CUMULATIVE DAMAGE HOTSPOT MODEL FOR USE WITH ARRHENIUS BASED IGNITION AND GROWTH MODEL

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The hot spot model described in this paper is based on the idea of cumulative damage that can be estimated from knowledge of the hysterisis of the material. This gives the energy deposited in the energetic material as a result of the work done in terms of a temperature rise. The additional temperature created by the work done is then added to a thin shell of energetic material surrounding the outer edge of the existing gas-filled pore that has already been heated by bulk effects. Although the model is really applicable to low strain rates, it can be used as a generic hot spot model even at high strain rates. In this case, the parameterisation can be obtained by matching to specific calibration data such as flyer, bullet impact, wedge test and run distance data and tested and validated against real weapon system results.

INTRODUCTION

We have previously reported details of our Arrhenius, temperature dependent homogeneous ignition and growth of reaction model, which includes heterogeneous effects modelled through a gas pore collapse mechanism[1]. The pore collapse mechanism implemented in the model only accounts for the contribution from compression of gas bubbles in the explosive matrix. The gas collapse is assumed to be adiabatic within the smallest time step in the model, which is typically that for heat conduction, but otherwise is non-adiabatic in terms of a hydrocode time step.

Shock compression of the gas has been shown experimentally to be an important hot spot mechanism[2,3], and in many ways resembles the phenomenon of sonoluminescence[4]. There is, however, experimental evidence that other mechanisms can be important when bubbles are shocked. For example, jetting of material across the cavity has been observed[5,6]. Additionally, it has been proposed that visco-plastic heating of the material around a cavity is more important for shock initiation[7] and this has been used as the basis for a number of hot spot models[8].

The existing pore collapse hot spot functionality is only expected to be relevant in the shock regime where the pore collapse

time is very short and hence the pore temperature very high. At lower shock amplitudes, such as lower velocity impacts, or where low velocity projectiles penetrate an explosive store, other hot spot mechanisms would be expected to play a role in controlling the response of the underlying homogeneous model. In these regimes, mechanisms such as shear or friction are likely to be more important than adiabatic compression of gas-filled pores.

In developing shear or frictional heating models consideration must be given to the fact the model is to be implemented into a hydrocode, and that it is necessary to link the model (as a sub-model) with the existing burn model. A one-dimensional solution would be preferred, but this needs to be reconciled against the fact that shear, or friction, are three-dimensional problems.

There are a number of papers in the literature that use the idea of cumulative damage models to describe the damage caused when energetic materials, such as propellants, are stressed. Moreover the method has been shown to be applicable to high-strain rates (10^3-10^4 s^{-1})[9]. The method allows relatively simple experimental techniques to be used to characterise the test material. Hopkinson bar experiments can give dynamic stress-strain data, and constant stress experiments can be performed using a dynamic mechanical thermal analyser, using either a parallel plate or shear sandwich fixture. From such measurements the overall mechanical response of the energetic material can be determined and the hysteresis energy losses in the material measured.

A knowledge of the hysteresis energy when an energetic material is deformed can be used as a measure of the damage (which is probably a mixture of shearing, plastic deformation, dewetting of crystals and binder and microvoid / cracking formation). Furthermore, it can be used as an additional heating term calibrated from experiment.

This paper describes the background and implementation of a new hot spot model. It has been designed to operate either with the existing pore collapse hot spot model or with a particle burn model. Only the pore collapse implementation will be considered in this work. The hot spot model is based on the idea of cumulative damage that can be estimated from knowledge of the hysteresis of the material. This gives the energy deposited in the energetic material as a result of the work done in terms of a temperature rise. The additional temperature created by the work done is then added to a thin shell of energetic material surrounding the outer edge of the pore that has already been heated by bulk effects. Although the model is really applicable to low strain rates, it can be used as a generic hot spot model even at high strain rates. In this case, the parameterisation can be obtained by matching to specific calibration data such as flyer, bullet impact, wedge test and run distance data and tested and validated against real weapon system results.

BACKGROUND

The hot spot model described in this paper is designed to simulate the contribution of hot spots formed in the energetic material as a shock wave passes through it. These hot spots may occur due to shear heating, visco plastic heating and the like. It is assumed that such processes occur around dislocations in the material's structure, so a perfectly uniform (idealised) material will not exhibit this behaviour. For the Arrhenius burn model, the only irregularities currently capable of being modelled are the gas pores. However, it should be noted that it is our intention to introduce a grain burning model for the explosive crystals which will use the same

methodology developed for the gaseous pores, at later date.

In the current pore collapse model, the gas filled pores are assumed to be spherical, and are surrounded by a thin shell of energetic material of constant mass. The purpose of the shell is to allow heat transfer from the pore gas to the bulk material (which is a mixture of energetic material and binder) through a simple conduction process. As shell material is consumed by reaction, mass is transferred from the bulk to the shell (to maintain constant mass) and from shell to gaseous products. It is therefore convenient to use the degree of distortion of the shell material for the shear model. It should be noted that homogeneous explosives cannot use the shear model because of their uniform structure (they have no pores present).

