Mathematical Models for the Prediction of Heat Flux from Fire Balls

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Abstract: - The aim of this article is to summarize two mathematical models for the prediction of heat flux from Fire Ball in the context of the flammable substances safety aspects. The contribution deals with possible scenarios of accidents associated with transport and storage facilities. The study presents the results of determination of hazardous zone in the event of two various chemicals of release. For calculations, the BLEVE static model, BLEVE dynamic models included in the program EFFECTS 9.0.8. were used and results obtained were compared with the modified Netherlands Organization for Applied Scientific Research model developed by authors and programmed in NetBeans 7.4 for this study. This model can make a contribution towards solving the problems facing the flammable alternative fuels. Scenarios modeled within this study represent a possible approach to the preliminary assessment of risk that should be verified by more detailed CFD modeling. These scenarios can also be used for a quick estimation of areas endangered by an incident or accident. The results of modeling of the hazardous zones contribute to a reduction in risk of major accidents associated with these potential alternative energy sources and with the environmental safety.

Key-Words: - Accident, Effect modeling, Fire Ball, Heat Flux, Liquid Flammable Gas, Safety

1 Introduction

The sudden release of superheated flammable liquid from a storage tank or process vessel is the beginning of a complex event that often ends in the formation of a short-lived Fire Ball. The event starts with a major failure of the container. Because the pressure in the container is greater than atmospheric pressure, much of the liquid is quickly expelled into the atmosphere. In response to this rapid drop in pressure, a portion of the liquid flashes to vapor nearly instantaneously. This vapor expands rapidly, shattering some of the remaining liquid into small drops, thereby creating a turbulent aerosol cloud consisting of vapor, liquid drops, and air. The aerosol cloud quickly increases in size, entraining more air as it grows. Ignition of this aerosol cloud results in a Fire Ball that exists until the vapor and liquid fuel within the cloud are consumed. The Fire Ball can emit a large amount of radiant energy during its brief life, and is capable of causing injuries and damage over an area several times greater than the size of the Fire Ball. Therefore, when conducting a hazards or risk analysis of process vessels or storage tanks that contain superheated flammable liquids, it is important to be able to accurately model the radiant heat effects of Fire Balls. Most Fire Ball radiation models ignore the dynamic nature of Fire Balls and simply treat them as static events. This simplification often causes such models to over predict the extent of potentially damaging or injurious radiant heat hazard zones. In spite of this dynamic behavior, most Fire Ball radiation models currently in use treat the Fire Ball as a static event in which the Fire Ball has a constant size, emits radiant heat at a constant rate, and is located at a fixed position relative to grade. Static models typically assume the Fire Balls reaches its maximum diameter instantaneously and maintains that size for the full duration of the Fire Balls. Nearly all of the static models calculate the Fire Ball diameter by using an equation of the following form, which relates maximum Fire Ball diameter to the mass of fuel involved in the Fire Ball [1].

1.1 Interest

A few instances which illustrate the variety of situations and focused on propane and butane LFG under which Fire Ball has occurred are presented below in Table 1.

Table 1 An illustrative list of some of the major accidents with Fire Balls occurrence

Date	Location	Fuel	Quantity	Damage
1957	Montreal, Canada	Butane	5100	1d
1958	Michigan, USA	Butane	55	1d
1959	Meldrin, USA	Propane	55	23d
1969	Laurel, USA	Propane	65	2d, 976i
1970	Crescent City, USA	Propane	275	66i
1972	Tewksbury, USA	Propane	28	a
1972	Lynchburg, USA	Propane	9	2d, 5i
1974	Oneonta, USA	Propane	288	25i
1975	Eagle Pass, USA	Propane	18	16d
1978	Waverly, USA	Propane	45	16d, 43i
1979	Pazton, USA	Propane	a	8i
1984	Mexico City, Mex.	Propane	3000	650d
1984	Romeoville, USA	Propane	a	15d, 22i
1996	Palermo, Italy	Propane	a	5d, 25i
1998	Alberta City, USA	Propane	40	2d, 7i
2002	Cairo, Egypt	Butane	a	373d
2004	Washington, USA	Propane	a	10d

Data are taken from [2-4]. In Table 1 the letter a means that the information is not available; all the quantities are in tones; i means injured and d means death. From the Table 1 of notable Fire Ball incidents and a literature survey on Fire Ball events we can summarize the type and amount of fuel and overall damage. This is a broad assessment, limited to a sample size of 17 comprising only of some of the major Fire Ball transportation incidents but they are enough to demonstrate the importance of the Fire Balls that have occurred in this period as an interest of this study.

