated value of the same was 2.56 bar gauge.

### 3. CFD simulation

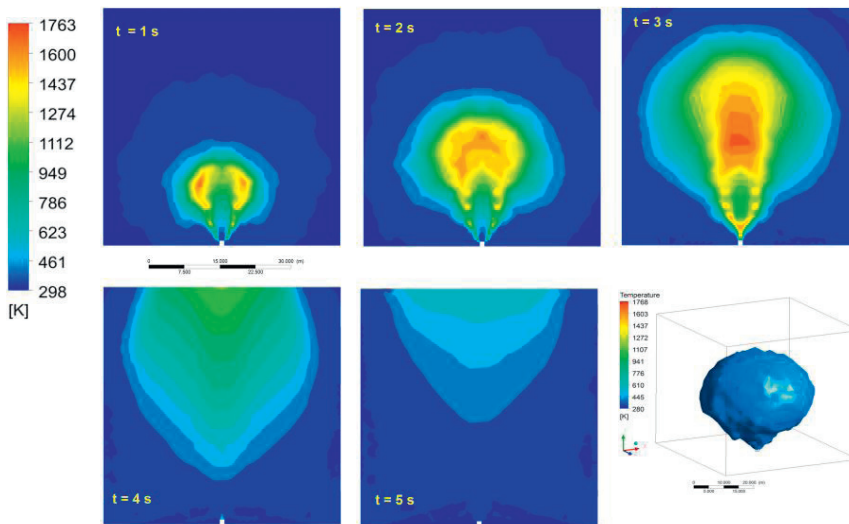
A 50 m<sup>3</sup> cube was used for modelling the effects of fireball originated from a 1 m<sup>3</sup> IBC located centrally (Fig. 3). Total numbers of tetrahedral cells were varied from 143844 to 750000 for the accuracy purposes.



The release velocity of fuel vapors was 25 m/s with a total release time of 2.5 s. Sub-models for turbulence, combustion and radiation were included to account the essential physics. Transient runs were performed for peroxy-fuel as well as for propane and Jet A. Time dependent reactive Navier-Stokes equations [21] were solved with commercial code Ansys CFX 14.5 [22].

Figure 3. Computational domain, mesh and boundary condition

CFD predicted evolution of a peroxy-fuel fireball (shown in form of isotherms) with time at the centre plane of the domain is shown in Fig. 4. In simulation the fireball was fully developed at t = 3 s and dissipated afterwards. The predicted temperatures matches well with the measured values (deduced from irradiance measurement).



CFD predicts the outer flame surface temperature as 400 K whereas the measured value was 390 K. For instance as indicated in section 2 the measured irradiance values at 225 m with four sensors were  $E = 0.8 \text{ kW/m}^2$  ( $T = 390 \text{ K}$ ) [20] which reproduced quite well by CFD as  $E = 1.3 \text{ kW/m}^2$  with a  $T = 400 \text{ K}$  (see bottom right of Fig. 4).

Figure 4. CFD predicted time evolution of a peroxy-fuel fireball (t = 1 s to 5 s are showing the contour plots of temperature at the centre plane). Bottom right is an iso-surface of 400 K.

#### 4. Conclusions

Experimental and computational investigations were performed on the BLEVE and fireball of a peroxy-fuel. Due to fast burning the peroxy-fuel fireball emitted higher thermal radiation and therefore demands for larger safety distances for storage and transportation. CFD simulation provided excellent insight on the time and space dependent near field characteristics and proved to be a powerful tool for safety distance estimations from incidents like BLEVEs and fireballs.

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