Turbulent Clustering of Particles and Radiation Induced Ignition of Dust Explosions

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ABSTRACT

Since detonation is the only established theory that allows rapid burning producing a high pressure that can be sustained in open areas, the generally accepted opinion was that the mechanism explaining the high rate of combustion in dust explosions is deflagration-to-detonation transition. In the present work we propose a theoretical substantiation of an alternative mechanism explaining the origin of the secondary explosion producing high speeds of combustion and high overpressures in unconfined dust explosions. We show that the clustering of dust particles in a turbulent flow ahead of the advancing flame front gives rise to a significant increase of the thermal radiation absorption length. This effect ensures that clusters of dust particles are exposed to and heated by radiation from hot combustion products of the primary ignited flame for a sufficiently long time to become multi-point ignition kernels in a large volume ahead of the advancing flame. The ignition times of a fuel–air mixture caused by radiatively heated clusters of particles is considerably reduced compared with the ignition time caused by an isolated particle. Radiation-induced multipoint ignitions of a large volume of fuel–air ahead of the primary flame efficiently increase the total flame area, giving rise to the secondary explosion, which results in the high rates of combustion and overpressures required to account for the observed level of overpressures and damage in unconfined dust explosions, such as for example the 2005 Buncefield explosion and several vapour cloud explosions of severity similar to that of the Buncefield incident.

KEYWORDS: Explosions, turbulence, detonation, radiation.

INTRODUCTION

Dust explosions occur when an accidentally ignited flame propagates through a cloud of fine particles suspended in gaseous fuel-air mixtures [1-3]. Dust explosions have been significant hazards for centuries in the mining industry and in grain elevators. Currently the danger of dust explosions is a permanent threat in all those industries in which powders of fine particles are involved. Despite intense investigations over more than 100 years the mechanism of dust explosions still remains one of the main unresolved problem. It is known that unconfined dust explosions consist of a relatively weak primary explosion followed by much more severe secondary explosions. While the hazardous effect of the primary explosion is relatively small, the secondary explosions may propagate with a speed of up to 1000 m/s producing overpressures of over 10 atm, which is comparable to the pressures produced by a detonation.

Currently there is no consensus on the mechanism of dust or vapor cloud explosions. Some researchers believe that that DDT occurs in large explosions like the 2005 Buncefield fuel storage explosion see e.g. [4, 5, 6, 7] and references within. In particular, it was widely believed that the formation of a spontaneous wave on a temperature gradient is a mechanism for switching to

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detonation mode [7]. However, recent experiments, progress in the development and understanding the detailed chemical models, and numerical simulations with detailed chemical models showed that the DDT mechanism is different from the gradient mechanism [8, 9, 10, 11].

The possibility that DDT occurs in large explosions in industrial accidents has generally only been recognised for highly reactive fuels such as hydrogen and ethylene, and models have been validated against a range of experimental data obtained from laboratory-scale experiments. Applying such data to industrial accidents is to take the models beyond their validation range, where they cannot be used as predictive tools. In the particular case of the 2005 Buncefield fuel storage explosion investigators and forensics teams were able to collect a large amount of data and evidences, providing a unique valuable information about the timings and damage data in the event [4, 5]. A detailed analysis of physical damage and data available from CCTV cameras led other researchers [12, 13] to conclusions that scenarios based on detonation and the type of the observed damage are not consistent with what would occur in a detonation, and that ‘the combustion in Buncefield was unsteady (episodic), with periods of rapid flame advance being punctuated by pauses.

In this paper we consider an alternative mechanism of dust (vapour cloud) explosions due to clustering of dust particles in a turbulent flow ahead of the advancing flame. We present an idealized theoretical model, assuming a dust cloud consisting of inert particle. We also do not consider either the pyrolysis of the dust particles, or mechanism of the advancing flame propagation. It is generally believed that in a in large explosions like the Buncefield explosion, the advancing flame causes turbulent flow ahead of the flame front. We show that in this case there is possibility of multipoint radiation induced ignition of a large volume of flammable gas ahead of the advancing flame due to turbulent clustering of particles ahead of the flame. The turbulent clustering of particles results in a significant increase of the thermal radiation absorption length. Therefore, clusters of dust particles are exposed to and heated by radiation from hot combustion products of the primary ignited flame for a sufficiently long time to become multi-point ignition kernels in a large volume ahead of the advancing flame. Radiation-induced multipoint ignitions of a large volume of fuel–air ahead of the primary flame may explain the origin of the secondary explosion with periods of rapid flame advance producing high local overpressures being punctuated by pauses.