1.2. Previous studies

Since the Fire Ball interest has been defined, experiments have been described to confirmed the different theories about the Fire Ball, but also to create an experimental database of Fire Ball experiments for comparison with correlations and models. Most of the experiments were performed at small scale, or at middle scale, but two main experiments were performed at large scale. In 1991, large scale experiments were performed by British gas in the frame of a European commission research project and published by [5]. The reference case was a 5.6 m^3 reservoir, filled at 22% (2 tons) with butane that was heated until a pressure of 15 bars, and then ruptured by detonation of a linear shape explosive. A parametric analysis of the fluid mass (changed to 1 ton) or type (changed to propane), of the reservoir volume (doubled), and of the rupture pressure (halved) was performed. The overpressure was measured at 25, 50, 75, 100 and 150 m from the source, in different directions. A few years later, the federal institute of material research and testing (BAM) in Germany performed a BLEVE test (Fig. 1) with a 45 m^3 reservoir, filled at 22% (5 tons) with propane [6]. It ruptured at 25 bars after being immersed in a hydrocarbon pool fire. The blast wave was recorded at 100, 150 and 200 m from the source.

Fig. 1 Fire Ball following rupture of 5 ton propane reservoir, BAM experiment [6]

1.3 Analysis

Large quantities of models have been published to estimate the Fire Ball geometrical parameters radius, height and radiation some of them summarized in Tables 2-3.

Presented semi-empirical models can be grouped in two different approaches: the static models and the dynamic models. For the calculation we modified the TNO model (modification denoted in equations 2,4,5,6,7,9,12,13) as follows: (i) take into account the temporal evolution of diameter and high of the Fire Ball centre, (ii) take into account the fraction of radiation that based on comparison with experimental results and (iii) take into account the air transmissivity defined by [7], which uses the amounts of CO_2 and H_2O in the path from the Fire Ball to the observer.

Table 2 Models for estimating t (s) and D (m)

Source	Duration	Diameter
Hardee[1]	$1.11 \cdot M^{0.167}$	$6.24 \cdot M^{0.333}$
Fay[2]	$2.53 \cdot M^{0.167}$	$6.28 \cdot M^{0.333}$
Lihou [3]	$0.45 \cdot M^{0.333}$	$5.72 \cdot M^{0.333}$
Roberts[4]	$0.45 \cdot M^{0.333}$	$5.80 \cdot M^{0.333}$
Pietersen[5]	$0.852 \cdot M^{0.260}$	$6.48 \cdot M^{0.325}$
Martinsen[6]	$0.9 \cdot M^{0.260}$	$8.66 \cdot M^{0.250} \cdot t^{0.333}$

[1] [8], [2] [9], [3] [10], [4] [11], [5] [12], [6] [1]

In Table 2 M: mass of fuel in Fire Ball (kg), t: duration of the Fire Ball (s) and D: diameter of the Fire Ball (m).

Table 3 Models for estimating H (m) and q (W/m^2)

Source	Height	Radiation
Hardee[1]	-	-
Fay[2]	$6.48 \cdot M^{0.325}$	-
Lihou [3]	$4.35 \cdot M^{0.333}$	-
Roberts[4]	-	-
Pietersen[5]	$4.35 \cdot M^{0.333}$	$E \cdot F \cdot \tau$
Martinsen[6]	$8.66 \cdot M^{0.250} \cdot t^{0.333}$	$0.0133 \cdot f \cdot H_c \cdot M^{0.083}$

[1] [8], [2] [9], [3] [10], [4] [11], [5] [12], [6] [1]

In Table 3 M: mass of fuel in Fire Ball (kg), t: duration of the Fire Ball (s), H: height of the Fire Ball center (m) q: heat radiation (W/m^2), E: surface emissive power (W/m^2), F: view factor (-), τ: atmospheric transmissivity (-), f: fraction of heat (-), Hc: combustion heat [J/kg].

