Theoretical Approach to Dust Explosion

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Abstract

A number of experimental researches on dust explosion have been published with measured data of the explosive characteristics such as the ignition temperature, the flame propagation velocity, the upper and lower limit explosible concentrations and the rate of pressure rise.

In this study the above-mentioned explosive characteristics are dealt with systematically based on a simple model of uniformly dispersed dust cloud consisting of particles of the same size, from the viewpoint of heat transfer process.

Comparing the computed results with the empirical law and the experimental data, it is assured that the explosive characteristics can be predicted theoretically. In addition, the analysis of the area for the pressure relief venting is conducted to minimize the damage, leading to a new dimensionless vent ratio.

1. Prediction of ignition temperature
1.1 Definition of ignition temperature

The ignition temperature is defined as the gas temperature at which a mass of particles begin to burn, when they are heated in an oven with a certain shape and size. It has been measured with a great number of materials. In Fig. 1, the surface temperature of solid $T_s$ is displayed on the abscissa and the heat of reaction $q_1$ and the heat emitting from the solid surface into the atmosphere by convection $q_2$ are taken on the ordinate. When $q_1$ is less than $q_2$, the reaction is always kept at the level of oxidation. On the other hand, when $q_1$ is more than $q_2$, the reaction of combustion makes continuous progress. A steady state can be kept only on the conditions of $q_1 = q_2$ and $dq_1/dT_s = dq_2/dT_s$. The reading of the horizontal axis $T$ (surrounding temperature) on this condition is experimentally defined as the ignition temperature.

1.2 Ignition temperature of dust cloud

The reaction rate of oxidation of a single spherical particle with a diameter of $D_p$ is given by Hottel et al. as follows:

$$- \frac{dm}{dt} = \frac{k_s}{T_s} \exp \left( \frac{-E}{RT_s} \right) C_g \pi D_p^2$$

where $m$ is mass of the particle, $t$ time, $k_s$ rate constant of reaction, $E$ activation energy and $C_g$ concentration of oxygen. The number of the particles $n$ in the dust cloud with a diameter $l$ and the dust concentration $C_d$ is

$$n = C_d l^3 / \rho_s D_p^3$$

for the particle of a density $\rho_s$. The generated heat $G$ in the lump of the particles and the emitted heat $U$ from them are calculated in the
following equations:

\[ G = nQ\left(- \frac{dm}{dt}\right) = n\pi D_p^2 \frac{A}{\sqrt{T_s}} \exp\left(- \frac{E}{RT_s}\right) \]  
(3)

\[ U = n\pi D_p^2 h(T_s - T) + n\pi D_p^2 \left(\epsilon_p a_G \sigma T_s^4 - a_p \epsilon_G \sigma T_s^4\right) + \pi l^2 \left(\epsilon_p a_w \sigma T_s^4 - a_p \epsilon_w \sigma T_s^4\right) \]  
(4)

Symbols \(A\), \(e\), \(a\), \(\sigma\) and \(h\) are a constant, blackness, absorptivity, Stefan-Boltzmann's constant and film coefficient of heat transfer, respectively. The suffixes \(P\), \(G\) and \(W\) represent particle, gas and wall respectively. The solution of \(T\) of the simultaneous equations

\[ G = U \quad \text{and} \quad \frac{dG}{dT_s} = \frac{dU}{dT_s} \]  
(5)

is compared with the empirical ignition temperature\(^{2,3}\) in Fig. 2. The value of \(A\) is plotted against the activation energy in Fig. 3.

\[ \text{Fig. 2A Comparison of empirical ignition point of some metals with predicted values} \]

\[ \text{Fig. 2B Comparison of empirical ignition point of some plastics with predicted values} \]

\[ \text{Fig. 3 Relationship between } A \text{ value and activation energy} \]

2. Prediction of flame propagation velocity.\(^{16}\)

2.1 Model of propagation

Let us consider a cloud of dust in the vast space where a series of particles can be regarded to line up in the direction of flame propagation.
excluding the case of a long pipe of small diameter. The average distance \( L \) between each particle with a diameter \( D_p \) is calculated as

\[
L = \left( \frac{\pi}{6} D_p^3 \rho_s / C_d \right)^{1/3}
\]

with the dust concentration \( C_d \) and the solid density \( \rho_s \). The time interval \( \Delta t_n \) between the ignition of the \( n \)th particle and that of the \( (n+1) \)th is the time required for the flame propagation. From these values, the so-called burning velocity is calculated. Meanwhile, if the left end of a vessel is closed and the right end is open, the particles in the second and the following sections will be pushed toward right owing to the pressure rise by the generated gas from the combustion of the 1st particle. The successive particles start burning one after another and cause the expansion of gas. In this way the expansion velocity is calculated as the sum of the transportation effect by the simultaneously burning particles.