In normal practice emissivity of combustion products and radiation absorption in a fresh unburnt gaseous mixture are small and do not influence the flame propagation. The situation is different for flames propagating through a cloud of fine particles suspended in a gaseous mixture. Thermal radiation emitted from the flame, propagating in a particle-laden fuel/air mixture, is absorbed and re-emitted by the particles ahead of the flame with heat being transferred from the particles to the surrounding gas by thermal conduction. It was shown [14, 15] that the radiative preheating may result in a strong increase in both the temperature of particles and of the gas of fuel/air ahead of the advancing flame and the advancing flame velocity. For evenly dispersed particles, the maximum increase in the temperature of the gas mixture immediately ahead of the flame front can be estimated as [14] $\Delta T \approx \left(\left(1-e^{-1}\right)\sigma T_b^4\right) \big/ \left(U_f\left(\rho_p c_p + \rho_g c_{v,g}\right)\right)$ where U_f is the normal laminar flame velocity, σT_b^4 is the blackbody radiative flux, ρ_g is the mass density of the gaseous mixture, and c_p and c_v are the specific heats of particles and the gas phase, respectively.

The intensity of the radiant flux decreases exponentially on the scale of the order of the radiation absorption length, $L_a = 1 \big/ \langle \kappa \rangle \approx d_p\, 2\rho_p \big/ \left(3\rho_d\right)$, in the case of evenly dispersed particles, where $\langle \kappa \rangle = \sigma_p \langle N \rangle$ is the mean particle absorption coefficient, $\sigma_p \approx \pi d_p^2 / 4$ is the absorption cross section of the particle, d_p is the particle size (diameter), $N_p \equiv \langle N \rangle$ is the mean particle number density, ρ_p is the material density of the dust particles, and ρ_d is the spatial particle mass density, and $\langle N\rangle$ is the mean number density of dispersed particles. Thus, if particles are evenly dispersed the dust cloud ahead of the advancing flame is opaque to thermal radiation within a few centimeters. Therefore, in case of the evenly dispersed particles, the radiation-induced ignition of the fuel-air by the radiatively heated particles is not possible [15]. The situation is completely different when particles are non-uniformly dispersed, for example, in the form of the optically thick dust layer, which is separated from the flame front by the transparent gap of gaseous fuel with very small concentration of particles. In this case the particles in the layer can be exposed to and heated by the radiation from the flame for sufficiently long time to become ignition kernels.

An explosion, producing a high overpressure and shock waves ahead of the advancing flame can occur as a result of ignition of a large volume of fuel-air mixture by the ignition kernels of particles heated by radiation from hot combustion products. It was shown [16, 17] that the turbulent clustering of particles increases strongly, up to 1000 times the penetration length of thermal radiation within a dust cloud. This is possible if the penetration length of radiation, L_{eff} , becomes so large, that the particles are sufficiently heated by the radiation in a large volume even far ahead of the advancing flame, so that sound waves have no time to equalize pressure, $\tau_{ign} << L_{eff} / a_s$, where a_s is the speed of sound in the flow ahead of the flame.

TURBULENT CLUSTERING OF PARTICLES; RADIATION HEAT TRANSFER

The mean radiation intensity

In a turbulent flow small particles with material density much larger than the gas density assemble in small clusters with sizes about several Kolmogorov viscous scales. The turbulent eddies, acting as small centrifuges, push the particles to the regions between the eddies, where the pressure fluctuations are maximum and the vorticity intensity is minimum. Therefore, suspended small particles in a turbulent flow tend to assemble in clusters with much higher number densities of particles than the mean particle number density. This effect has been investigated in a number of analytical, numerical, and experimental studies [18-23].