2 Problem Formulation

The reason for the presented analysis was the evaluation of the heat flux from Fire Ball in comparison with the results of the experimental simulations. The analysis was made by comparing the result of applications of the experimental results and accidents observations with the results obtained by tools of mathematical modeling on the basis of modification of currently available type point source and solid flame models.

3 Problem Solution

By their nature, the presented models depend heavily on experimental data. Correlations may describe the gross features of the fire. For example, to represent the location of a fire in space, correlations for the flame length and the trajectory of the centre line of the fire may be derived. Alternatively the fire may be represented by coupling the fire geometry obtained from such correlations with secondary correlations for surface emissive power or the fraction of combustion energy input to the flame that is emitted as radiation.

3.1 Solid flame (modified T.N.O.) model

The dynamic T.N.O. model is described in [1, 13] by Eq. 1 - 15. Surface emitter models, which assume that heat is radiated from the surface of a solid object (usually tilted cone or cylinder). The solid flame approach is used, which means that part of the combustion heat is radiated through the visible flame surface area of the flame. However, flames do not really emit radiation from their surface area only. The emitted heat flux varies with the distance over which emission occurs. Thus the use of SEPs is a two-dimensional simplification of a very complex three-dimensional heat radiation phenomenon.

The amount of liquefied gas released in case of complete failure of the tank:

$$m = V_{rel} \cdot \rho = f \cdot V \cdot \rho \qquad (1)$$

where m = mass of the flammable material [kg]; f = fraction of the volume of the pressure tank, filled with the flammable liquefied pressurized gas [-]; V = volume of the tank [m^3]; V_{rel} = amount of dangerous substance which will be released in case of a complete tank failure [m^3]; ρ = density of the flammable material in the pressure tank [kg/m^3].

The radius of the Fire Ball amount of liquefied gas released:

$$r = 4,33 \cdot M^{0.25} \cdot t^{1/3} \qquad (2)$$

where r = radius of the Fire Ball [m]; m = mass of the flammable material [kg].

The duration of the Fire Ball (could be also listed in [14]):

$$t = 0.9 \cdot m^{0.26} \qquad (3)$$

where t = duration of the Fire Ball [s]; m = mass of the flammable material [kg].

The lift-off height of the Fire Ball:

$$H = 2 \cdot r = 8.66 \cdot M^{0.25} \cdot t^{1/3} \quad (4)$$

where H = height from the center of the Fire Ball to the center of the ground under the Fire Ball [m]; r = radius of the Fire Ball [m]; m = mass of the flammable material [kg].

Calculation of the distance X from the center of the Fire Ball to the object:

$$X = (x^2 + H^2)^{1/2} \quad (5)$$

where X = the distance measured over the ground from the projected center of the Fire Ball on the ground under the Fire Ball [m]; H = height from the center of the Fire Ball to the center of the ground under the Fire Ball [m]; x = distance from the center of the Fire Ball to the radiated object [m].

Calculation of the maximum value of the view factor at a distance X (used calculation does not include the moving from gas dispersion phenomena [15]):

$$F = \left(\frac{8,66 \cdot m^{0.25} \cdot t^{1/3}}{2 \cdot y} \right)^2 \quad (6)$$

where F = geometric view factor [-]; r = radius of the Fire Ball [m]; X = distance from the center of the Fire Ball to the radiated object [m].

Calculation of the fraction of the generated heat radiated by a Fire Ball:

$$f = 0.27 \cdot P^{0.32} \quad (7)$$

where f = fraction of the generated heat radiated by a Fire Ball [-]; P = vapor pressure of flammable material inside the vessel [bar].

The net available heat for radiation:

$$\Delta H = \Delta H_c - \Delta H_v - C_p \cdot \Delta T \quad (8)$$

where ΔH = net available heat [J/kg]; ΔH_C = combustion heat of the flammable material at its boiling point [J/kg]; ΔH_v = vaporization heat of the flammable material at its boiling point [J/kg]; C_p = specific heat capacity at constant pressure [J/kg.K]; ΔT = temperature difference between flame and ambient temperature [K].

The Surface Emissive Power is the heat flux due to heat radiation at the surface area of the flame in W/m^2. The surface emissive power can be estimated from the combustion energy generated per second, which can be determined from the combustion burning-rate, the heat of combustion of the material and the surface area of the flame.