The shear model monitors the change in shape (i.e. strain) of the shell of energetic material surrounding each pore as a shock wave propagates through it. A look-up table of energy vs. strain rate is then used to calculate the heating in the shell.

The leading edge of a pressure wave acts to compress the pore and shell, therefore the shell will be subjected to compressive strain. During this phase, the pressure wave will be losing energy to the shell, but it is assumed that:

- the shell does not heat up (by any more than the bulk heating effect);
- the reduction in energy of the pressure wave is negligible compared to its total energy.

After the peak of the pressure wave has passed, the pore and shell expand out. The resulting tensile strain causes energy gained from the shock wave to be liberated in the material, manifesting itself as a temperature rise. The strain rate of the shell material, once calculated, leads directly to a quantity of energy being dispersed in the material as heat. This quantity of energy is read from a table of energy vs. strain rate supplied by the user.

MODEL SPECIFICATION

The specification detailed here can be regarded as the initial stage in an iterative process of analysing the shear model's performance and changing its functionality to improve results. The specification has been kept deliberately straightforward so as not to introduce unnecessary complexities at the first iteration.

Strain Calculation

Strain is the change in length of a material along a single dimension. The strain is thus resolved into 3 Cartesian components. One component addresses the increase in shell thickness, and is therefore perpendicular to the tangential plane of the shell material's surface. The other two components are within (or at least parallel to) the tangential plane of the shell's surface, thus measuring the stretching of the shell's 'skin'. Due to the shell being spherically symmetrical, the last two components are equal. The total strain is assumed to be the sum of the 3 components, and this total strain is converted to an energy value using the look-up table.

The shell's dimensions are deduced both before and after straining. Due to the spherical symmetry of the shell, its shape is completely described by its inner and outer radius. Information required to deduce these radii is given in Table 1.

TABLE 1. PARAMETERS REQUIRED TO CALCULATE SHELL DIMENSIONS

Parameter symbol	Meaning
η_σ	mass fraction of pore shell
η_β	mass fraction of bulk
r_ϕ	current pore radius

ϕ	current porosity

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Pore shell Radii

The radius of the bulk region, r_β, is given by:

$$r_\beta = \frac{r_\phi}{\sqrt[3]{\phi}} \qquad (1)$$

It is assumed that the shell and bulk have the same density. This volume ratio then follows, where V denotes the volume of a region specified by its subscript:

$$\frac{V_\sigma}{V_\sigma + V_\beta} = \frac{\eta_\sigma}{\eta_\sigma + \eta_\beta}$$

For each region Ω, substituting V_Ω for $^4/_3\pi r_\Omega^3$ and re-arranging gives the radius (outer) of the shell, r_σ:

$$r_\sigma = \sqrt[3]{\frac{\eta_\sigma}{\eta_\sigma + \eta_\beta}\left(r_\beta{}^3 - r_\phi{}^3\right) + r_\phi{}^3}$$

The inner radius of the shell is equal to the radius of the pore, r_ϕ, which is already known.

Strain calculation from radii

The strain that the shell undergoes is calculated as 3 mutually perpendicular Cartesian components. The x and y components deal with stretching within the plane parallel to the shell's tangential surface. If the plane in which stretching is measured is actually on the shell's outer surface, then the strain will be overestimated as the inner surface will not be stretched by as much. Similarly, considering the inner surface will underestimate the strain. Therefore, the stretching will be measured in the spherical surface that is midway between the inner and outer radii. The radius of the surface in question is therefore given by r_s:

$$r_s = \frac{r_o + r_i}{2}$$

where r_o and r_i are the outer and inner radii of the shell respectively. The area of this surface is A_s:

$$A_s = 4\pi r_s{}^2$$

Hence given an updated value of r_s, an updated A_s can be deduced. The two perpendicular dimensions within the surface area, being equal, will each change by the same factor. The standard equation for strain along a length l is:

$$\varepsilon_l = \left|\frac{l'' - l'}{l'}\right|$$

where l'' and l' are the latest and previous values of the length respectively. The modulus ensures that the equation is valid for compression as well as expansion. However, the model will use the following modified equation for strain:

$$\varepsilon_l = f_l\left|\frac{l'' - l'}{l_0}\right| \qquad (2)$$

where l_0 is the original value of l, and f_l is a multiplication factor for the strain. Making the change in length relative to l_0 rather than l' means that the strain value will be independent of the number of time-steps that the strain is split into. A side effect of using l_0 rather than l' for the denominator means that the latest length is compared against a value that is several iterations old. Using a long timespan introduces the possibility of mass transfer and other non-pressure effects altering the length. The multiplication factor is present to compensate for these effects. If material is transferred out of the shell so that its length along a certain axis is halved, all subsequent length measurements will be half of what they would otherwise have

been. Therefore all future measurements will need to be doubled.

