

PREDICTION OF BURNING RATE OF AN ACCIDENTALLY RELEASED FLAMMABLE FUEL BY MEANS OF CFD SIMULATION

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ABSTRACT

Depending on the length of combustion zone, average mass flow rate of fluid crossing the interface (imaginary source of equivalent size) of combustion and plume zone can be represented as average mass loss rate of any fuel during steady burning period. A model based on this is suggested to predict the mass burning rate of an accidentally released flammable liquid fuel by means of CFD (Computational Fluid Dynamics) simulation. Two organic peroxides tert-butyl peroxy benzoate (TBPB) and tert-butyl peroxy-2-ethylhexanoate (TBPEH) widely used for polymerization are taken as reference fuels. The model simply assumes complete consumption of fuel (single step chemistry) in the combustion zone i.e. there are no intermediate products. The fundamental reasons behind relatively fast burning and large flame lengths of organic peroxides based on fuel Froude number (Fr_f) are also explored.

Keywords: mass burning rate; CFD simulation; TBPB; TBPEH; turbulent fire; fuel Froude number.

NOMENCLATURE

d Pool diameter (m)
 r Pool radius (m)
 \dot{m} Mass burning rate [kg/s]
 \dot{m}_a Mass of air entrained [kg/s]
 \dot{m}_g Mass of hot gases crossing the clear flame zone [kg/(m²s)]
 \dot{m}_f Mass burning rate of a finite diameter pool [kg/(m²s)]
 \dot{m}_∞ Mass burning rate of an infinite diameter pool [kg/(m²s)]
 H_{cl} Height of clear flame zone (m)
 H_p Height of plume zone (m)
 H Height of flame (m)
 ρ Density of air (1.2 kg/m³)
 g Gravitational acceleration (9.8 m/s²)
 A, B Constants (21, 38)
 x Axial length along flame (m)
 T Flame temperature (K)

v Velocity of hot gases
 y Length normal to flame axis (m)
 Fr_f Fuel Froude number

$(\bar{\quad})$ Time averaged quantity

Subscript

a ambient conditions
 f fuel
 g gas
 $f-f$ fuel surface
 $g-g$ gas surface
 CFD Computational Fluid Dynamics

INTRODUCTION

Pool fire is the most common consequence of any accidentally released flammable liquid. The occurrence of such scenario may appear in a storage facility or during the transportation of dangerous goods. A number of measures have been developed for specifying the safety distances from such fires for the people and places. The characteristics of large pool fire e.g. burning rate, flame length and radiation are the most common parameters of interest. There have a lot experimental work (Thomas, 1963, Mudan, 1984, Fay, 2007) been done on the measurement of these characteristics. Recently some computational work has also been reported by various groups (Sinai, 2000, Sinai 1995, Vela et al., 2009). The prediction of flame temperature, velocity, irradiance and surface emissive power were carried out by using CFD simulation with various sub-models for turbulence and chemistry. What was not tried to look at is the burning rate of the fuel being spilled. Almost all numerical work carried out so far concentrate on the dynamics of fire plume and the burning rate of the fuel was overlooked. Since it requires the modelling of the evaporation and the model complexity in a multiphase problem extends furthermore when natural convection also involved with it so most of the simulation only considers the gas phase combustion in pool fires and ignores the evaporation phase. We also carry out the gas phase combustion simulation and report the way to predict the burning rate following the mass balance across the combustion zone. Flame lengths and temperature predicted by the simulation are also discussed. A schematic of a large pool fire can be seen in Fig. 1 where three zones are shown in axial direction.