The surface emissive power:

$$E = \frac{\Delta H \cdot m \cdot 0.27 \cdot P^{0.32}}{4 \cdot \pi \cdot r^2 \cdot 0,852 \cdot m_f^{0,25}} \quad (9)$$

where E = surface emissive power which is the average radiation emittance of the flame surface [W/m^2]; ΔH = net available heat [J/kg]; m = mass of the flammable material [kg]; f = fraction of the generated heat radiated by a Fire Ball [-]; r = radius of the Fire Ball [m]; t = duration of exposure [s].

Actual path length between the surface area of the Fire Ball and the object:

$$x = X - r \quad (10)$$

where x = distance from the center of the Fire Ball to the radiated object [m]; X = the distance measured over the ground from the projected center of the Fire Ball on the ground under the Fire Ball [m]; r = radius of the Fire Ball [m].

Partial vapor pressure of water in air at a relative humidity:

$$P_w = 101325 \cdot (\mathrm{RH}) \cdot e^{(14,4114 - \frac{5328}{T_a})} \quad (11)$$

where P_w = partial vapor pressure of water in air at a relative humidity RH [Pa; N/m^2]; RH = relative humidity of air [%rel/100]; T_a = absolute temperature of ambient air at standard conditions [K].

Calculation of the atmospheric transmissivity:

$$A = 0,001171 \cdot \log_{10}\left(\frac{H \cdot p_w}{T_a} \right) + 0,02368 \cdot \log_{10}\left(\frac{H \cdot p_w}{T_a} \right)^2 \quad (12)$$

$$B = 0,03188 \cdot \log_{10}\left(\frac{273 \cdot r}{T_a} \right) - 0,001164 \cdot \log_{10}\left(\frac{273 \cdot r}{T_a} \right)^2 \quad (13)$$

$$\tau = 1,006 - A - B \quad (14)$$

where τ = atmospheric transmissivity [-]; P_w = partial vapor pressure of water in air at a relative humidity RH [Pa; N/m^2]; H = height from the center of the Fire Ball to the center of the ground under the

Fire Ball [m]; r = radius of the Fire Ball [m], T_a = temperature of the air [°C].

The heat flux q at a certain distance from the fire is experienced by the receiver per unit area:

$$q = E \cdot F \cdot \tau \tag{15}$$

where q = heat flux at certain distance [W/m^2]; E = surface emissive power which is the average radiation emittance of the flame surface [W/m^2]; τ = atmospheric transmissivity [-].

3.2 Point source (static C.C.P.S.) model

Point source models do not attempt any shape prediction and assume that the source of the heat radiation is a point [16] by Eg. 16 - 23.

The following equation is then used to calculate the intensity of the thermal radiation at any specific "target" location outside the flame:

$$q = \frac{2.2 \cdot \tau_a \cdot R \cdot H_c \cdot m_f^{0.67}}{4 \cdot \pi \cdot L^2} \tag{16}$$

where q = radiation per unit area received by the receptor [W/m^2]; τ_a = atmospheric transmissivity [-]; R = radiative fraction of heat of combustion [-]; H_c = heat of combustion [J/kg]; m_f = mass of fuel in the Fire Ball [kg]; and L = distance from Fire Ball center to the receptor [m].

Distance from the Fire Ball center to the specific target is than receptor:

$$L = \left(\frac{2.2 \cdot \tau_a \cdot R \cdot H_c \cdot m_f^{0.67}}{4 \cdot \pi \cdot q} \right)^{1/2} \tag{17}$$

where L = distance from Fire Ball center to the receptor [m]; q = radiation per unit area received by the receptor [W/m^2]; τ_a = atmospheric transmissivity [-]; R = radiative fraction of heat of combustion [-]; H_c = heat of combustion [J/kg]; and m_f = mass of fuel in the Fire Ball [kg].

Height of the Fire Ball center from the ground:

$$H = 0{,}75 \cdot D \quad = 4{,}35 \cdot m_f^{1/3} \tag{18}$$

where H = height of the Fire Ball center from the ground [m]; D = Fire Ball diameter [m]; and m_f = mass of fuel in the Fire Ball [kg].

