

A simple model for the pressure field from a distribution of hotspots

B D Lambourn, H J Lacy, C A Handley and H R James

AWE Aldermaston, READING, Berkshire RG7 4PR, United Kingdom

Email: brian.lambourn@awe.co.uk

Abstract. At the APS SCCM in 2009, Hill, Zimmermann and Nichols showed that assuming burn fronts propagate at constant speed from individual point hotspots distributed randomly in a volume, the reaction rate history could be determined. In this paper a simple analytic approximation is found for the time history of the pressure in the volume. Using acoustic theory, the time history of the pressure field for burning from a single spherical, isolated hotspot of finite radius is developed. Then at any point in the volume, the overall pressure history is determined from the sum of the pressure fields from all the individual hotspots. The results are shown to be in qualitative agreement with 1D mesoscale hydrocode calculations of the reaction and burning from a finite size spherical hotspot.

1. Introduction

As part of developing a better understanding of the relationship between mesoscale and continuum models of reactive burn in a heterogeneous explosive, this paper investigates how the pressure field from a distribution of hotspots varies with time. It is an extension of the work by Hill, Zimmermann and Nichols [1], who considered the bulk reaction history for burning from hotspots distributed randomly in a volume. They assumed that each of the burn fronts was initiated at time zero from individual hotspots of initial radius, a , and propagates at constant speed, b . By considering the probability that any point in a volume containing a distribution of burning hotspots has not yet reacted, Hill, Zimmermann and Nichols allowed for the gradual overlapping of burn fronts and showed that the time history of the bulk extent of reaction is

$$\alpha = 1 - \exp\left\{-\frac{4\pi\eta(bt+a)^3}{3}\right\} \quad (1)$$

where α is the volume fraction of reaction, η is the number of hotspots per unit volume and t is time. In their analysis, Hill et al assumed that the hotspots were point sources ($a=0$); equation (1) is a simple generalisation.

The development of the pressure field is a hydrodynamic problem, in which information about burning propagates away from each hotspot at the velocity of sound, ahead of the burn front. Typically the ratio of burn front speed to sound speed is ~ 0.001 , which has a significant effect on the resulting pressure field. Initially, the pressure field for a single isolated hotspot is developed and then the problem of a distribution of hotspots is considered. A simple analytic model and 1D mesoscale hydrocode calculations with heat conduction and Arrhenius kinetics are used to address the problem.



2. The analytic model for an isolated spherical hotspot

Analytically, it is not possible to simultaneously model the burning process and develop the hydrodynamics of the overall pressure field. Since the main aim of this paper is to develop the hydrodynamic field, a simplifying assumption is made that reaction is instantaneous. The burn front then becomes a constant velocity discontinuity that converts non-reacted material ahead into reaction products behind the burn front.

The problem is analysed by writing the parameters in the 1D spherical equations of motion as scaled deviations from the bulk explosive state, i.e. particle velocity (u'/c_1), density (ρ'/ρ_1) and pressure ($p'/\rho_1 c_1^2$), where ρ_1 is the bulk density and c_1 is the bulk sound speed. The assumption is made that the scaled parameters and their derivatives are all first order small, so that to first order, products of these terms can be neglected. The equations of motion then reduce to the wave equation, which can be solved using a velocity potential method [2].

At time zero, the material in the hotspot is assumed to instantaneously change into reaction products at pressure deviation $p' = \rho_1 c_1^2 \sigma$, where σ is the thermicity parameter. To simplify the analysis further, the sound speed in the products and non-reacted explosive are both assumed to equal c_1 , so that the $p' - \rho'$ relation for the two components can be summarised by

$$p' = c_1^2 \rho' + \rho_1 c_1^2 \sigma \alpha \quad (2)$$

where $\alpha = 0$ for the non-reacted explosive and $\alpha = 1$ for the reaction products.

Using the same approximations, the pressure difference across the burn front reduces to

$$p_g' - p_s' = -\frac{\beta^2}{1 - \beta^2} \rho_1 c_1^2 \sigma \quad (3)$$

where subscript s refers to non-reacted explosive, subscript g to the gaseous reaction products, and β is the ratio of the constant burn front speed, b , to the bulk explosive sound speed, c_1 . Equation (3) implies that pressure ahead of the burn front is greater than the pressure behind.

3. Mesoscale calculations

The mesoscale calculations used a one-dimensional Lagrangian hydrocode, to which heat conduction and a single step Arrhenius reaction rate have been added [3]. A linear Gruneisen equation of state (EOS) is assumed for the non-reacted explosive, a JWL EOS for the reaction products, and pressure and temperature equilibrium is assumed for partially reacted explosive. The hotspot calculations consist of a central higher temperature region, representing a generic hotspot, surrounded by cooler, bulk explosive. Reaction begins in the hotspot and propagates outwards as a burn wave.