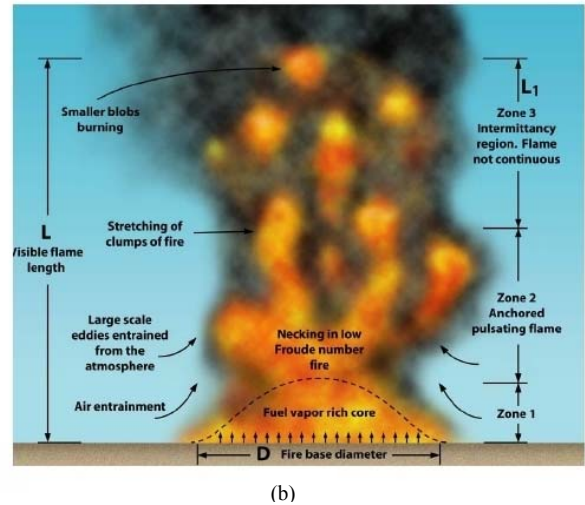
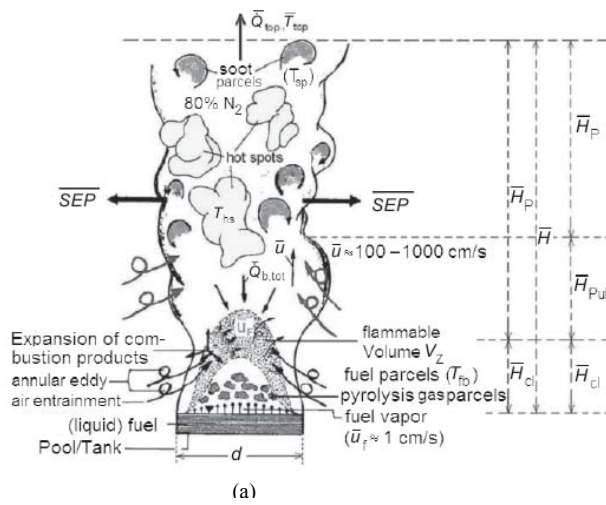


Figure 1: Three well defined zones in a large pool fire [Schönbucher et al., 2009 (a) and Raj, 2005 (b)]



Figure 2: Instantaneous photographic images of TBPB $\left(\frac{\bar{H}}{d} = 9\right)$ and TBPEH $\left(\frac{\bar{H}}{d} = 8\right)$ pool fires ($d = 3.4$ m)

The clear flame zone or sometimes called combustion zone defines the location where most of the chemical reactions occur. Above this a pulsating or intermittent zone has been observed where the continuous flame starts breaking into parts and becomes fully buoyant in plume zone i.e. third zone.

Organic peroxides are hazardous substances liable to decompose due to exothermic reactions when exposed to uncontrolled temperature, contamination, confinement and quantity. They have been used by the chemical industries for many years as free radical polymerizing agents. Their safe storage and transportation are the prime concern of chemical industries and regulating authorities. The decision about the distance for their safe storage and transportation is made on the basis of standard fire tests. Burning rate, flame temperature and irradiance are the important parameters of concern. In this work we present the estimation of these parameters

for two organic peroxides (TBPB and TBPEH) by means of CFD simulation.

EXPERIMENTAL OVERVIEW

The measurement of burning rate was carried out with weight loss measuring instruments based on the principle pressure signals which then converted into fuel loss per unit time. The \bar{m}_f of TBPB and TBPEH are found to be 6 to 8.5 times higher than a corresponding optically thick pool fire of diesel.

The ratio of time averaged visible flame length to pool diameter \bar{H}/d for both peroxides [Fig. 2] are almost 4 to 4.5 larger to a corresponding hydrocarbon pool flame e.g. diesel, gasoline, kerosene ($\bar{H}/d \approx 2$).

The details about the experimental methodology, instruments used and results could be found in references

(Mishra et al., 2008, 2009a, 2009b)

MODEL DESCRIPTION

A schematic of the physics of a pool fire of diameter d is shown in Fig. 3. The clear flame zone (combustion zone) shown as yellow colour can be separated by a section g-g above which there are only hot combustion products. The time averaged liquid fuel mass loss rate \dot{m}_f'' must be equal to the mass of hot gases crossing the interface g-g i.e. \dot{m}_g'' in order to satisfy the mass conservation principle.