The equation for the intensity of radiation in the two-phase flow reads (see, e.g., [24, 25]):

$$(\hat{\mathbf{s}}\cdot\nabla)\,I(\hat{\mathbf{s}},\mathbf{r}) = -\big(\kappa_g(\mathbf{r})+\kappa_p(\mathbf{r})+\kappa_s(\mathbf{r})\big)I(\hat{\mathbf{s}},\mathbf{r})+\kappa_g\,I_{b,g}+\kappa_p\,I_{b,p}+\frac{\kappa_s}{4\pi}\int_\Omega \Phi(\mathbf{r},\hat{\mathbf{s}};\hat{\mathbf{s}}')I(\hat{\mathbf{s}}',\mathbf{r})d\Omega', \qquad (1)$$

where $\kappa_g(\mathbf{r})$ and $\kappa_p(\mathbf{r})$ are the absorption coefficients for the gas and particles, $\kappa_s(\mathbf{r})$ is the particle scattering coefficient, $\Phi(\mathbf{r},\hat{\mathbf{s}};\hat{\mathbf{s}}')$ is the scattering phase function, $I_{b,g}(\mathbf{r})$ and $I_{b,p}(\mathbf{r})$ are the black body radiation intensities for gas and particles, $\hat{\mathbf{s}}=\mathbf{k}/k$ is the unit vector in the direction of radiation. Taking into account that the scattering and absorption cross sections for gases at normal conditions are very small, the contribution from the gas phase is negligible in comparison with that of particles, Eq. (1) is reduced to

$$(\hat{\mathbf{s}}\cdot\nabla)I(\hat{\mathbf{s}},\mathbf{r}) = \kappa(\mathbf{r})\big(I_b(\mathbf{r})-I(\hat{\mathbf{s}},\mathbf{r})\big), \qquad (2)$$

where $\kappa \equiv \kappa_p(\mathbf{r})$ and $I_b \equiv I_{p,b}$ depend on the local temperature.

In the mean-field approach all quantities are decomposed into the mean and fluctuating parts: $I=\langle I\rangle+I'$, $I_b=\langle I_b\rangle+I_b'$, $\kappa=\langle\kappa\rangle+\kappa'$. The particle absorption coefficient is $\kappa=\sigma_a n$, and the fluctuations of the absorption coefficient are $\kappa'=n'\sigma_a=n'\langle\kappa\rangle/\langle N\rangle$. Averaging Eq. (2) over the ensemble of the particle number density fluctuations, we obtain the equation for the mean irradiation intensity $\langle I(\hat{\mathbf{s}},\mathbf{r})\rangle$:

$$(\hat{\mathbf{s}}\cdot\nabla)\langle I(\hat{\mathbf{s}},\mathbf{r})\rangle = -\langle\kappa\rangle\left(\langle I\rangle - \langle I_b\rangle\right) - \left\langle\kappa' I'\right\rangle + \left\langle\kappa' I_b'\right\rangle . \tag{3}$$

Subtracting Eq. (3) from Eq. (2), we obtain the equation for fluctuations I' :

$$(\hat{\mathbf{s}}\cdot\nabla + \langle\kappa\rangle + \kappa')\, I'(\mathbf{r},\hat{\mathbf{s}}) = I_{source} , \tag{4}$$

where

$$I_{source} = -\kappa'\left(\langle I\rangle - \langle I_b\rangle\right) + \left\langle\kappa' I'\right\rangle + (\langle\kappa\rangle + \kappa')\, I_b' - \left\langle\kappa' I_b'\right\rangle . \tag{5}$$

The solution of Eq. (5) is

$$I'(\mathbf{r},\mathbf{s}) = \int_{-\infty}^{+\infty} I_{source} \exp\left(-\left|\int_{s'}^{s}[\langle\kappa\rangle + \kappa'(s'')]ds''\right|\right)ds' . \tag{6}$$