\[
\frac{\partial T(x, t)}{\partial t} = \kappa \frac{\partial^2 T(x, t)}{\partial x^2} \tag{7}
\]

\[
T(x, t) = (T_f - T_o) \text{erfc} \left( \frac{x}{2\sqrt{\kappa t}} \right) + T_o \tag{8}
\]

where \( T \) is the gas temperature with the suffix \( f \) for the flame and \( 0 \) for the initial stage and \( \kappa \) represents the coefficient of thermal diffusion. The radius \( R_b \) of the flame is given as

\[
R_b = \left( D_p / 4 \right) \left[ 1 + \sqrt{1 + \left( 2k^*/D_p \right)} \right] \tag{9}
\]

for a liquid droplet with a diameter \( D_p \) and equilibrium constant \( k^* \) (\( k^* = 1 \sim 10 \text{ cm}^2 \))

Taking dynamic heat balance of a particle,

\[
\frac{\pi}{6} D_p^3 \rho_s C_p \frac{dT_{dl}}{dt} = \pi D_p^2 h(T_{dl} - T_{dl}) + \frac{\pi}{2} D_p^3 (a_p \varepsilon_f \sigma T_f^4 + a_p \varepsilon_{el} \sigma T_{el}^4) - \pi D_p^2 \rho_p \sigma T_{dl}^4 \tag{10}
\]

The suffixes \( g \) and \( dL \) represent the gas and the particle at the point of \( L \) respectively. The time required for the complete combustion of a single particle \( \tau \) is given as

\[
\tau = K_D D_p^2 \tag{11}
\]

with the burning constant \( K_D = 100 \sim 1000 \text{ (sec/cm}^2) \)

2. 3 Expansion velocity, overall flame propagation velocity

The mass of a single particle \( m \) changes with time \( \theta \) as follows:

\[
m(\theta) = m_o \left[ 1 - \left( \frac{D_p(\theta)}{D_p_o} \right)^3 \right] \tag{12}
\]

therefore

\[
\frac{dm(\theta)}{d\theta} = \frac{3m_o}{\tau} \left( 1 - \left( \frac{\theta}{\tau} \right)^2 \right) \tag{13}
\]

When net \( n_C \) moles of gas is generated by the combustion of one mole of the particles, the volume increases at the same pressure \( P \) and the temperature \( T_G \) from \( V_1 = (n_N RT_o / P) \) to

\[
V_2 = (n_N + n_C)RT_G / P \tag{14}
\]

Where \( n_N \) is the number of mole of air per one mole of particle and \( n_C \) the number of mole of gas evolved by the combustion of one mole of the particle. The velocity due to this expansion \( v(\theta) \) is

\[
v(\theta) = \frac{R}{L^2 MP} [(n_N + n_C)T_G - n_N T_o] \frac{dm}{d\theta}
\]
\[ M \text{ is the molecular weight of the particle.} \]

\[ V(t) = \sum_{i=1}^{n-1} v(t - i\Delta t) \quad (16) \]

\[ V(t) \text{ is the overall propagation velocity (approximately equals the expansion velocity). As an example, } V(t) \text{ is calculated for cellulose acetate with density of 1.28 g/cc, } C_p = 0.35, \quad E_p = 0.8 \text{ as well as with the settings of } \epsilon = a, \quad T_f = 1600K \quad \text{and } T_0 = 293K \quad \text{and depicted in Fig. 6. These predicted values show good agreement with the empirical values of deflagration}^{10}. \]

\[ \text{Fig. 6 Overall expansion velocity} \]

3. Prediction of upper and lower limit explosible concentration

3.1 Theory of lower limit explosible concentration

Dust cloud is regarded as a group of uniformly dispersed particles in the vast space with a constant mutual distance of \( L \) as shown in Fig. 7. The distance between each particle is given as

\[ L = \left( \frac{\rho_s}{C_d} \right)^{1/3} D_p \quad (17) \]

