Simple Analytical Model for Metal Particle Ignition in Condensed Explosive

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Introduction

It has now become common practice to add reactive metal particles (typically, magnesium, aluminum, etc.) to explosives to enhance blast performance. Metal combustion can be very energetic (as much as 3 or 4 times the energy release of typical explosives). Although the total energy released by the metal combustion is significant and comparable to the total energy released by the explosive itself, the timescale of this energy release (timescale for particle reaction) for typical particle sizes (1 to 100 μm), is most probably too long to contribute directly to the detonation front itself. Instead, the metal particles may react with air or even with the detonation products behind the blast wave. It has been shown that the metal particle reaction can significantly increase the strength of the blast and the total impulse delivered to nearby objects or structures (Frost et al. 2002, 2003).

Frost et al. (2002) have conducted many experiments with packed beds of metal particles in charges of nitromethane. It was shown that sufficiently rapid particle ignition was critical to the blast enhancement. In the case of magnesium, for a given particle size, there is a critical charge size below which the metal particles do not ignite or ignite on a timescale too long to reinforce the blast. It was also found that larger particles require larger charges for particles to ignite. Since the detonation products of smaller charges expand and cool faster, the above results suggest that particles should be heated for a sufficiently long time for ignition to occur promptly enough to enhance the blast. Obviously, it would be of interest to identify the scaling laws responsible for this behavior and understand the parameters that determine if particle reaction will occur.

To date, multi-phase computational fluid dynamics models have been used (Frost et al. 2002) to predict the conditions for metal particle reaction in explosives. While such models can, in principle, model a great amount of detail in the phenomena of interest, they are not as useful for engineering calculations or for identifying the dominant scaling laws. In this paper, an alternative approach is taken to develop a highly simplified model that incorporates the minimum details necessary to capture the governing physical processes that determine if particles will react in a given explosive dispersal event. This model is also useful to assess the relative contributions toward particle ignition made by the detonation front itself, the subsequent product expansion, and the shock heated air the particles will encounter if they leave the detonation products.

The Model

The approach taken here is to model a single particle. In other words, the effect of the particle on the expansion of the detonation products is neglected. This should be valid for small particle

loadings. The detonation wave is assumed to be a discontinuous CJ detonation propagating in a homogeneous explosive, followed by an ideal Taylor wave. The subsequent expansion of the products is modeled using a highly simplified planar geometry with the products treated as a perfect gas with constant γ. With this analytical model of the flow field, the particles are introduced and their trajectories and convective heating histories are solved. A simple reaction criterion (critical temperature) is used to determine if particles ignite.

The model developed here has a number of shortcomings due to the simplifying nature of the assumptions made. Further, considerable uncertainty exists in a number of parameters invoked in the development of the model (e.g., transport properties of high temperature/pressure detonation products). Yet, the very simplicity of the model (straightforward integration of ordinary differential equations) permits the sensitivity of these assumptions and models to be quickly and easily assessed.

Model of Detonation Products

Consider a planar slab of explosive of length $2L$. A planar discontinuous CJ detonation is assumed to form instantaneously in the center (at the plane of symmetry) at $t = 0$ and propagate outward. Once the detonation reaches the end of the charge, the products are assumed to expand to vacuum. The CJ state is calculated for nitromethane using the equilibrium code Cheetah 2.0 (Fried et al. 1998). As mentioned above, the detonation products are treated as a perfect gas with constant γ. Cheetah 2.0 predicts a γ of 2.69 (from a $pv^{\gamma} = constant$ fit at the CJ point). However, in the special case of $\gamma = 3$ for planar homentropic ($s = constant$) flow, the governing equations for the flow are dramatically simplified: the right running and left running characteristics become independent (straight lines) (Stanyukovich 1960). As a consequence, the solution of the entire flow field of detonation products expanding to vacuum can be expressed algebraically. Therefore, for simplicity, γ is taken to be 3 in the present model. Figure 1 shows the six different regions of the flow field on an x-t diagram. Region 0 is the unreacted high explosive. Region 1 is vacuum. Region 2 is the Taylor wave behind the detonation. Region 3 is the quiescent region behind the Taylor wave. Region 4 is affected by both the extension of the Taylor wave and the left-running expansion generated when the detonation reaches the edge of the explosive. Region 5 is also the left-running expansion. Finally, region 6 is the interaction of the left-running expansion and its reflection from the plane of symmetry. This flow field extends to infinity in both space and time.