Expanding the exponent in Eq.(6), multiplying the obtained equation by κ' and averaging over the ensemble of fluctuations, we obtain for the one-point correlation function $\left\langle\kappa' I'\right\rangle$

$$\begin{aligned} \left\langle\kappa' I'\right\rangle &= 1 + \int_{-\infty}^{+\infty}\left(\int_{s'}^{s}\kappa'(s)\kappa'(s'')ds''\right)\exp(-\langle\kappa\rangle\left|s-s'\right|)ds' = \\ &= -\left(\langle I\rangle - \langle I_b\rangle\right)\int_{-\infty}^{+\infty}\langle\kappa'(s)\kappa'(s')\rangle\exp(-\langle\kappa\rangle\left|s-s'\right|)ds' \end{aligned} . \tag{7}$$

Substituting the correlation function $\left\langle\kappa' I'\right\rangle$ into Eq. (3), we obtain an equation for the mean radiation intensity

$$(\hat{\mathbf{s}}\cdot\nabla)\langle I(\hat{\mathbf{s}},\mathbf{r})\rangle = -\kappa_{eff}\left(\langle I\rangle - \langle I_b\rangle\right), \tag{8}$$

where κ_{eff} is the effective absorption coefficient, which takes into account the particle clustering in a temperature stratified turbulence

$$\kappa_{eff} = \langle\kappa\rangle\left(1 - \frac{2\beta J_1}{1 + 2\beta J_2}\right). \tag{9}$$

The integrals J_1 and J_2 in Eq. (9) are given by integrals of the two-point correlation function of the particle number density fluctuations $\Phi(t,\mathbf{R}) = \left\langle n'(t,\mathbf{x})n'(t,\mathbf{x}+\mathbf{R})\right\rangle$. Calculation details can be found in [21, 22].

Effect of particle clustering on the effective penetration length of radiation

The two-point correlation function that accounts for particle clustering in temperature stratified turbulence was derived in [21]:

$$\Phi(R) = (n_{cl}/\langle N\rangle)^2 \text{, for } 0 \le R \le \ell_D \text{ ; } \Phi(R) = \left(\frac{n_{cl}}{\langle N\rangle}\right)^2\left(\frac{R}{\ell_D}\right)^{-\mu}\cos\left(\alpha\ln\frac{R}{\ell_D}\right) \text{ for } \ell_D \le R < \infty , \tag{10}$$

where $R = \mathbf{R}\cdot\hat{\mathbf{s}}$, $\ell_D = a\ell_\eta / Sc^{1/2}$ is the size of a cluster, $\ell_\eta = \ell_0 / \mathrm{Re}^{3/4}$ is the Kolmogorov turbulent scale, $Sc = \nu / D$ is the Schmidt number, $\alpha = 3\pi(1+\sigma_{\mathrm{T}})/(1+3\sigma_{\mathrm{T}})\ln\mathrm{Sc}$, $\sigma_{\mathrm{T}} = (\sigma_{\mathrm{T}0}^2 + \sigma_{\mathrm{v}}^2)^{1/2}$ is the degree of compressibility of the turbulent diffusion tensor, σ_v is the degree of compressibility of the particle velocity field and μ is expressed as a combination of the degree of compressibility of the turbulent diffusion tensor and the degree of compressibility of the particle velocity field $\mu = \left(3 - \sigma_T + 20\sigma_v(1+\sigma_T)/(1+\sigma_v)\right)/\left(2(1+3\sigma_T)\right)$. The value of the numerical factor $a \approx 5-10$ corresponds to the values obtained in the laboratory experiments and the atmospheric measurements. It was shown [21] that the maximum number density of particles attained inside the cluster is

$$\frac{n_{cl}}{\langle N\rangle} = \left(1 + \frac{e\mu}{\pi} Sc^{\mu/2} \ln Sc\right)^{1/2}. \tag{11}$$

Calculating integrals J_1 and J_2 in Eq. (9) using Eqs. (10, 11) we obtain the effective penetration length of radiation $L_{eff} \equiv 1/\kappa_{eff}$ in the form

$$L_{eff}/L_a = 1 + \frac{2a}{Sc^{1/2}}\left(\frac{n_{cl}}{\langle N\rangle}\right)^2 \left(\frac{\ell_\eta}{L_a}\right)\left(1 + \frac{\mu - 1}{(\mu-1)^2 + \alpha^2}\right). \tag{12}$$

where L_a is the radiation absorption length for the case of evenly dispersed particles.