Placing the dust cloud in the spherical co-ordination, first the particle in the center begins to burn and then the particles in the 2nd shell are heated by the emitted heat from the central particle. Supposing the particles in the 2nd shell reach the ignition temperature \( T_{ig} \) and ignite at the moment when the central particle has finished its combustion, gives the limit condition for the flame propagation to be possible. The limit concentration \( C_d \) is calculated from the \( L \) satisfying the above-mentioned condition and the equation (17). This is the theoretical lower limit explosible concentration. From the equation of heat conduction

\[ \frac{\partial T(r, t)}{\partial t} = \kappa \left( \frac{\partial^2 T(r, t)}{\partial r^2} + \frac{2}{r} \frac{\partial T(r, t)}{\partial r} \right) \quad (18) \]

and the boundary conditions of \( T = T_f \) at \( r = R_b \) and \( T = T_i \) at \( t = 0 \), the solution is

\[ T(r, t) = \frac{(T_f - T_i) R_b}{r} \text{ erfc} \left( \frac{r - R_b}{2 \sqrt{\kappa t}} \right) + T_i \quad (19) \]

From the heat balance of the particles,

\[ \frac{\pi}{6} D_p^3 \rho_s \frac{dT_d}{dt} = \pi D_p^2 h(T_{gL} - T_{dL}) \]

\[ + \frac{\pi}{2} D_p^2 a_p \epsilon_f F o T_f^4 - \pi D_p^2 \epsilon_p a T_d^4 \quad (20) \]

Assuming the relations

\[ \eta = \frac{t}{\tau} \quad (21) \]

and

\[ \tau = K_D D_p^2 \quad (22) \]

\[ T_{gL}(\eta) = \frac{(T_f - T_i) R_b}{L} \text{ erfc} \left( \frac{L - R_b}{2 \sqrt{\kappa K_D D_p^2 \eta}} \right) + T_i \quad (23) \]

The predicted \( C_d \) with \( \eta = 1 \) (lower limit explosible concentration) is compared with the
experimental values in Fig. 8. As for the cellulose compounds both values agree well when $k^*$ is 10 cm$^{-1}$.

3.2 Theoretical consideration on upper limit explosible concentration$^{12)}$

Oxygen in a limited area must diffuse to catch up with the combustion of some particles in the dust cloud for the continuous burning. First the total amount of oxygen in the considered space is shared evenly among all the particles in it. Each particle must get enough heat for ignition from the adjoining burning particle, by the time it consumes its assigned oxygen. The upper limit explosible dust concentration is clearly defined as the one at the state where all the particles at least begin to burn, not to say have finished burning. The equations are developed in the same way as in the last section except the consideration on the quantity of oxygen. An example of the comparison of the predicted values and the experimental data$^{13, 14)}$ is shown in Fig. 9. In this case explosion cannot take place with the oxygen concentration under 10%. Thus it is possible to conduct the fundamental calculation for "inerting".

4. Maximum rate of pressure rise$^{20)}$

4.1 Cubical law

The pressure and the rate of pressure rise of dust explosion in a closed vessel are most immediate characteristics to show the degree of hazard.

$$V_0^{1/3} \left. \frac{dP}{dt} \right|_{\text{max}} = K_{GC}$$

(24)

where $V_0$ is the volume of a spherical vessel and $dP/dt$ is the rate of pressure rise.

Recently the above equation has become agreed empirically$^{15)}$. $K_{GC}$ has been found to be a constant for each dust, but to differ depending on the kind of material, particle size, dust concentration and so on, although the details of it still remain unknown. In the present
report it will be discussed to understand the meaning of the constant \( K_G \) and to enable to predict it for unknown materials and under any condition. Besides the effect on scale-up by the extension to the case of unspherical vessels and the possibility of comparing experimental data obtained with the testers of different size and shape will be also discussed in the followings.

4. 2 Modeling of dust cloud in vessel

When the particles are dispersed as shown in Fig. 11,

\[
L = (\rho_s/C_d)^{1/3} D_p
\]

\[
N(n) = 24n^2 - 48n + 26
\]

\( N \) is the number of the particles on the \( n \)th spherical surface from the center \( (n \geq 2) \).