Distance from the Fire Ball centre projection to the ground to the receptor:

$$X = (L^2 - H^2)^{1/2} \tag{19}$$

where X = distance from the Fire Ball center projection to the ground to the receptor [m]; L = distance from Fire Ball center to the receptor [m]; and H = height of the Fire Ball center from the ground [m].

For the evaluation of the exposure duration for Fire Ball model we used relationships, which are given in [17]. The equation for Fire Ball duration normally has the following form, which relates the duration or lifetime of the Fire Ball to the mass of fuel involved in the Fire Ball:

$$t = k \cdot m_f^n \tag{20}$$

where t = Fire Ball duration [s]; k, n = constants [-]; and m_f = mass of the flammable material in the Fire Ball [kg].

In published models, values of the constants k and n range from 0.23 to 2.61, and from 0.0966 to 0.333, respectively. Some examples of semi-empirical models are depicted in Tables 2-3. The [17] version of this equation used in this article is as follows:

$$t = 0.45 \cdot m^{0.333} \tag{21}$$

where t = Fire Ball duration [s]; and m_f = mass of fuel in the Fire Ball [kg].

The seriousness of injuries and extent of damage that can be caused by thermal radiation from a fire depend on the intensity of the incident radiation, and the duration of exposure to that level of heat flux. Since fireballs exist for only a few seconds, the duration of exposure is commonly set equal to the duration of the fireball. The evaluation of the damage caused by the thermal radiation is proportional to radiation intensity of exposure [17]:

$$D = t \cdot q^{4/3} \tag{22}$$

where D = thermal radiation dose [(W/m^2)$^{4/3}$.s]; t = duration of exposure [s]; and q = radiation per unit area received by the receptor [W/m^2].

The probit functions for the thermal "dose" that could cause the first-degree burns:

$$P = -36.38 + 2.56 \ln(q^{4/3} t) \tag{23}$$

where P = probit function [-]; t = duration of exposure [s]; and q = radiation per unit area received by the receptor [W/m^2].

These models can only be applied to the specific type of fire examined in the experiments which form the basis of the model. Also, although dimensional analysis may have been used in deriving the correlations within the model, the range over which those correlations apply will be limited (e.g. in terms of flammable material, mass flow rate, etc.).

3.3 Result and discussions

As calculation example comparable with the experimental results of [5-6] that could be compared to some non-transportation accidental scenarios like [18] (with LPG) we considered 5.6 m^3 reservoir, filled at 40% (2 tons) with pressurized liquefied butane (C_4H_{10}) that was heated until a pressure of 15 bar and 45 m^3 reservoir, and we considered 45 m^3 reservoir filled at 22% (5 tons) with propane (C_3H_8) standing within a large fire. After some time the vessel ruptures totally and two-phase mixture, instantaneously released, is ignited immediately. Due to external fire the vessel is locally weakened. Therefore it is almost probable that it will break. As impacts we will look for the heat radiation at a large storage tank, located 25, 50, 75, 100, 150 (this value is presented in Table 4-5) and 200 m from the vessel. In the calculation we will not considered the estimation of the pressure waves and fragmentation. The results of the calculations are summarized in Tables 4-5.

Table 4 Comparison of experimental simulation by British Gas with presented models

Quantity	Unit	B.G. simulation	T.N.O. Model	E.P.A. Model
d	m	74	75	73
t	s	6.1	5.9	6.1
H		85	84	54
E	kW/m^2	356	352	350

In Table 4 the name of chemical is butane; V = 5,6 m^3; filling degree = 40%, m = 2000 kg, t: duration of the Fire Ball (s), d: diameter of the Fire Ball, H: height of the Fire Ball center (m) E: heat radiation (W/m^2).

Table 5 Comparison of Fire Ball simulation by B.A.M. with presented models

Quantity	Unit	B.A.M. simulation	T.N.O. Model	E.P.A. Model
d	m	100	100	104
t	s	7.2	7.3	7.8
H	m	100	102	50
E	kW/m^2	-	353	350

In Table 5 the name of chemical is propane; V = 45 m^3; filling degree = 22%, m = 5141 kg, t: duration of the Fire Ball (s), d: diameter of the Fire Ball, H: height of the Fire Ball center (m) E: heat radiation (W/m^2).