Two physical effects affect the radiation transfer: (i) transparent for radiation windows are formed between particle clusters (ii) particles inside optically thick clusters are screened from the radiation and therefore do not participate in the radiation absorption. The present theory takes into account the collective effects of turbulent clusters on radiation transfer, but do not consider the screening effect of optically thick clusters. Therefore, the obtained results give a lower limit for the increase in the penetration length of radiation, whereas the overall effect can be much stronger.

RADIATION-INDUCED EXPLOSIONS

In the early stage of dust explosions, the combustion mode is an accidentally ignited deflagration. The pressure waves produced by the accelerating flame run ahead giving rise to turbulence in the flow ahead of the advancing flame. With the increase in the primary flame surface and flame velocity, the parameters of the turbulent flow ahead of the advancing flame, i.e. u_0, ℓ_0, Re, St, $\nabla\langle T\rangle$ change continuously. The dust particles in the turbulent flow ahead of the flame front assemble in clusters during a time of the order of milliseconds. Figure 1 shows the ratio L_{eff}/L_a versus particle size calculated for the case of isothermal turbulence for the turbulent methane-air flow at normal conditions; ν = 0.2 cm^2/s, a_s = 450 cm/s, $n_{cl}/\langle N\rangle$ = 500, σ_{T0} = 1/2.

It was shown in [21] that for temperature stratified turbulence the ratio $n_{cl}/\langle N\rangle$ can increase up to three orders of magnitude. Therefore, clustering of particles in the temperature stratified turbulent flow ahead of the primary flame may increase the radiation penetration length by up to 2–3 orders of magnitude, as it is shown in Figure 2. This effect ensures that clusters of particles are exposed to and heated by the radiation from the primary flame for a sufficiently long time to become ignition kernels in a large volume ahead of the flame. The multi-point radiation-induced ignition of the surrounding fuel–air increases effectively the total flame area, so the distance, which each flame has to cover for a complete burn-out of the fuel, is substantially reduced. It results in a strong increase of the effective combustion speed, defined as the rate of reactant consumption of a given volume, and overpressures, required to account for the observed level of damages in unconfined dust explosions. If, for example, the radiation absorption length of evenly dispersed particles with spatial mass density 0.03 kg/m^3 was in the range of a few centimeters, dust particles assembled in the clusters of particles, are sufficiently heated by radiation at distances up to 10–20 m ahead of the advancing flame. The ignition time of the fuel–air by the radiatively heated particles measured in experiments [26] is 100 ms for 10 μm inert particles. The level of thermal radiation of hot combustion products in dust explosions, $S \sim 400 kW / m^2$ is sufficient to raise the temperature of particles by $\Delta T_p \approx 1000\,K$ during $\tau_T \approx d_p \rho_p c_p \Delta T_p / S < 10\,ms$.

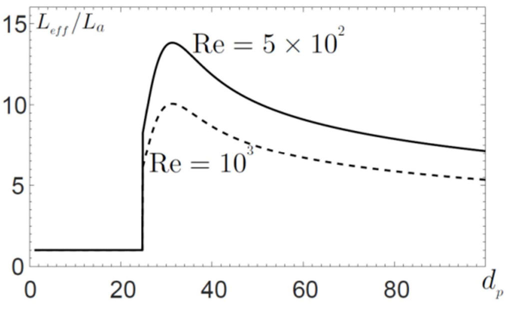

Fig. 1. The ratio L_{eff} / L_a versus particle size for the particle clustering in isothermal turbulence with different Reynolds numbers: 5 × 10^2 (solid line) and 10^3 (dashed line).

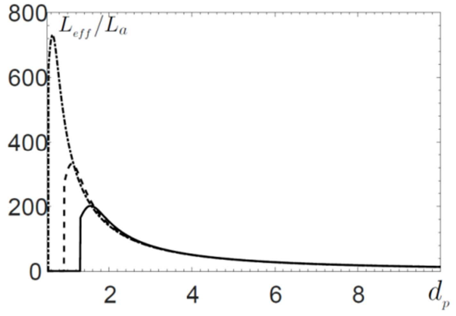

Fig. 2. The ratio L_{eff} / L_a versus particle size for different mean temperature gradients: $|\nabla T|$ = 0.5 K/m (solid), 1 K/m (dashed), 3 K/m (dashed-dotted).The particle diameter is in microns.

