

## ABSTRACT

Time averaged mass burning rate ( $\overline{\dot{m}}_f''$ ), flame length ( $\overline{H}$ ), temperature ( $\overline{T}$ ), irradiance ( $\overline{E}$ ) and surface emissive power ( $\overline{SEP}$ ) of TBPB (tert-butyl peroxybenzoate) and TBPEH (tert-butyl peroxy-2-ethylhexanoate) pool fires are measured for six pool diameters ( $d = 0.059$  m, 0.107 m, 0.18 m, 0.5 m, 1 m and 3.4 m) at BAM in house and outside test facility.

The measured heats of combustion ( $-\Delta h_c$ ) of TBPB and TBPEH are 30113 kJ/kg and 34455 kJ/kg and the specific heat capacities at constant pressure ( $c_p$ ) are 1.8 kJ/(kg K) and 2.1 kJ/(kg K) respectively.

The measured  $\overline{\dot{m}}_f''$  of TBPB and TBPEH pool fires are in the range of  $0.37 \text{ kg}/(\text{m}^2 \text{ s}) \leq \overline{\dot{m}}_f'' \leq 0.83 \text{ kg}/(\text{m}^2 \text{ s})$  and show little dependence on the pool diameter  $d$ , and are four to sixty times higher (for  $d = 1$  m) than that of hydrocarbon pool fires. It is shown that the mass burning rates of the investigated organic peroxides can be represented as an exponential function of the self-accelerating decomposition temperature (SADT). Low SADT implies that the organic peroxide pool fires burn at a much higher  $\overline{\dot{m}}_f''$  than hydrocarbon pool fires.

Fuel Froude numbers ( $Fr_f$ ) of TBPB and TBPEH are 5 to 100 times (depending on  $d$ ) higher than for hydrocarbon pool fires. Due to higher  $Fr_f$  the  $\overline{H}$  of TBPB and TBPEH (measured with a S-VHS Videocamera) are found to be two times larger ( $d = 1$  m) than corresponding pool fires of hydrocarbons. Heskestads flame length correlation predicts the  $\overline{H}/d$  ( $d = 3.4$  m) of TBPB and TBPEH pool fires much better than Thomas and Fay correlations.

The measured time averaged flame temperatures  $\overline{T}$  ( $d = 3.4$  m) for TBPB and TBPEH pool fires are in the range of  $1400 \text{ K} \leq \overline{T} \leq 1500 \text{ K}$  and are 200 K to 300 K higher than for JP-4, kerosene and gasoline.

The irradiances of the TBPB and TBPEH pool fires measured by radiometers are  $\overline{E}$  ( $\Delta y/d = 0.3$ ) = 45 kW/m<sup>2</sup> and  $\overline{E} = 98 \text{ kW}/\text{m}^2$  which are two to ten times higher in comparison to the corresponding n-pentane, super gasoline and diesel pool fires. So the thermal safety distances for organic peroxide pool fires are larger by a factor four in comparison to the hydrocarbon pool fires.

An infrared thermography system is used for the determination of  $\overline{SEP}$  of TBPB and TBPEH pool fires. The values of surface emissive power for TBPB and TBPEH are  $\overline{SEP}$  ( $d = 3.4$  m) = 196 kW/m<sup>2</sup> and  $\overline{SEP} = 258 \text{ kW}/\text{m}^2$  and thus the  $\overline{SEP}$  are by a factor of approximately two higher than for hydrocarbon pool fires.

A self-sustained pulsating  $\overline{H}/d$  ('W'-Effect) is found in TBPB pool flames and is further analysed to explain the reason of occurrence on the basis of chemical structure of the fuel and discontinuous heat flux back from flame to the liquid pool.

CFD simulations of TBPB and TBPEH pool fires at  $d = 0.18$  m, 0.5 m, 1 m, 3.4 m and 8 m are carried out using the Unsteady Reynolds Averaged Navier Stokes (URANS) equations. The three-dimensional geometries have been discretized with unstructured hybrid grids, with the number of cells in the range of 1 million. Depending on the grid resolution and the pool diameter time steps of  $0.0001 \text{ s} \leq \Delta t \leq 0.01 \text{ s}$  for the CFD simulations are used. For solving the discretized equations a finite volume based implicit solver ANSYS CFX has been used. For modelling the combustion, stoichiometric combustion for both peroxides are assumed. The temperature dependence of the reaction rate has been determined by the Arrhenius approach. For modelling the combustion eddy dissipation concept (EDC) model has been used. For turbulence buoyancy modified k-  $\epsilon$  and SAS (Scale Adaptive Simulation) turbulence models are used. For the thermal radiation and soot mass fraction discrete transfer radiation model and Magnusson soot model have been used.

A new method is suggested for the prediction of mass burning rate ( $\overline{m}_f''$ ) by CFD simulation. Both peroxide pool fires show approximately constant mass burning rate independent of  $d$  whereas  $\overline{m}_f''$  of TBPEH are under predicted at the beginning but show relatively good agreement with measurements for large pool diameters ( $d = 1$  m). In case of TBPB the CFD simulation over predicts the mass burning rate  $\overline{m}_f''$  of small TBPB pool fires and shows a continuous decrease with  $d$ . CFD predicts the flame length  $\overline{H}$  close to the measured data provided that the constants in Thomas equation are modified.

The CFD predicted time averaged surface emission flame temperatures of TBPB and TBPEH pool fires ( $d = 3.4$  m, 1437 K and 1542 K) are in good agreement with the measured time averaged flame temperatures.

The CFD predicted  $\overline{SEF}$  for TBPB and TBPEH pool fires ( $d = 3.4$  m, 217 kW/m<sup>2</sup> and 288 kW/m<sup>2</sup>) are also in agreement with the measured values. From the CFD predicted irradiance  $\overline{E}_{\text{CFD}}$  it is possible to determine the thermal safety distances from large pool fires of hydrocarbons and organic peroxides.