Model of Particle Kinematics

Neglecting body forces, the only force acting on a particle in the detonation products flow is a drag force. Therefore, the governing equation becomes:

$$\frac{d^2x}{dt^2} = \frac{3}{4}\frac{C_D\rho(x,t)}{d_p\rho_p}\left|u(x,t) - \frac{dx}{dt}\right|\left[u(x,t) - \frac{dx}{dt}\right].$$

Of course, an expression for the drag coefficient, C_D, is required. In this model, the correlation of (Igra & Takayama, 1993) is used. This correlation valid for Reynolds numbers ranging from 200 to 101,000 was obtained for unsteady particles in shock tubes and is given below:

$$\log C_D = a + b(\log Re) + c(\log Re)^2 + d(\log Re)^3 .$$

It is found that the results are relatively insensitive to the drag coefficient. Integrating the governing equation subject to the flow field solution obtained before, with given initial conditions (position and velocity) yields the trajectory of the particle. Figure 1 shows the trajectories of 9 particles with zero initial velocities and different initial positions.

Zhang et al. (2001) have found that a significant amount of momentum was transferred to the particle during the interaction of the particle with the detonation front. This implies that the particles in this model should be given a non-zero initial velocity after crossing the detonation. However, it was found that an initial velocity as high as 1000 m/s had a negligible effect on the results. This is because the particles are relatively small and come to near mechanical equilibrium with the dense flow of detonation products quite rapidly. Therefore, the initial velocity of the particles was kept at zero in the present study.

Model of Particle Heating and Ignition

In this study, the particle ignition is considered as the onset of gaseous reaction. For simplicity, it is assumed that this happens at a critical particle temperature. For metals such as magnesium, this temperature is usually taken as the metal boiling point, whereas for aluminum, the oxide melting point is usually used (Roberts et al. 1993). Only magnesium particles are considered in this investigation. In general, until the critical temperature is reached, a particle is subject to convective and radiative heat transfer from (or to) the detonation products. Furthermore, heterogeneous surface reactions between the products and the particle also contribute to heating the particle.

In cases where the rate of convective heat transfer to the particle is much less than the rate of conductive heat transfer into the particle, a lumped capacitance analysis can be used (temperature gradients can be neglected inside the particle). The criterion usually used is that the Biot number, $Bi < 0.1$, where

$$Bi \equiv \frac{h d_p}{k} .$$

In this study, the Biot number for the particles considered tends to be higher than 0.1. In fact the Biot number can be as large as 1 in some cases. This means that temperature gradients are small but not negligible and should, in principle, be considered. However, for simplicity, a lumped capacitance analysis is used nevertheless. This means that in reality, it should be easier to ignite particles than is predicted since the entire particle mass does not need to be heated to the critical temperature. With the lumped capacitance analysis, the energy equation for the particle is:

$$\frac{dT_p}{dt} = \frac{6}{d_p \rho_p C_p}\left[h(T - T_p) + \varepsilon\sigma(T^4 - T_p^4) + \omega Q \right].$$

A correlation is needed for *h*, the average convective heat transfer coefficient. In this study, the correlation from Whitaker (1972) for spheres is used:

$$Nu = 2 + (0.4\,\mathrm{Re}^{1/2} + 0.06\,\mathrm{Re}^{2/3})\,\mathrm{Pr}^{0.4}\left(\frac{\mu_\infty}{\mu_w}\right)^{0.25}.$$

The heterogeneous surface reaction rate is taken from Roberts et al. (1993):

$$\omega = A\exp\left[\frac{-E_a}{RT}\right].$$

The melting of the particle is taken into account in the calculation. When the temperature of the particle reaches the melting point, the particle temperature is kept constant until an amount of heat equal to the latent heat of fusion is transferred to the particle.

Integrating the energy equation, subject to both the flow field and the particle trajectory obtained earlier, one obtains the temperature evolution of the particle. The solution shows the temperature first increase, reach a maximum and subsequently decrease. The location and time where the particle reaches its maximum temperature is indicated by a point on the particle trajectories in Fig. 1.

A simple comparison of the particle peak temperature and the ignition temperature determines if the particle successfully ignited. Since particles with different initial positions show different temperature histories, several particles are considered in the calculations. For a given charge size, some particles may ignite while others may not. In experiments however, one cannot make this distinction: a relatively sharp transition is observed between ignition and no ignition. Thus, to compare with experimental data, a simple criterion is used: in this case, if more than 50% of particles reach the ignition temperature, the particles are considered to have ignited. Once again, the results prove to be quite insensitive to this arbitrary fraction.