Figure 3 shows the dependence of L_{eff} / L_a on Reynolds numbers calculated for particles of different diameter. It is seen that a significant increase of the radiation penetration length caused by particle clustering occurs within a rather narrow interval of turbulent parameters. The effect is much weaker if the flow parameters ahead of the flame front are changed and appear outside the 'range of transparency'. Such a dependence of L_{eff} / L_a versus Reynolds numbers suggests possible explanation for the episodic nature of the explosion in the Buncefield incident described by Atkinson and Cusco [12].

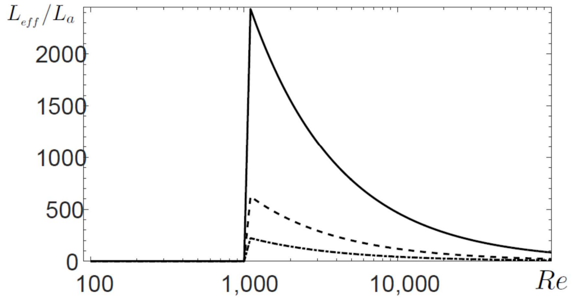

Fig. 3. The dependence of L_{eff} / L_a on the Reynolds number for different particle diameters: 1μm (solid), 5 μm (dashed), 10 μm (dashed-dotted); the temperature gradient is 3K/m.

According to the analysis of the Buncefield explosion [12]: 'The high overpressures in the cloud and low average rate of flame advance can be reconciled if the rate of flame advance was episodic, with periods of very rapid combustion being punctuated by pauses when the flame advanced very slowly. The wide spread high overpressures were caused by the rapid phases of combustion; the low average speed of advance was caused by the pauses.' From the beginning, the parameters of the turbulent flow, ahead of the advancing flame, vary continuously and finally fall within the 'range of transparency' when the radiation penetration length increases considerably. Since the primary flame is a deflagration, propagating with a velocity in the order of a few meters per second, the duration of this stage is the longest timescale in the problem. During this time the particle clusters ahead of the flame are exposed to and heated by the forward radiation for a sufficiently long time to become ignition kernels in a large volume ahead of the flame initiating the secondary explosion. Since the parameters of the turbulent flow are changed after the secondary explosion, the rapid phase of combustion is interrupted until the shock waves produced by the secondary explosion dissipate. The next phase continues until the parameters of turbulence in the flow ahead of the combustion wave fall again within the interval corresponding to the 'transparent window', such that the increased ratio L_{eff} / L_a caused by particle clustering provides conditions for the next secondary explosion.

CONCLUSIONS

It is shown that the mechanism of the secondary explosion in unconfined dust explosions and large vapour cloud explosions can be explained by the turbulent clustering of dust particles. The latter include the effect of a considerable increase in the radiation penetration length, the formation of ignition kernels in the turbulent flow caused by the primary flame, and the subsequent formation of secondary explosions, which are caused by the impact of forward thermal radiation. The mechanism of multi-point radiation induced ignitions due to the turbulent clustering of particles ensures that ignition of the gas mixture by the radiatively-heated clusters occurs rapidly and within a large volume ahead of the primary flame. The secondary explosion acts as an accelerating piston producing a strong pressure wave, which steepens into a shockwave. The intensity of the associated shock wave depends on the rate of progress of the secondary explosion and can be determined by using numerical simulations. The described scenario of unsteady combustion consisting of rapid combustion producing high overpressures, punctuated by subsequent slow combustion, is consistent with the analysis [5] of the Buncefield explosion. Although details of the real physical processes could be different, the proposed theoretical model describes the episodic nature of combustion in dust explosions observed in [12], and more importantly it captures the most important relevant physics. More detailed analysis, i.e. taking into account the particle size distribution, inter-particle collisions, possible coalescence of particles inside the clusters, and the effect of gravitational sedimentation of large particles, can only be done using numerical simulations. The obtained analytical solution can serve as a benchmark for numerical simulations of dust explosions, which do not need to rely on the simplifying assumptions.

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