4. Single isolated spherical hotspot

Figure 1 is a wave diagram for the evolution of the pressure field for a single isolated spherical hotspot in the analytic model. At time zero, the hotspot OA, of radius a , instantaneously reacts and a pressure deviation $\rho c^2 \sigma$ is generated. It is assumed that a burn front AB is created instantaneously and that it propagates at constant velocity b , behind which are reaction products and ahead is non-reacted explosive.

The pressure discontinuity at A is resolved by a shock AS propagated into the non-reacted explosive and a rarefaction AC propagated into the hotspot, which is reflected at the axis as a rarefaction CR. Because the sound speed has been assumed to be equal between the reactants and products, there are no further reverberations in the hotspot.

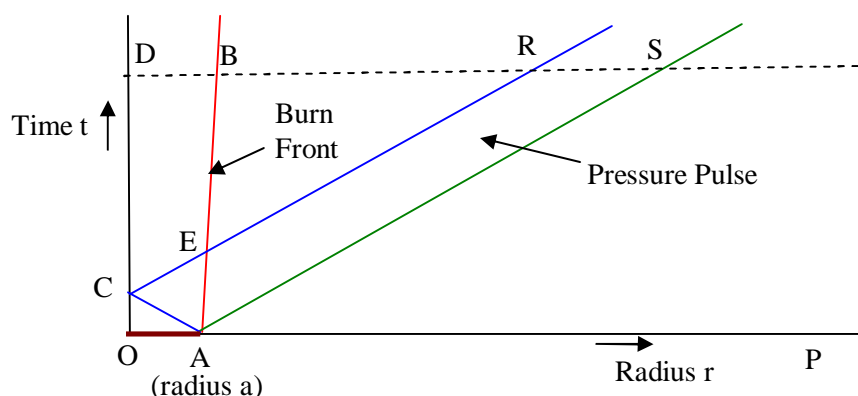


Figure 1. Wave diagram for a spherical isolated hotspot.

The analytic solution for the velocity potential is successively built up in the regions OAC, ACE, SAER, etc., until the pressure profile along a constant time line, for example DBRS, is defined. The pressure profile consists of three regions – a constant width, leading pressure pulse RS of width $2a$, a reacted burn region DB behind the burn front of growing radius $(bt+a)$ and the main pressure field BR, ever expanding at rate $(c_1 - b)$.

A schematic pressure profile along DBRS is shown in figure 2. The pressure deviation, Δp , inside the burn front, p'_{burn} , is constant in space and time, increases with burn front velocity, and is proportional to β^2 .

$$p'_{\text{burn}} = \left(\frac{\beta}{1+\beta} \right)^2 \rho_1 c_1^2 \sigma \quad (4)$$

Immediately ahead of the burn front the pressure is higher (equation (3)), but between the burn front and the shock pulse, pressure deviation, p'_{field} , in region BR decays like $1/r$, but again increases with burn front velocity and is overall proportional to β^2 .

$$p'_{\text{field}} = 2 \left(\frac{\beta}{1 - \beta^2} \right)^2 \left\{ \frac{a + bt}{r} - \beta \right\} \rho_1 c_1^2 \sigma \quad (5)$$

The pressure pulse, of constant width $2a$, has a leading shock and trailing rarefaction and also decays in amplitude as $1/r$

$$p'_{\text{pulse}} = \frac{1}{(1-\beta)^2} \left\{ \frac{(1-2\beta)(r-c_1 t) + \beta a}{r} \right\} \frac{\rho_1 c_1^2 \sigma}{2} \quad (6)$$

In any interval of time δt , the burn front increases its radius by $b\delta t$, but the overall profile expands by the much greater increase in radius $c_1\delta t$. The energy released during δt is rapidly spread at velocity c_1 and sustains the burn front and the pressure distribution both behind and ahead of the burn front.

Following Handley [3], the material simulated in the mesoscale calculations was HMX, shocked to ~ 20 GPa. However, to find the pressure field from an isolated hotspot, it was necessary to artificially speed up the burn front by increasing the thermal conductivity, in order to avoid interference from the pressure pulse being reflected from the outer boundary of the computational domain.

Figure 3 shows a pressure profile from a mesoscale calculation with an inset showing more detail (circled) inside the burn front. The hotspot was initially of $2.4\text{ }\mu\text{m}$ radius with a temperature of 2600 K . The results show that, despite the simplifying assumptions of the analytic model, including the assumptions of instantaneous reaction and a common sound speed, there is qualitative agreement with the mesoscale hydrocode calculations. This includes: a constant pressure inside the burn front, a narrow burn front with higher pressure immediately ahead, decaying to an inverted N-shaped pressure pulse, albeit spread out because of the time for the reaction to occur in the hotspot.

