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VAPOUR CLOUD EXPLOSION MODEL

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Summary

Over the last few years vapour cloud explosions have become a subject of major concern. The effects, loss of life and damage to property, have been shown to be very severe. The authorities responsible for safety have need of methods and models to estimate the possible damage from accidental explosions so as to be able to estimate the risk of certain installations or activities.

In this paper a model is presented which makes it possible to estimate the overpressure and positive phase duration as a function of the distance for an explosion, whether it is a detonation or a deflagration, on the basis of the reactivity (= sensitivity for flame acceleration) of the combustible mixture under consideration.

Introduction

Vapour cloud explosions have become a subject of major concern [1] over the last few years. The consequences, i.e. loss of life and damage to property, have been shown to be very severe. Therefore authorities responsible for safety, from government as well as from industry, are now involved in the estimation of the possible damage of a vapour cloud explosion resulting from industrial activities such as handling, storing and transporting combustible gases and liquids. From the whole chain of events that occur in the case of accidental release of a combustible gas or liquid, this article confines itself to the vapour cloud explosion, i.e. the presence of a combustible cloud is assumed as well as the presence of an adequate ignition source within the cloud.

After a description of the combustion phenomena involved, a model is presented and described in detail indicating ways of estimating the blast parameters, peak overpressure and positive phase duration of a vapour cloud explosion.

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Combustion phenomenology

In a premixed fuel—air mixture a flame may proceed due to different propagation mechanisms. If propagation is caused by heat transfer and diffusion of radicals from the reaction zone to the fresh mixture one speaks of a deflagration, whereas in the case of the flame being coupled to and supporting a shock wave which compresses and heats the unburned mixture almost instantaneously the explosion is called a detonation. Typical gaseous detonations show propagation velocities of the order of 2000 m/s and peak overpressures of the order of 20 bar. For a mixture of constant composition the detonation process is steady. After the reaction front has consumed the combustible mixture the shock expands in the ambient air.

Since an ordinary building will be demolished at an overpressure as low as a few tenths of a bar, a detonation in the open could cause great damage. However, a detonation in air will not easily be initiated [2]. Unless the fuel is very reactive as is the case with acetylene or ethylene oxide, it requires an intense shock wave. With other fuels such as methane, it is even doubtful whether a vapour cloud detonation is possible, although in closed systems this has been observed.

Much easier to initiate are deflagrations. Sparks with an energy content of the order of as little as a milliJoule are capable of starting a deflagration, at least in mixtures of optimum concentration, which are usually near the stoichiometric point. If the mixing ratio approaches the explosion limits the reactivity of the mixture decreases and the minimum ignition energy goes up. In a quiescent fuel—air mixture the flame velocity is of the order of a few metres per second. Due to the free expansion of the hot reaction products in the open the flame velocity is composed of the burning velocity (= velocity of the flame relative to the moving gas) and the expansion velocity (ratio is ca. 1 : 7 for stoichiometric mixtures). Flames with velocities of the order of a few metres per second do not produce peak overpressures in the open of any significance.

The flame velocity, though, may increase due to turbulence [3] in the gas ahead of the flame. This turbulence may be generated when the mixture ahead of the flame is flowing around obstacles. This will not only increase the turbulence but also the velocity of the moving gas. The velocity of the unburned gas ahead of the flame is an important part of the observed flame velocity. The above considerations lead to the following blast generating mechanisms.

Deflagration

A deflagration is the effect of a reaction front that propagates through a combustible mixture by means of heat conduction and convection from the burned to the unburned gas. The burned gas will expand and this expansion can be regarded as the movement of an imaginary permeable piston. This virtual piston movement is in fact creating the blast wave. So the rate of expansion of the burned gas is for the deflagration the blast generating mechanism.

Detonation

A detonation wave consists of a shock wave of such a strength that a chemical reaction starts directly behind the discontinuity. The energy released during the combustion process maintains the shock wave which loses energy due to its spherical expansion and its non-isentropic process. When the detonation wave reaches the edge of a combustible cloud the energy release behind the shock wave stops and the shock wave will decay in strength as it propagates through the inert atmosphere.