Figure 2 shows the critical charge size for magnesium particle ignition versus particle size as predicted by the analytical model as well as obtained experimentally by Frost (2002). The model captures the right trend of increasing critical charge size for increasing particle size. The model also comes within one order of magnitude of the experimental data. This is quite encouraging, considering the crudeness of the assumptions and the simplicity of the model. The model does overestimate the minimum charge size for successful ignition of the particles.

Spherical Geometry

It is interesting to note that the maximum temperature is reached just after the leading edge of the left-running expansion that is generated when the detonation reaches the surface of the explosive

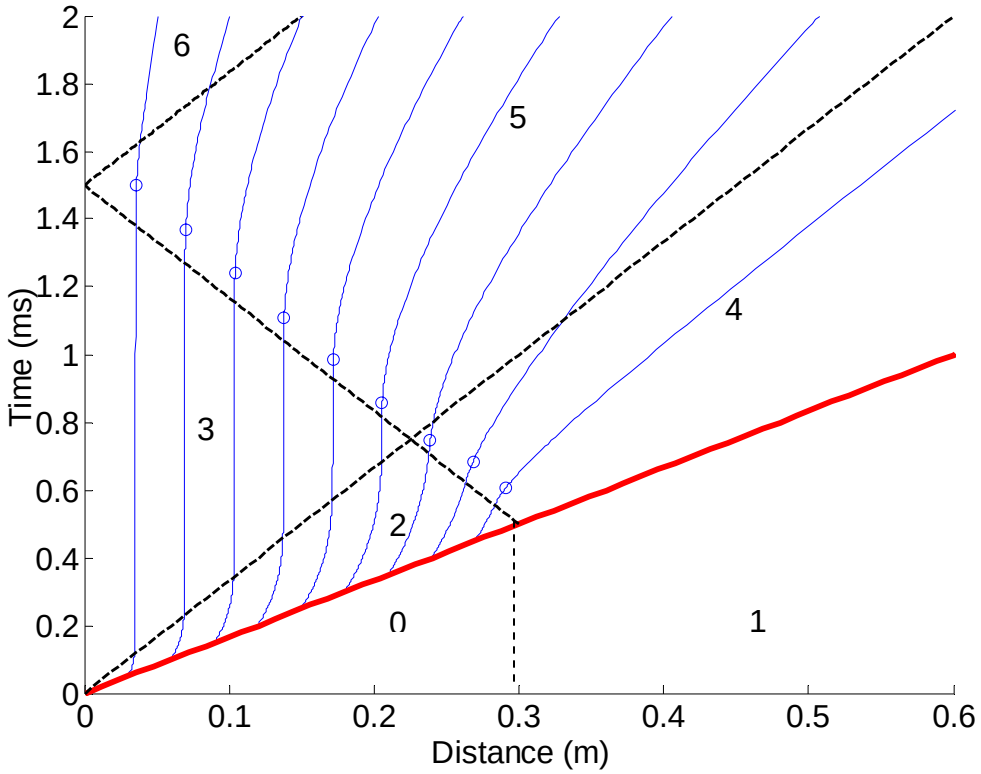

Figure 1. Trajectories of particles in flow field behind the detonation. A point indicates the where the particle reaches its maximum temperature.

(see Fig. 1). This is quite convenient because it implies that only regions 2 and 3 of the flow field are necessary to determine whether or not particles ignite in the products. Assuming that this is the case in other geometries as well, some of the previously mentioned restrictions can now be relaxed. For example, regions 2 and 3 (the Taylor wave and the quiescent region behind it) of the flow can be solved analytically in any geometry (planar, cylindrical or spherical) (Taylor 1949). Furthermore, the specific heat ratio no longer needs to be 3. A more realistic value of gamma can now be used. This should make a significant difference since the value of 3 results in a significant underestimation of the detonation products temperature along the isentrope (as compared to the values given by Cheetah 2.0). While keeping the perfect gas and constant specific heat ratio assumption for simplicity, a value of γ is chosen such that in the range of interest, temperature and pressure are in better agreement with the prediction by Cheetah 2.0. This value of the specific heat ratio is 1.9. The higher temperature of the products should lower the minimum charge size for particle ignition while the spherical geometry should raise it due to the steeper Taylor wave.

Figure 2 shows the predictions for both the planar case (with $\gamma = 3$) and the spherical case (with $\gamma = 1.9$). Clearly the effect of the specific heat ratio (higher temperature of the products) is more important than the effect of geometry since the spherical curve is lower than the planar one. It is also in better agreement with the experimental data where it now comes within a factor of 2-5.