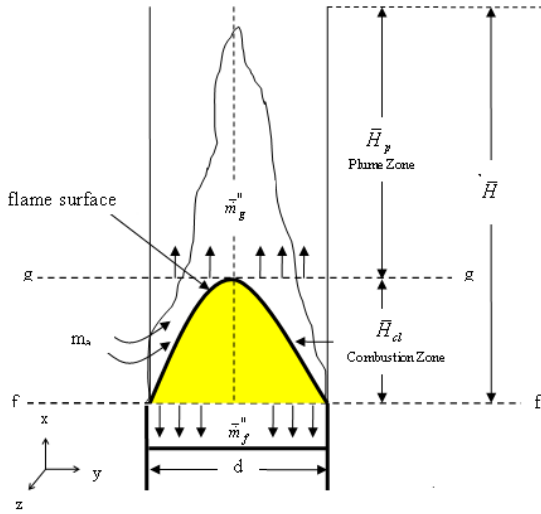


Figure 3: Mass balance across the combustion zone

Writing continuity equation across g-g

$$\dot{m}_g = \dot{m}_a + \dot{m}_f \quad (1)$$

Mass flow rate of fuel vapours leaving pool surface (above f-f):

$$\dot{m}_f = \dot{m}_f'' \times \left(\frac{\pi}{4} d^2 \right) \quad (2)$$

Mass flow rate of air entering

$$\dot{m}_a = \rho_a \times d \times \bar{H}_{cl} \times \sqrt{g \bar{H}_{cl}} \quad (3)$$

Since the mass of air entrained and mass of fuel vapour are proportional to each other; comparing equation (2) and (3) yields

$$\bar{H}_{cl} \propto d^{2/3} \quad (4)$$

Fay (2006) also provides an equation for clear flame zone i.e.

$$\frac{\bar{H}_{cl}}{d} = (13.8 \pm 2.15) Fr_f^{2/3} \quad (5)$$

Where fuel Froude number is defined as

$$Fr_f = \frac{\dot{m}_f''}{\rho_a \sqrt{gd}} \quad (6)$$

Additionally the air entrainment rate in equation (1) can be found from (Fay, 2006)

$$\dot{m}_a = A_e dx^{2/3} \quad (7)$$

Where A_e is the entrainment coefficient = 3.95 kg/(s-m^{5/3}) is calculated using the chemical and thermodynamic properties of TBPB.

Mass flow rate of burnt gases leaving upward (per unit pool surface area) (above g-g)
= mass flow average density of combustion products x mass flow average velocity of hot gases

$$\dot{m}_g'' = \rho_g \times v_g \quad (8)$$

The variables in equation (8) can be computed with the help of 3-D reactive Navier–Stokes equations (described below) with reliable turbulence models provided length of combustion zone \bar{H}_{cl} is known. Now this mass flow must be in agreement with the fuel mass loss rate for a finite diameter pool i.e. \dot{m}_f'' .

Computational Domain

Numerical pool and flow domain [Fig. 4] are modelled as axisymmetric geometry of diameters 1 m and 3.4 m and heights of 0.025 m and 7.65 m. For other pool diameters ($d = 0.18$ m, 0.5 m) appropriate scaled mesh was used. The pool wall (pan wall) is of 0.02 m thick. The mesh details and boundary conditions applied are shown in Table 1.

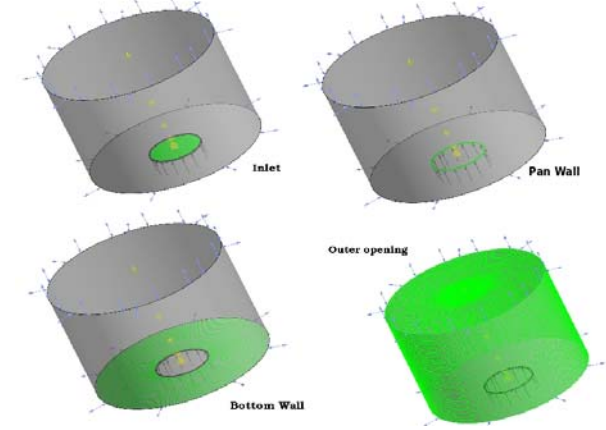


Figure 4: Mesh and boundary conditions

Part	Number of Elements	Boundary Condition
Pool	3441	Inlet (mass flow rate) (1 kg/s, T=400 K)
Pool wall	1440	No slip, Adiabatic
Bottom wall	5580	No slip, Adiabatic
Out	19821	Opening Pressure

Table 1: Mesh and Boundary Conditions

The minimum cell distance from wall to pool is 0.0046 m. Altogether 1,147,312 control volumes are used for the solution of transport equations described below. The other pool diameters are simply the scaled reduction of the above geometry and mesh size.