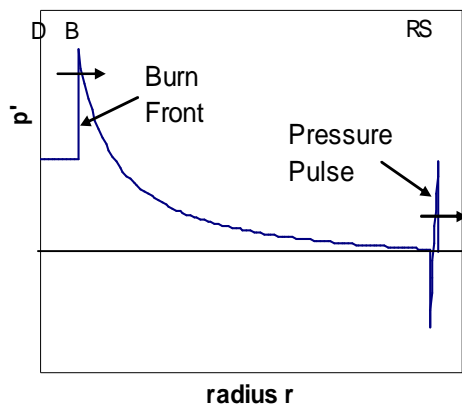


Figure 2. Analytic pressure profile.

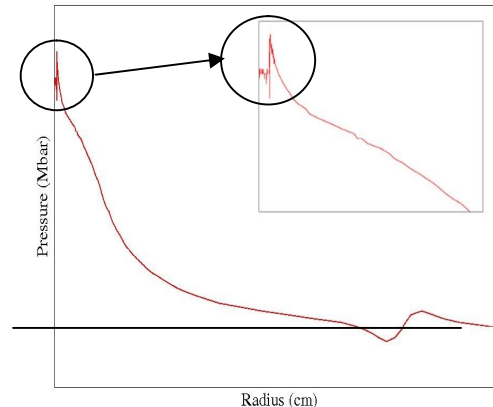


Figure 3. Mesoscale calculation.

5. Pressure field for a distribution of hotspots

The pressure fields in the analytic approximation are solutions of the wave equation. It follows that the pressure fields of individual hotspots can be added together to determine the pressure field for a distribution of hotspots in a volume. Like the derivation of the reaction rate by Hill et al [1], it is assumed that there are η hotspots per unit volume, all of initial radius a , and all activated at time zero.

At time t , at any point A in the volume, the hotspots whose burn fronts have expanded to reach or pass A will lie at zero time in a sphere of radius $(bt+a)$ surrounding A ; hotspots whose leading pressure pulse encloses A lie in a spherical shell between radii (c_1t-a) and (c_1t+a) , and finally hotspots that lie between radii $(bt+a)$ and (c_1t-a) will contribute from the general pressure field between the burn front and the pressure pulse. Because their pressure pulses have not yet reached A , hotspots lying outside radius (c_1t+a) at time zero do not contribute to the current value of pressure deviation at A .

Allowance needs to be made that some of the burn fronts have overlapped at time t . Analysis in planar geometry shows that at the intersection of two burn fronts, burning ceases and rarefactions are propagated outwards at speed c_1 . In spherical geometry this suggests that the contribution of hotspots is reduced by the degree of overlap of the hotspots. Hence to allow for overlaps, the assumption is made that the pressure contribution from those hotspots is reduced to the same extent as in the analysis by Hill et al [1]. In any volume V containing ηV hotspots, the spherical burn surfaces at time t have notionally expanded to volume $4\pi\eta(bt+a)^3V/3$. Allowing for burn front overlap, the total volume of reaction products is αV . Thus the factor to multiply the sum of the pressure integrals is the ratio $\alpha/\{4\pi\eta(bt+a)^3/3\}$. Hence at any time t the total pressure deviation from multiple hotspots is

$$p'(t) = \frac{\alpha(t)}{4\pi\eta(bt+a)^3/3} 4\pi\eta \left[\int_0^{bt+a} r^2 p'_{\text{burn}} dr + \int_{bt+a}^{c_1t-a} r^2 p'_{\text{field}} dr + \int_{c_1t-a}^{c_1t+a} r^2 p'_{\text{pulse}} dr \right] \rho_1 c_1^2 \sigma \quad (7)$$

Figure 4 shows an example of the contributions to the total pressure for a calculation with $1 \mu\text{m}$ radius hotspots, at average separations of $\sim 16 \mu\text{m}$, assuming $\beta = 0.001$. The contribution from the reaction products in the neighbourhood of A , p'_{burn} , is negligible. After $\sim 0.7 \mu\text{s}$, the contributions from the regions between the burn front and the pressure pulse, p'_{field} , dominates the total pressure. The contribution from the pressure pulses, p'_{pulse} , reaches a maximum at $\sim 2.8 \mu\text{s}$, after which the attenuation factor $1/r$ begins to dominate the increasing number of hotspots that contribute to p'_{pulse} .