Calculation methods for vapour cloud explosions

The aim of the calculation methods for vapour cloud explosions as presented in this paper is to estimate the pressure-time history of the shock wave caused by the explosion as a function of distance to the explosion centre. This pressure-distance relation should enable one to estimate the damage with the proper damage criteria.

The starting point of the calculations is the existence of a cloud of combustible composition. The amount of combustible material should be the result of the dispersion calculation. The assumed central ignition of the combustible cloud will result in a deflagration or a detonation depending on several parameters such as the strength of the ignition source, the size of the cloud, the presence of obstacles and, mainly, on the reactivity of the fuel. This section will be divided into two sections, one covering the calculation methods for a deflagration, and one for the detonation-type of combustion, but both methods will assume a hemispherical cloud lying on the ground and ignited in the centre of the ground plane. The reason for this model is that other shapes cannot be covered with adequate accuracy although some estimation methods have been brought forward [4,5].

Deflagration

As has been described earlier, the velocity of a deflagration wave is not a fixed value for a certain type of combustible gas when it is dispersed in a cloud. Therefore calculations have been made for a number of assumed flame front velocities, and depending on the actual situation a flame front velocity is estimated. Methods that have been presented in the past such as Kuhl et al. [6] assume a constant flame velocity, and will give self-similar solutions. As a logical consequence these methods do not describe the effect of an extinguishing flame as the flame reaches the edge of the cloud. A recent study by Luckritz [7], however, does incorporate this effect, but still uses a constant flame velocity. The calculation method developed by the Prins Maurits Laboratory TNO, however, makes it possible to use as an input variable any flame front velocity as a function of time. This method is based on an article by Strehlow et al. [8] describing how to determine the energy release rate of an explosion once a pressure—time profile at some distance from an explosion centre is known. This method was inverted so that, assuming a certain

arbitrary energy release rate (= a flame front velocity as a function of time), the pressure-distance relation could be established.

Description of the deflagration model

A hemispherical homogeneous cloud of combustible material with a volume V_0 will expand during the combustion process to a hemisphere with a volume V_1. The energy added to the unburned gas during this process is assumed to be added by a hemispherical piston, which in fact replaces the combustion process. This energy E_0 is equal to:

$$E_0 = \int_0^\infty p \left(\frac{dV}{dt}\right) dt \cong p_0(V_1 - V_0) = n_1 R_g T_1 - n_0 R_g T_0 \tag{1}$$

where the subscript 0 denotes the initial conditions and 1 the final ones. Eq. (1) leads to:

$$E_0 = p_0 V_0 \left[\frac{n_1 T_1}{n_0 T_0}\right] - 1 \tag{2}$$

This energy E_0 is, during the equivalent piston motion, added to the gas ahead of the piston.

The pressure field ahead of the moving piston is calculated by means of the well-known method of characteristics [9]. Introduction into the characteristic equations of the characteristic explosion length $L^\star$, which is defined as

$$L^\star = (E_0/p_0)^{1/3} \tag{3}$$

and the variable λ, which is

$$\lambda = L^\star/t_b \tag{4}$$

called the characteristic explosion velocity, where t_b represents the time in which the expansion process is completed, and introduction of the following reduced dimensionless variables:

$$\bar{t} = t/t_b \quad \text{(reduced time)} \tag{5}$$

$$\bar{R} = R/L^\star \quad \text{(reduced distance)} \tag{6}$$

$$\bar{u} = u/\lambda \quad \text{(reduced particle velocity)} \tag{7}$$

$$\bar{c} = c/\lambda \quad \text{(reduced sound velocity)} \tag{8}$$

$$\bar{p} = \frac{p - p_0}{p_0} \quad \text{(reduced overpressure)} \tag{9}$$

leads to the following characteristic equations:

$$\frac{\partial \bar{p}}{\partial \bar{t}} + (\bar{u} + \bar{c}) \frac{\partial \bar{p}}{\partial \bar{R}} + \gamma \frac{(\bar{p}+1)}{\bar{c}} \left[\frac{\partial \bar{u}}{\partial \bar{t}} + (\bar{u} + \bar{c}) \frac{\partial \bar{u}}{\partial \bar{R}} + 2 \frac{\bar{u}\bar{c}}{\bar{R}} \right] = 0 \tag{10}$$

$$\frac{\partial \bar{p}}{\partial \bar{t}} + (\bar{u} - \bar{c}) \frac{\partial \bar{p}}{\partial \bar{R}} - \gamma \frac{(\bar{p}+1)}{\bar{c}} \left[\frac{\partial \bar{u}}{\partial \bar{t}} + (\bar{u} - \bar{c}) \frac{\partial \bar{u}}{\partial \bar{R}} - 2 \frac{\bar{u}\bar{c}}{\bar{R}} \right] = 0 \tag{11}$$