The following important assumptions have been made in these simulations:

1. It is assumed that mixture consists of different components i.e. a multicomponent flow is modelled and thermal and mass diffusivity of all each component is equal (Le=1).
2. Reaction takes place only in single step i.e. fuel and oxidizer mix and burnt immediately. 'Mixed is burnt' hypothesis is employed.
3. Soret and Dufour effects are neglected.

Transport Models

For solving turbulent combustion problem one has to solve two additional equations (for species and energy) along with the classical Navier-Stokes equations. In short equations describing transport phenomena together with chemical reactions are written below in tensorial notation.

Mass conservation

$$\left(\frac{\partial \rho}{\partial t}\right) + \left(\frac{\partial(\rho u_j)}{\partial x_j}\right) = 0 \quad (9)$$

Momentum conservation

$$\left(\frac{\partial \rho u_i}{\partial t}\right) + \left(\frac{\partial(\rho u_i u_j)}{\partial x_j}\right) = -\frac{\partial p}{\partial x_j} + \frac{\partial \tau_{ij}}{\partial x_j} + \rho g_j \quad (10)$$

Scalar conservation

$$\left(\frac{\partial \varphi}{\partial t}\right) + \left(\frac{\partial(\rho u_j \varphi)}{\partial x_j}\right) = \frac{\partial}{\partial x_j} \left(\Gamma \frac{\partial \varphi}{\partial x_j} \right) + q_\varphi \quad (11)$$

Where ρ denotes mixture density; u_j is the components hydrodynamic velocity; p is the pressure and τ_{ij} is the viscous stress tensor components and g_j is the j^{th} component of the external force; φ stands for scalar variable i.e. species concentration and temperature ; Γ is diffusivity of scalar φ ; q_φ is the source or sink of scalar φ .

In addition to above set of equations perfect gas law reads:

$$p = \rho \frac{R}{M} T \quad (12)$$

Where p, T and M are defined as pressure, temperature and molar mass. R is perfect gas constant = 8.314 kJ/ (kg K). Reynolds stress terms appearing in transport equations are modelled by buoyancy modified standard k- ϵ turbulence model.

Chemistry Model

The single step chemistry is modelled by Arrhenius reaction rate law (used to calculate source or sink term in the scalar conservation equation) which states:

$$k = AT^\beta \exp\left(-\frac{E_a}{RT}\right) \quad (13)$$

Where k is the reaction rate; A is pre exponential factor; E_a is activation energy; β is reaction dependent parameter. These parameters for both fuels are listed in Table 2.

Fuel	E_A (kJ/mol)	A(1/s)	β
TBPB	151.59	2.23×10^{16}	0
TBPEH	124.9	1.54×10^{14}	0

Table 2. Chemical kinetic parameters.

The eddy dissipation model co-efficient A and B are set to 4 and -1 respectively.

The following sub-models were used in the CFD simulation:

1. k- ϵ and SAS (Scale Adaptive Simulation) turbulence models.
2. Eddy dissipation combustion model
3. Discrete transfer radiation model
4. Magnussen soot model.

Solution strategy

Time dependent transport equations are solved by using second order backward Euler method with an implicit finite volume based on commercial CFD code CFX-11 with time steps size of 0.01 second. Total time of simulation was 10 s. Five coefficient loop iteration for each time step is set with 8 CPU's of 2 GB of memory each for a target criterion of 10^{-4} for all variables.