From the results presented in Tables 4-5 we can discussed that for the radius of the Fire Ball, d, are the results of the modeling consistent with the results made by B.G. and B.A.M. (on average 7% difference). For the duration of the Fire Ball parameter, t, the results differs for about 5%. By comparing the parameter height from the centre of the Fire Ball to the centre of the ground under the Fire Ball, H, we can observed that the results of the point source model differs by approximately 3% and the results of the static models differs by approximately 36% for the B.G.

The results of the comparison are illustrated in Fig. 2-3:

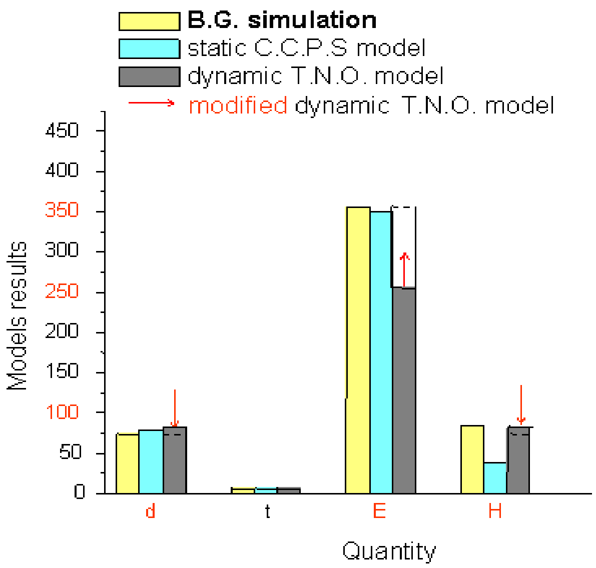

Fig. 2 Comparison of Johnsons (B.G.) experiment with the static C.C.P.S. and modified T.N.O.

Models for the B.A.M. experiment is the difference between the results of the modeling and the experimental results slightly higher

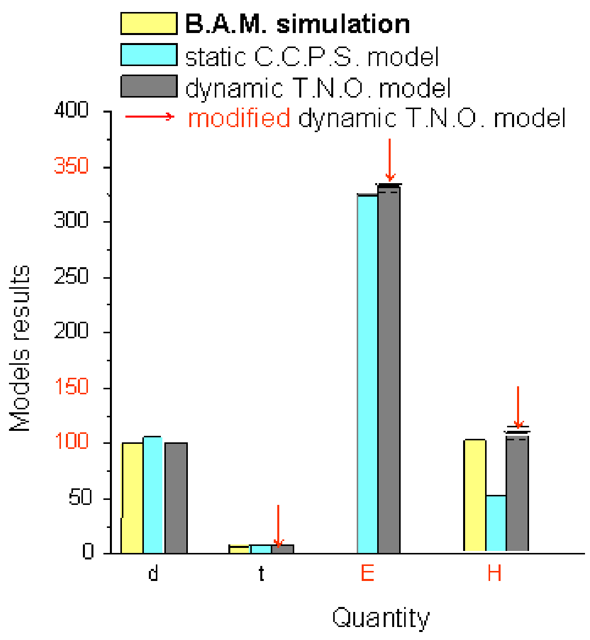

Figure 3 Comparison of Ludwigs (B.A.M.) experiment with the static C.C.P.S. and modified T.N.O. models

4 Conclusion

This study conducted with the previous studies of [1, 4, 19] introduces step-by-step development of a methodology for the estimating the fundamental parameters of Fire Ball in the context of accidents specific for transportation and storage of flammable substances. An calculation has been presented for a For these reasons the dynamic TNO model was modified and applied for testing with propane and butane Fire Ball events. Thermodynamic changes that occur during the release of superheated liquids are also incorporated into the model, making it suitable for predicting the radiant heat effects of Fire Ball formed as a result of cold catastrophic failures of pressure vessels, as well as Fire Balls created by BLEVE incidents and accidents. Predictions of the time-varying radiant heat flux incident upon targets located outside the Fire Ball are shown to agree well with results from large-scale experiments. The advantage of this modified model is that it is still quite easy to calculate. Scenarios modeled within this study represent a possible approach to the preliminary assessment of risk that should be verified by more detailed CFD modeling [20] and/or the results could be further used for a domino effect escalation [21].

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