Substitution in the equation of $L^{\star'} = \alpha L^{\star}$, where α equals a constant so that $\bar{t}' = \bar{t}/\alpha$, $\bar{R}' = \bar{R}/\alpha$ and so on, leads to the conclusion that if λ is constant the equations are invariant. This means that for every λ there exists a unique solution of the equations. When the solution of eqns. (10) and (11) is presented in the $\bar{p} - \bar{R}$ domain there exists only one curve for each value of λ.

The boundary condition for the characteristic equations is the piston movement, which is determined by the following equations:

piston path: $$\frac{d\bar{R}}{d\bar{t}} = \bar{u} \tag{12}$$

energy: $$\frac{d\bar{E}}{d\bar{t}} = 2\pi \bar{R}^2 (\bar{p} + 1)\bar{u} \tag{13}$$

where $$\bar{E} = E(\bar{t})/E_0 \tag{14}$$

Eqn. (13) gives through the function $d\bar{E}/d\bar{t}$ the dimensionless form of the energy release rate function.

The characteristic equations together with eqns. (12) and (13) describe and determine the flow field once the energy release rate function is given as an input variable. The formation and location of shock waves in that flow field is solved by the adoption of the "area balancing technique" as extensively described by Whitham [10], and therefore not discussed in this paper.

The energy release rate function that has been adopted in our calculation is given in dimensionless form as:

$$d\bar{E}/d\bar{t} = (\pi/2)\,(\sin \pi \bar{t} + \tfrac{1}{2} \sin (2\pi \bar{t})) \tag{15}$$

which satisfies the condition:

$$\int_{\bar{t}=0}^{\bar{t}=1} \frac{d\bar{E}}{d\bar{t}}\, d\bar{t} = 1 \tag{16}$$

The relation between the value of λ and the average flame velocity may be obtained in the following way. The expansion process from a hemisphere with radius R_0 to a hemisphere with radius R_1 is governed by eqn. (2). With

$n_1 T_1 / n_0 T_0 = 7$, as is used in our calculations, the energy added per unit volume equals 6×10^5 J. This results, together with the definition of λ and by assuming the average flame velocity $\bar{v}_{fl}$ to be equal to R_1/t_b, in:

$$\bar{v}_{fl} = 0.82\,\lambda \tag{17}$$

Results of the calculations

Calculations have been performed with a computer program developed by Haverdings [11], based on the aforementioned equations for $n_1 T_1 / n_0 T_0 = 7$ and average flame velocities of 40, 80 and 160 m/s. The energy added to the gas during the expansion process has already been determined to be 6×10^5 J/m^3. In fact, the available combustion energy E_c in a combustible mixture is for stoichionetric conditions roughly equal to 3.5×10^6 J/m^3 so that about 17% of the available combustion energy is used for shock wave formation.

The results of the calculations are presented in Fig. 1 as the reduced peak overpressure of the created shock wave $\bar{P}\bar{S}$ as a function of the reduced distance $\bar{R}$ for several average flame velocities. Note that the energy used for the scaling of $\bar{R}$ is the total available combustion energy.