![Fig. 11 Model of dust particles with notation](image)

4. 3 Flame propagation time

The equation of heat conduction is as shown formerly

\[
\frac{\partial T_g}{\partial t} = \kappa \left( \frac{\partial^2 T_g}{\partial r^2} + \frac{2}{r} \frac{\partial T_g}{\partial r} \right)
\]

When solved with the previous boundary conditions,

\[
T_g (r, t) = (T_f - T_{io}) \frac{R_b}{r} \text{erfc} \left( \frac{r - R_b}{2\sqrt{kt}} \right) + T_{io}
\]

\( T_f \) : temperature of flame

\( T_{io} \) : initial temperature

\( R_b \) : radius of flame

\( \kappa \) : thermal diffusion coefficient

\( F \) : shape factor

\( \sigma \) : Stefan-Boltzmann’s constant

\( L \) : distance between particles

The time \( \Delta t \) when \( T_d (\Delta t) = T_{ig} \) (ignition temperature) in the equation (30) is the one required for the flame to transfer from the \( (n - 1) \)th surface to the \( n \)th, namely the flame propagation time. When the vessel is spherical and \( n \) is large enough, the propagation velocity \( v \) is

\[
v = \frac{L}{\Delta t}
\]

4. 4 Quantity of burned out dust

As \( \theta/\tau \approx 1 - D_p(\theta)/D_p0 \) where the combustion completing time \( \tau = KDP_p^{2} \), the quantity of the burned out dust by the time \( \theta \) is

\[
m(\theta) = m_o \left[ 1 - (1 - \theta/\tau)^3 \right]
\]

\( m_o = (\pi/6)D_p^3 \rho_s \)

Therefore, the total mass of the material which started burning at \( t = 0 \) and has burned out by the time \( t \) is

\[
M(t) = m_o \sum_{i=1}^{n} N(i) \left[ 1 - \left\{ 1 - \frac{t - (i-1)\Delta t}{\tau} \right\}^3 \right]
\]

\[ \approx 8m_o (t/\Delta t)^3 \] (31)

In case the oxygen is enough, the maximum amount \( M_o \) of the burned out material in a vessel of volume \( V_o \) and with the concentration \( C_d \) is

\[
M_o = C_d V_o
\]

If \( C_d \) is rather large and the oxygen is not...
where

\[ \frac{dM(t)}{dt} \bigg|_{t=t_0} = \frac{24m_0}{(\Delta t)^3} \left( \frac{aV_o}{8m_o} \right)^{2/3} \Delta t^2 \]

\[ = \frac{6}{\Delta t} m_0^{1/3} (aV_o)^{2/3} \]

Therefore

\[ V_o^{1/3} \frac{dP}{dt} \bigg|_{t=t_0} = \gamma D \left( \frac{36\pi \rho_2^{1/3}}{a} \right) P_{\text{max}} \left[ 1 - \left( \frac{P_o}{P_{\text{max}}} \right)^{1/\gamma} \right] \]

This equation shows that the empirical cubic law has been deduced theoretically and that when the properties of the dust (chemical formula, concentration, particle size) are known, the value \( K_{GC} \) in the equation (24), namely the right hand side of the equation (39) is apparently constant. Though a spherical vessel has been dealt with here, the cubical law including a shape factor can be adaptable also for vessels of approximately cylindrical shape, which suggests the possibility of exchanging data with vessels of various shapes. Figs. 13 and 14 show the predicted value by the equation (39) and (35) respectively and Fig. 15 displays the comparison of the theoretical and experimental values\(^{18,19}\).
\[
\frac{dP}{dt} = \gamma P^{1-\gamma} (P_m^{1/\gamma} - 1) \frac{dM(t)}{dt} - \gamma P^{1-\gamma} (P_m^{1/\gamma} - P) \left( \frac{W_b}{\rho_m V_o} + \frac{W_u}{\rho_o V_o} \right) \quad (40)
\]

For \( P < 1/0.53 \)
\[
W = C_s S \left( \frac{2\gamma}{\gamma - 1} \right) g_c P_o (\gamma P - P_v^{\gamma-1})^{1/2}
\]
and for \( P > 1/0.53 \)
\[
W = C_s S \left( \frac{2\gamma}{\gamma + 1} \right) g_c P_o \gamma P_v^{\gamma-1/2}
\]

If \( P \) in the equation (40) reaches the maximum achievable pressure \( P_v \), \( dP/dt \) must become 0. The area of the relief vent should be designed in such a way that \( P_v \) is kept under the strength of the material constructing the vessel. The value \( C_s \) is called coefficient of discharge.