When the pressure components from equations (4) to (6) are substituted into equation (7) and the integration is carried out, terms cancel and equation (7) greatly simplifies to give the mean bulk pressure deviation history as

$$p'(t) = \rho_1 c_1^2 \sigma \cdot \alpha(t) \quad (8)$$

This equation has the same form as that given by CIM [4], a continuum level reactive burn model that also uses a linearised partially reacted equation of state. CIM is an exact analytic solution to the nonlinear reactive burn equations of motion, which was used to simulate the initial stages of the sustained shock to detonation transition. In the case considered in this paper and the paper by Hill et al, in which reaction starts at time zero, CIM gives the same growth of pressure deviation as equation (8), with $\alpha(t)$ replaced by $\lambda(t)$, where λ is the extent of reaction per unit mass. However in this case, where there is no bulk motion and the bulk density is constant, α and λ are identical.

The only way of simulating the pressure field from multiple hotspots in the 1D mesoscale calculations is to make the outer boundary rigid, corresponding to assuming a series of spherical shell hotspots surrounding a central hotspot. Figure 5 shows the growth of pressure with time for a calculation in which a 1.2 μm -radius spherical hotspot initially at 1600 K, is surrounded by a 9 μm -thick shell of ambient temperature HMX. The configuration was identical to the cylindrical simulations described in the Flame Propagation section of [3], and corresponds to the analytic simulation in figure 4. The rise of pressure deviation using the analytical model is again qualitatively similar to the mesoscale hydrocode-calculation.

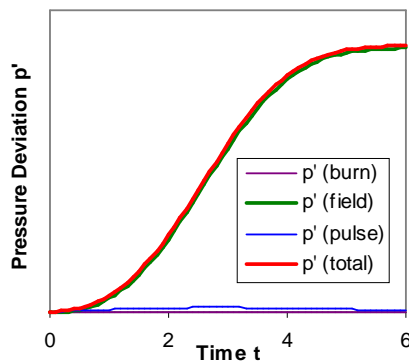


Figure 4. Total pressure history.

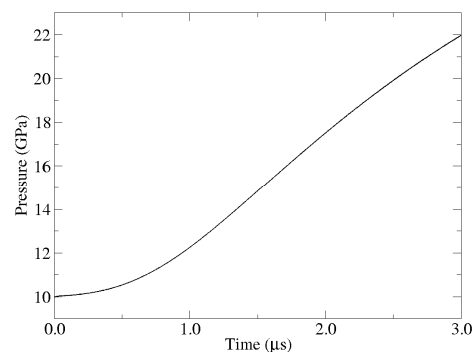


Figure 5. Mesoscale calculation.

Quantitative comparisons are not possible because the simple model uses an extremely simplified equation of state with only two constant parameters, the same sound speed in the reactants and products and assumes a constant burn speed. The mesoscale calculations used proper equations of state, and it was found [3] that the burn speed decreases because the temperature in the products cools as the burn front propagates. In addition the simple model assumes a random distribution of hotspots across a volume, while the mesoscale calculation assumes the spherical symmetry of a hotspot surrounded by a series of equally separated spherical shell hotspots.

6. Discussion and Conclusions

Making a number of simplifying assumptions, an analytic model has been developed for the pressure field surrounding an isolated, spherical, burning hotspot. The solution depends on the ratio, β , of the assumed constant burn front speed to the local sound speed, where typically $\beta \sim 0.001$. The pressure deviation is constant behind the burn front, is slightly higher immediately ahead of the burn front and decays like $1/r$ between the burn front and an inverted N-shaped leading pressure pulse propagated into the explosive. One dimensional mesoscale hydrocode calculations, with Arrhenius kinetics and heat conduction, show that the pressure distribution agrees qualitatively with the simple model, including the general form of the pressure pulse.

The simple model has been used to determine the time history of the pressure field at any point in a distribution of hotspots, by adding the contributions from each hotspot up to a distance of $\sim c_1 t$ from A. It is shown that the total pressure deviation is:

- a. dominated by the summation of the pressure fields lying between the burn front and the pressure pulse for each hotspot, and
- b. reduces to the simple relationship (8) that agrees with the pressure field deduced at continuum level using the analytic reactive model CIM [4].

The Hill, Zimmerman, Nichols model [1] for the reaction rate from a distribution of hotspots shows that reaction rate is a local phenomenon, depending on the closure of burn fronts from adjacent hotspots, i.e. over distances of a few micro-metres. On the other hand, the development of the pressure field depends on contributions from burning hotspots up to millimetres away.

At least in the simple configuration of a field of hotspots simultaneously starting to react at time zero, the Hill et al paper and this paper have shown that there is a direct equivalence between the bulk reaction rate history and pressure deviation history from a distribution of hotspots and reactive hydrodynamics at the continuum level. It is reasonable to assume that such equivalence applies to other shock initiation configurations, where the initiation of hotspots may be time dependent and/or if the field of hotspots is of limited extent.

References

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