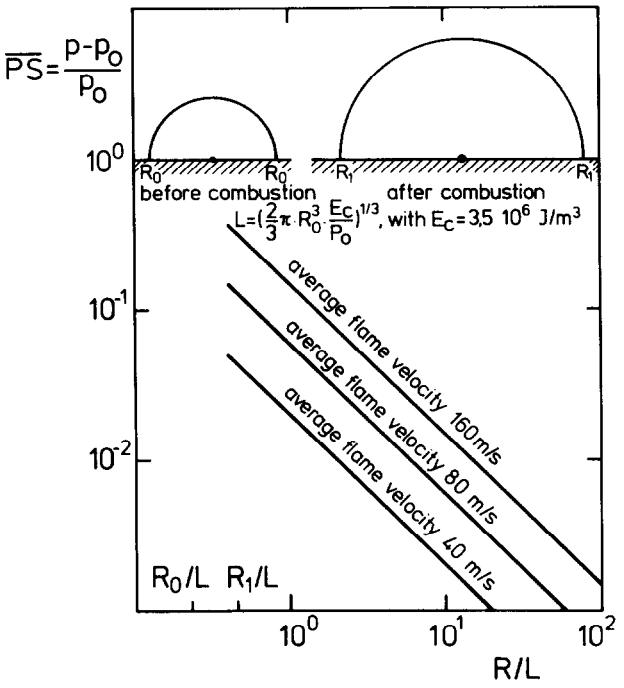

Fig. 1. Overpressure $\overline{PS}$ as a function of the distance $\bar{R}$.

TABLE 1

Peak overpressure—distance relation for average flame front velocities

Average flame velocity, $\bar{v}_{fl}$ (m/s)	Peak overpressure, $\overline{PS}$
40	$2 \times 10^{-2} \frac{L}{R}$
80	$6 \times 10^{-2} \frac{L}{R}$
160	$15 \times 10^{-2} \frac{L}{R}$

The dependence of the peak overpressure on the distance may also be given with the formulas presented in Table 1.

Estimation of the positive phase duration

An estimation of the positive phase duration of the blast wave created by a deflagration in a hemispherical volume may be obtained as shown in Fig. 2. Central ignition of a hemispherical cloud results, according to this model, in a flame front propagating with an average flame velocity $\bar{v}_{fl}$ and a sound wave with a velocity c_0 which will finally result in a shock wave. The expansion, due to complete combustion at $R = R_1$ and $t = t_b$, will be responsible for the decay behind the shock wave. The zero overpressure level behind the shock wave will propagate with the local sound velocity c_0. The propagation of the leading shock wave is governed by its peak overpressure. This overpressure as a function of the distance is, for the several average flame velocities, in general

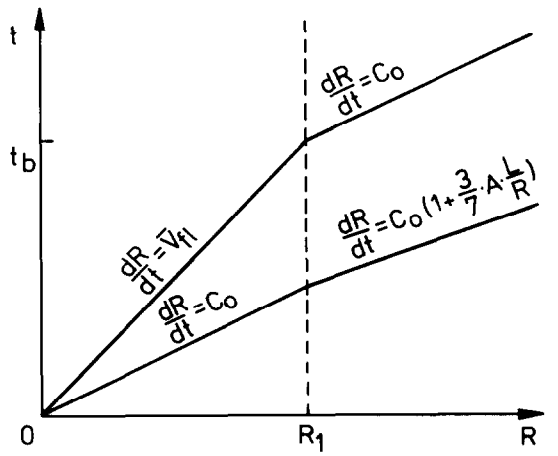

Fig. 2. Calculation of the positive phase duration.

given by the formula

$$\overline{PS} = \frac{p - p_0}{p_0} = A \frac{L}{R} \tag{18}$$

where A represents a constant which is dependent only on the average flame velocity (Table 1).

Using elementary shock wave theory [9] it is approximated that the velocity of a shock wave, U_{sw}, is related to its peak overpressure by:

$$U_{sw} = \frac{dR}{dt} = c_0 \left(1 + \frac{\gamma + 1}{4\gamma} \overline{PS}\right) \tag{19}$$

where γ represents the ratio of specific heats and is equal to 1.4 for air. Combination of eqns. (18) and (19) leads to

$$\frac{dR}{dt} = c_0 \left(1 + \frac{3}{7} A \frac{L}{R}\right) \tag{20}$$

With the derived equations as schematically presented in Fig. 2 the positive phase duration, t_+, can be estimated.

At the edge of the expanded cloud ($R = R_1$) the positive phase duration equals:

$$t_+(R_1) = R_1 \left(\frac{1}{\bar{v}_{fl}} - \frac{1}{c_0}\right)$$

The growth of t_+ as a function of R is obtained after integration of eqn. (20) and is determined by the difference at a location R of the arrival times of the leading shock wave and the sound wave (Fig. 2).