RESULT AND DISCUSSIONS

Mass burning rate

For the prediction of the burning rate from simulation one needs to know the length of combustion zone where all the fuel and oxidizer has been fully consumed and what is left is only hot combustion products. We assume that the infinite diameter pool burns with the same rate as $d=1$ m. Doing so and using equation (2) and (3) leads to an estimation of \bar{H}_{cl} of an infinite diameter pool. Furthermore an equation deduced from equation (2) and (3) provides a relation between \bar{H}_{cl} and d and is independent of the fuel type. The same is also written in terms of Fr_F in equation (5). In this way an estimation about the \bar{H}_{cl} for a given d can be established which finally helps to predict the \bar{m}_g'' by using the equation (5).

Such an approximation made for TBPB and TBPEH pool fires ($d = 0.18$ m, 0.5 m and 1 m) is shown in Fig. 5.

Where CFD results are shown as straight lines. These predictions were made when the flame has reached fully developed steady burning conditions. Both organic peroxides more or less show constant burning rate irrespective of the d whereas CFD over predicts the \bar{m}_f'' of small TBPB pool fires and shows a continuous decrease with d . On the other hand the CFD predicted \bar{m}_f'' of TBPEH pool fires are under predicted at the beginning but shows relatively good estimation for large pool diameters i.e. $d = 1$ m. Since the model largely depends on the way adopted for the calculation of \bar{H}_{cl} which is a strong function of chemical reactions which finally produces an impression about the velocity and density of burnt gases leaving upwards so it might be due to the fact that there are not enough chemical energy liberated due to the exothermic reactions in the combustion zone and therefore the velocity is largely under predicted. A unique self pulsating effect of TBPB pool fire observed experimentally could also be the reason for under prediction in simulation.

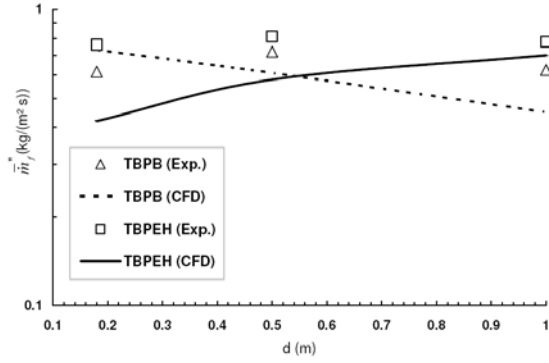


Figure 5: Mass burning rate vs. pool diameter

Flame Length

A number of semi empirical models developed are based on the correlations of flame height data of many hydrocarbon fuel pool fires. Most of them indicate that there is a dependency of flame length on fuel Froude number as written in equation (14). The definition of Fr_f can also be written as a function of \bar{m}_f'' .

$$\frac{\bar{H}}{d} = A \left(Fr_f \right)^B \quad (14)$$

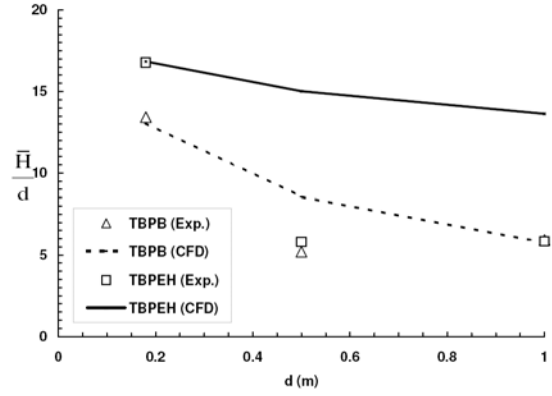


Figure 6: Time averaged measured and CFD predicted flame lengths

The constants A and B on the right hand side of the equation (14) can be adjusted according to the fuel type and its properties. Thomas performed experiments on the wood crib fires and reported the value of A and B as 42 and 0.61 respectively. Such an approximation for TBPB and TBPEH leads to the following values of constants shown in the Table 3.

Fuel	A	B
TBPB	21	0.61
TBPEH	38	0.61

Table 3: Constants used in equation (14)

Without changing the power i.e. B in the equation (11) estimates the $\frac{\bar{H}}{d}$ for TBPB quite satisfactorily whereas the prediction of TBPEH needs further adjustment of B [Fig. 6]. More experimental data will certainly help to develop precise values of A and B and finally a general relationship for organic peroxides could be realized.