Using the above-mentioned \( K_{GC} \)
\[
\left[ \frac{S}{V_o^{2/3}} \right]^{-1} = \frac{P_v}{K_{GC}} \left( \frac{g_c P_o}{\rho_o} \right)^{1/2} f(\gamma) g(P_v) \quad (42)
\]
Here for \( P_v < 1/0.53 \)
\[
f(\gamma) = \gamma \left( \frac{2\gamma}{\gamma - 1} \right)^{1/2},
\]
\[
g(P_v) = P_v^{1-\gamma} (P_v^{1-1/\gamma} - 1)^{1/2}
\]
and for \( P_v > 1/0.53 \)
\[
f(\gamma) = \gamma \left( \frac{2}{\gamma + 1} \right)^{(\gamma+1)/(\gamma-1)^{1/2}}
\]
\[
g(P_v) = P_v^{(3\gamma-1)/2\gamma}
\]

The theoretical values and the experimental ones\(^{18,22,23}\) of \( S/V_o^{2/3} \) are compared in Fig. 16 with different symbols for the various kinds of material. The theoretical values seem larger to some extent than the experimental ones, as the first term of rate of pressure rise in Eq. (40) is replaced by the maximum one to assure safety. But it is clearly understood from the figures that the tendency of the predicted values is in accordance with that of the experimental ones. Besides, the compared values range over the second power of 10, which suggests the theoretical equation can be applied to the wide range of practical cases.

5. **Design of pressure relief vent\(^{21}\)**

5.1 **Vent ratio**

The vent ratio is defined conventionally as the one of the area \( S \) of the pressure relief vent to the volume \( V_o \) of the vessel. Empirically it is used for designing pressure relief vent but not sound because it is not dimensionless.

5.2 **Pressure rise at explosion relief venting**

From the equation of dynamics for pressure rise,
Fig. 16 Comparison of calculated $S/V_o^{2/3}$ with experimental $S/V_o^{2/3}$

range of design of relief vent.

**Nomenclature**

$A$: constant

$a$: a constant regarding dust concentration $= C_d$

$C_d$: dust concentration

$C_g$: concentration of oxygen

$C_s$: coefficient of discharge

$C_{ps}$: specific heat of solid

$D_p$: particle diameter

$E$: activation energy for oxidation

$F$: view factor

$G$: generated heat

$g_c$: gravitation conversion factor

$h$: heat transfer coefficient

$k_D$: burning constant

$K_{GC}$: constant for cubical law

$k_s$: rate constant

$k^*$: equilibrium constant

$L$: average distance between two particles

$l$: diameter of dust cloud

$M$: molecular mass

$m$: mass of particle

$N(n)$: number of particles at nth spherical surface

$n$: number of assumed spherical surface

$n$: number of particles

$n_C$: mole number of gas produced by combustion per one mole of particle

$n_N$: mole number of air per one mole of particle

$P$: pressure

$P$: pressure ratio

$P_{max}$: maximum pressure

$P_v$: maximum achievable pressure = strength of material

$Q$: heat of reaction per gram

$q_1, q_2$: heat generated and emitted

$R$: gas constant

$R_b$: radius of flame

$R$: distance for spherical co-ordinates

$S$: vent area

$T$: temperature of gas

$T_{GL}$: gas temperature at a distance $L$

$T_f$: flame temperature

$T_{dL}$: solid temperature at a distance $L$

$T_s$: temperature of solid surface

$T_i, T_0$: initial temperature

$t$: time

$Δt$: time interval for propagation

$U$: heat left

$V$: overall expansion velocity

$V_o$: volume of equipment

$v$: velocity

$W$: mass velocity of gas

$X$: distance

$α$: absorptivity

$γ$: specific heat ratio

$ε$: blackness

$ρ_s$: density of solid

$κ$: thermal diffusivity

$σ$: Stefan-Boltzmann’s constant

$τ$: time for completing reaction

$θ$: time

$η$: $t/τ$

**Subscripts**

$G$: gas

$p$: particle

$w$: wall

$b$: burnt

$u$: unburnt

$o$: initial

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