With k as integration constant, integration of eqn. (20) leads to:

$$t = \frac{R}{c_0} - \frac{3}{7} A \frac{L}{c_0} \ln\left(1 + \frac{R}{L} \frac{7}{3A}\right) + k \tag{21}$$

The second term in the equation gives the difference in arrival times between the sound wave and the shock wave. The integration constant k is given by the positive phase duration at location $R = R_1$.

$$k = R_1 \left(\frac{1}{\bar{v}_{fl}} - \frac{1}{c_0}\right) + \frac{3}{7} A \frac{L}{c_0} \ln\left(1 + \frac{R_1}{L} \frac{7}{3A}\right) \tag{22}$$

Thus the positive phase duration t_+ as a function of R is determined by the formula for $R > R_1$:

$$t_+ = R_1 \left(\frac{1}{\bar{v}_{fl}} - \frac{1}{c_0}\right) + \frac{3}{7} A \frac{L}{c_0} \ln\left[\frac{1 + \frac{7}{3A} \frac{R}{L}}{1 + \frac{7}{3A} \frac{R_1}{L}}\right] \tag{23}$$

Introduction of a dimensionless positive phase duration $\overline{TS}$ according to Baker [12]

$$\overline{TS} = c_0 t_+ \frac{1}{L}$$

reduces eqn. (23) to

$$\overline{TS} = 0.456 \left(\frac{c_0}{\bar{v}_{fl}} - 1 \right) + \frac{3}{7} A \ln \left[\frac{1 + \frac{7}{3A} \frac{R}{L}}{1 + \frac{1.064}{A}} \right] \tag{24}$$

where R_1/L is assumed to be equal to 0.456 in accordance with their definitions. Fig. 3 is a graphical representation of eqn. (24) for the adopted average flame velocities.

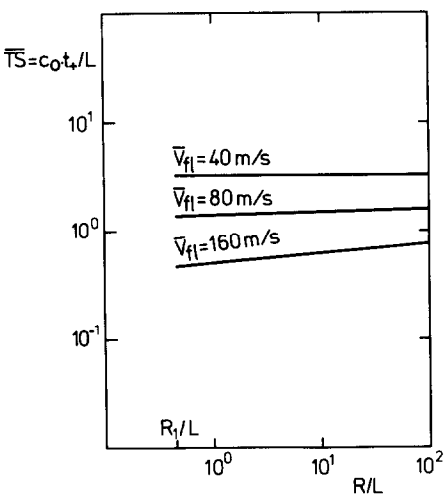

Fig. 3. The dimensionless positive phase duration TS as a function of R/L for a deflagration.

Detonation

The piston model as used for the deflagration cannot be used to estimate the shock wave overpressure as a function of the distance to the explosion centre for a detonation. Contrary to the deflagration, experimental evidence is available through the tests of Kogarko [13] for the detonation case. The validity of his experimental results has been checked by the Brinkley—Kirkwood method [14]. The calculation indicated that about 25% of the total available combustion energy is found back in the shock wave at the edge of the combustible volume. His results adopted for a hemispherical cloud and put into

the variables used in this article are for the overpressure $\overline{PS}$:

$$\overline{PS} = 0.518\,(R/L)^{-1.7} \text{ for } 0.29 < R/L < 1.088 \tag{25}$$

$$\overline{PS} = 0.2177\,(R/L) + 0.1841/(R/L)^2 + 0.1194/(R/L)^3 \text{ for } R/L > 1.088 \tag{26}$$

and for the positive phase duration TS:

$$\overline{TS} = 0.1853\,\sqrt{(R/L)} \text{ for } 0.36 < R/L < 12.6 \tag{27}$$

The upper limit for $\overline{TS}$, $R/L = 12.6$, stems from the fact that Kogarko did not publish $\overline{TS}$ for $R/L > 12.6$. Nevertheless the same procedure as proposed for the deflagration may be used for the detonation to calculate $\overline{TS}$. Hence eqn. (26) may be approximated for the low peak overpressure regime by:

$$\overline{PS} = 0.2177/(R/L) \tag{28}$$

and the equivalent equation of eqn. (23) for $\overline{TS}$ in the case of a detonation is:

$$\overline{TS} = 0.20 + 0.0933 \ln (1 + 10.7\,R/L) \text{ for } R/L > 12.6 \tag{29}$$