Flame Temperature and Velocities

An extensive validation of the present model has been shown in (Mishra et al., 2009). Where the centreline temperature and velocities of hot gases in a large pool fire were compared with the standard experimental data reported in literature. Here we follow the same validation methodology and compare the present results with the real measurements. The maximum flame temperature predicted by CFD simulation (~1400 K) shown in Fig. 7 is in agreement with the measured one but the radial temperature profiles [Fig. 8] still deviate from the thermographic and thermocouple measurements.

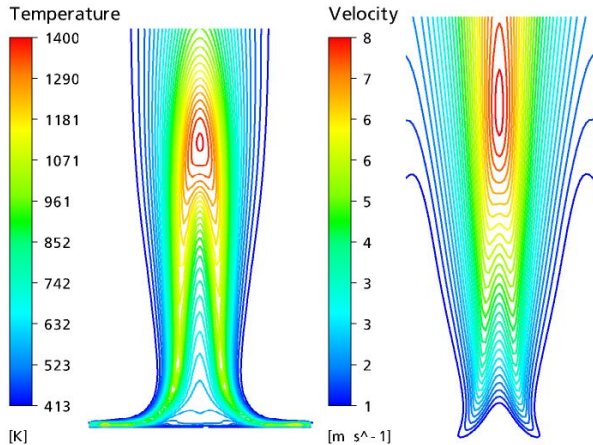


Figure 7: Instantaneous temperature and velocity profile predicted by CFD simulation ($d = 1$ m)

The mass flow average velocity with which the peroxide vapours leave the liquid pool surface is (~ 1 m/s). CFD simulation also estimates the velocities within the same range [Fig. 7]. A comprehensive validation of present simulations were reported in (Mishra et al., 2009c) where the computed radial velocity profiles of fully developed flame were found to be good in agreement except in the clear flame i.e. combustion zone. The lack of detailed chemistry did not let the flame broadened near the base of the pool.

A comparison between measured and CFD predicted time averaged radial temperature profiles at three axial locations are shown in Fig. 8. The time averaging is done by taking an average of ten instantaneous thermo graphic images of flame during steady burning period. Thermocouple measured time averaged temperatures at centre of the flame were found to be always 50-150 K lower than thermo graphic measurements whereas CFD predicted \bar{T} are quite good in agreement near to the pool

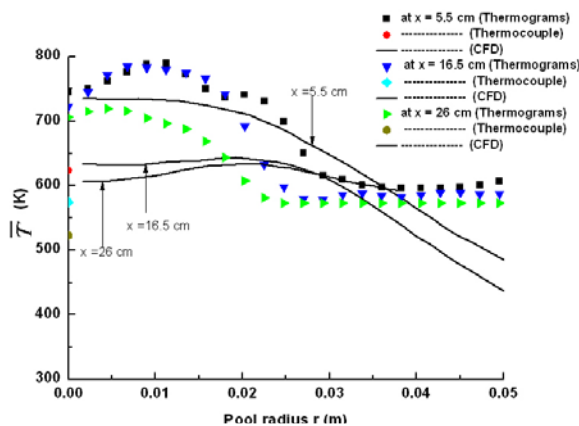


Figure 8: Time averaged measured and CFD predicted radial temperature profiles ($d = 0.18$ m)

surface and qualitatively comparable at the increased axial distances from the pool surface. Since the experiments for $d = 0.5$ m and 1 m were made outside under influence of cross wind so the true comparison was only possible for $d = 0.18$ m. Nevertheless the radial temperature profiles expect to be follow the similar pattern.

CONCLUSION AND FUTURE WORK

A model for predicting the mass burning rate of an accidentally released flammable fuel is developed and applied for two organic peroxide pool fires. Single step chemistry and the present turbulence model do not provide required mixing and therefore the burning rates are underestimated by the CFD simulation. Flame temperature and velocities of hot gases are qualitatively in agreement with the present simulation. Employment of the better chemical reaction model e.g. Flamelet and proper turbulence model e.g. LES (Large Eddy Simulation) might improve the quality of present predictions.

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