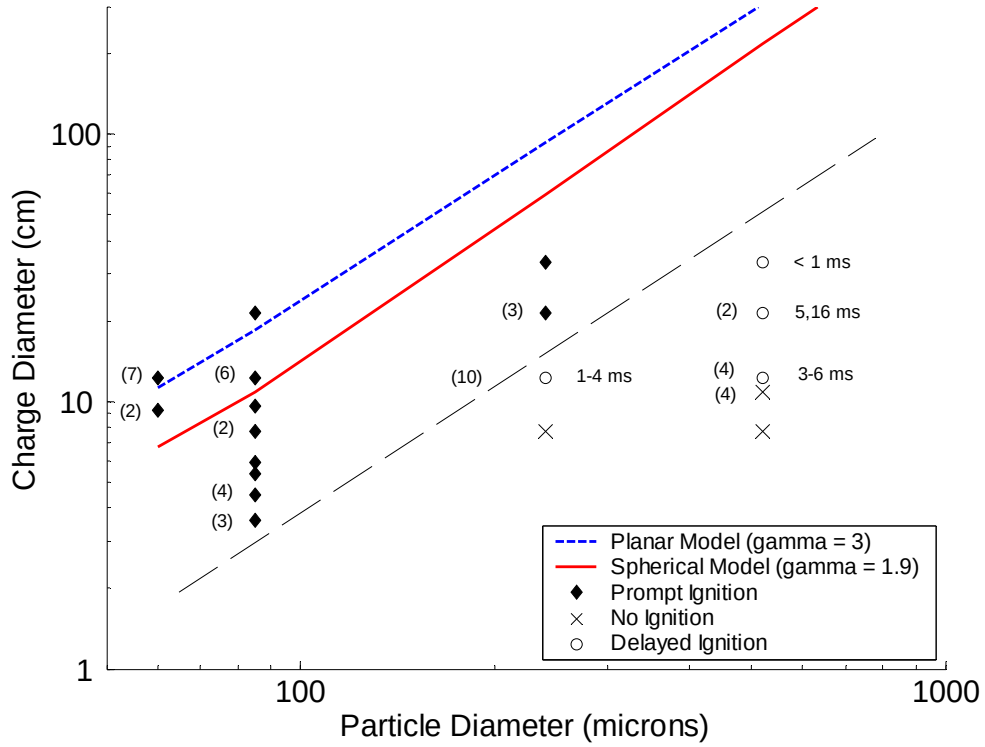

Figure 2. Critical charge size for particle ignition as a function of particle size. Both the results of the planar and spherical models are shown as well as experimental data from Forst et al. (2002). Numbers in parentheses indicates number of experiments performed.

Discussion

It should be noted that although they were included in the present analysis, the contributions of radiation and heterogeneous surface reaction are negligible. Most of the heating of the particle to its critical temperature for ignition is done by convective heat transfer from the products to the particle.

Even though the model does not predict exactly the minimum charge diameter for particle ignition, it is in relatively good agreement with the experimental data of Frost (2002). It overestimates the data by a factor of 2 to 5. Also it appropriately captures the dependence of the minimum charge size on the particle size. This suggests that the governing physical mechanisms responsible for the phenomenon are appropriately captured by the model.

It appears as though radiative heat transfer is negligible. Most of the particle heating is achieved by convection and occurs in the Taylor wave and in the quiescent region behind it. Since the particles start to cool near the leading edge of the left-running expansion wave, one may conclude that the assumption of expansion to vacuum is reasonable. In fact, by considering only regions 2 and 3, the results would be unchanged if the expansion was not to vacuum. In other words, if the explosive sphere is placed in an atmosphere with a finite initial pressure, a blast

wave will be transmitted into the atmosphere. However, regions 2 and 3 will not be affected by this. In fact, the leading edge of the left-running expansion will not be affected either. The only result is that the expansion fan will not expand all the way to the contact surface.

Also, in the present model, surface reactions have a negligible contribution to the particle heating. Of course this conclusion depends on the parameters used (mainly the activation energy). It may be that the activation energy is lower than the value that was used. There is no consensus in the literature on what theses values are. The effect of the high pressure and the composition of the detonation products are also not well understood. Also, it may be that the high intense stresses applied to the particle during the interaction with the detonation front have an effect. It could break a protective oxide layer and significantly lower the activation energy. A more significant contribution of chemical heat release would lower the minimum charge size for particle ignition which would improve the agreement of the model with the experimental data.

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