Vapour cloud explosion model

With the methods described and the calculation results obtained a model may be presented to estimate the blast parameters, i.e. the peak overpressure and the positive phase duration, of the shock wave originating from a hemispherical vapour cloud explosion. For that purpose the overpressure and the positive phase duration for the case of a deflagration and a detonation are given in the same graph (Fig. 4), together with a short description of the variables involved.

Three regimes are indicated in Fig. 4 applicable to fuel—air mixtures of low, medium or high reactivity respectively. If for instance a fuel—air mixture of low reactivity is considered the blast wave parameters will vary for a certain distance between the upper and lower boundary of the regime. In the actual situation for which this estimation of the blast parameters is performed the lower boundary will be used where there is no reason to expect a relatively high flame acceleration. But if reasons do exist, the upper boundary of the regime should be used. Of course, intermediate values could be chosen as well, as long as they are consistent, i.e. for one specific explosion there exists only one curve in the $\overline{PS}$—$\overline{R}$ and $\overline{TS}$—$\overline{R}$ plane which should be consistent with the formulas presented in this paper (eqns. (18) and (24)).

The criteria which determine the reactivity of the fuel—air mixtures are still under investigation at our laboratory [15], but nevertheless some fuel—air mixtures may already be placed in groups of different reactivity. In our view reactivity may be defined as sensitivity to flame acceleration.

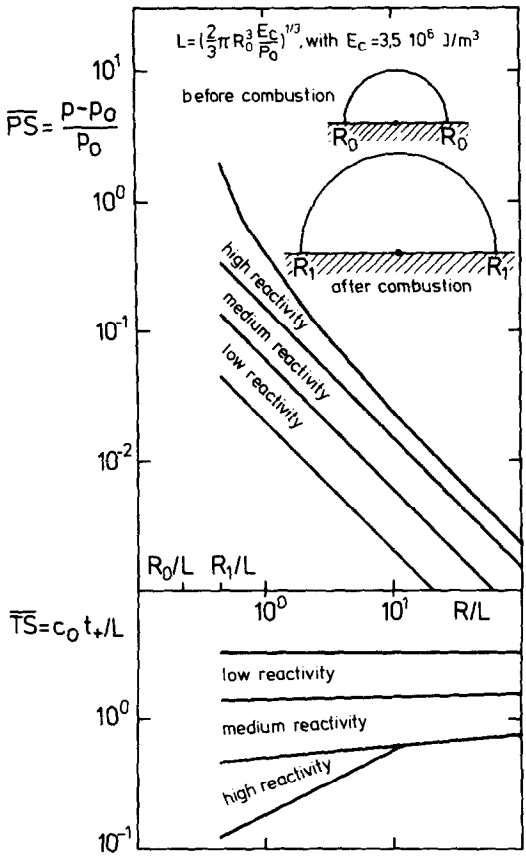

Fig. 4. Peak overpressure and positive phase duration as a function of the distance.

We consider methane, for instance, as a fuel of low reactivity, and ethane and butane as fuels of medium reactivity, whereas hydrogen, ethylene oxide and acetylene are considered to be fuels of high reactivity.

Conclusion

A model is presented for estimating the blast parameters of the shock wave originating from a vapour cloud explosion on the basis of reactivity, which has been defined as sensitivity to flame acceleration. Three regimes are given for the overpressure and positive phase duration—distance relationships, each regime being valid for a fuel—air mixture of a different reactivity. For a fuel—air mixture for which this model has to be adopted experimental data should indicate whether it is a fuel mixture of a reactivity comparable to, for instance, methane, ethane or acetylene. These experimental data should give information on the explosion parameters of the mixture.

Further, it will depend on the actual situation whether flame accelerations may be expected so that a curve near the upper or lower boundary of the regime must be chosen. Flame accelerations are generally speaking enhanced by the presence of obstacles which create, when located inside the cloud, increased flow velocities and turbulence.

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