The multiplication factor is simply deduced by dividing the previous length by the latest length:

$$f_l = \frac{l'}{l''}$$

where the change in length is due to mass transfer etc. If such a factor already exists for a given dimension of the shell, the new factor that replaces it will be derived using the formula for *f* above, and by multiplying this by the existing factor:

$$f_l'' = f_l' \frac{l'}{l''} \qquad (3)$$

The factor will continue to be used to calculate strain until the dimension starts to compress due to pressure, in which case the material is deemed to have finished undergoing strain for the present time, and *f* will be reset to unity.

The latest value of x will be given by:

$$x'' = \sqrt{A_s''} \qquad (4)$$

The strain along each of the components in the surface will be:

$$\varepsilon_x = \varepsilon_y = f_x \left| \frac{x'' - x'}{x_0} \right|$$

where x_0 is the value since the expansion along the *x* direction began. The strain along the third component (relating to changes in the shell's thickness) is given by:

$$\varepsilon_z = f_z \left| \frac{z'' - z'}{z_0} \right|$$

The 'z length' is defined as difference between the outer and inner radii of the shell. The latest value of z will simply be the outer shell radius minus the inner shell radius.

The total strain is arrived at by adding together the individual components:

$$\varepsilon_T = \varepsilon_x + \varepsilon_y + \varepsilon_z \qquad (5)$$

The total strain rate is calculated by dividing this by the current burn model time-step:

$$\dot{\varepsilon}_T = \frac{\varepsilon_T}{\Delta t} \qquad (6)$$

Note that there will be a separate value of $\dot{\varepsilon}_T$ for the explosive and metal shells.

Heating Term

The total strain value ε_T is divided by the current burn model time-step to get a strain rate for the shell. This rate is then looked up in a table of strain rate vs. energy. The strain rate value will generally lie between two entries in the table, so the energy value will need to be interpolated (linearly, for simplicity) between the two entries. Once an energy value has been derived from the table, it is multiplied by the number of pores or metal particles (as appropriate) to arrive at the total energy contribution of shells of that type in that element. To illustrate, the energy supplied by shearing of all explosive shells in a given element, E_s, is given by:

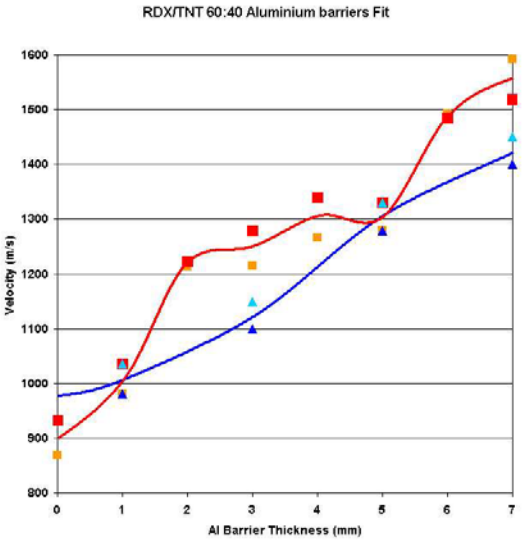
$$E_s = n_\phi E_L \qquad (7)$$

where n_ϕ is the number of pores in the element and E_L is the energy corresponding to $\dot{\varepsilon}_T$ in the lookup table. The resulting energy term is added to the energy in the shell, which will filter through as a temperature rise in the shell.

TESTING THE MODEL

Although the model has been developed based on the notion of cummulative damage, and it was intended to parameterise the model from hysterisis data, this has not been possible to date due to lack of experimental data. The testing has therefore been concentrated on checking the mathematical flow of data through the equations and the ability of the model to add control to the sensitivity of impact simulations of explosive charges covered with aluminium.

FIGURE 1. FRAGMENT IMPACT OF 13.15MM DIAMETER STEEL PROJECTILES AGAINST RDX/TNT CHARGES COVERED BY ALUMINIUM BARRIERS. THE EXPERIMENTAL RESULTS ARE SHOWN IN RED AND THE CALCULATED VALUES IN BLUE



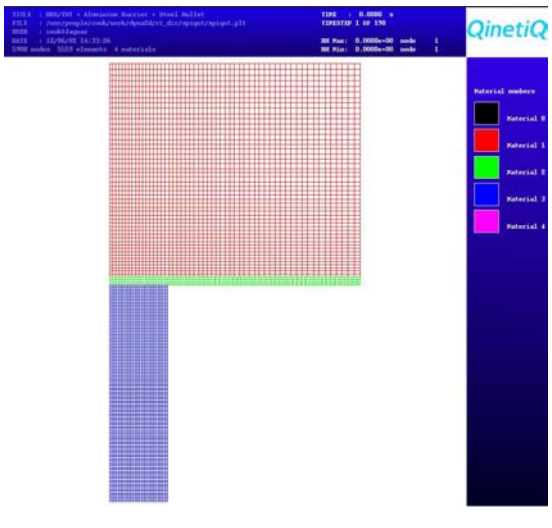
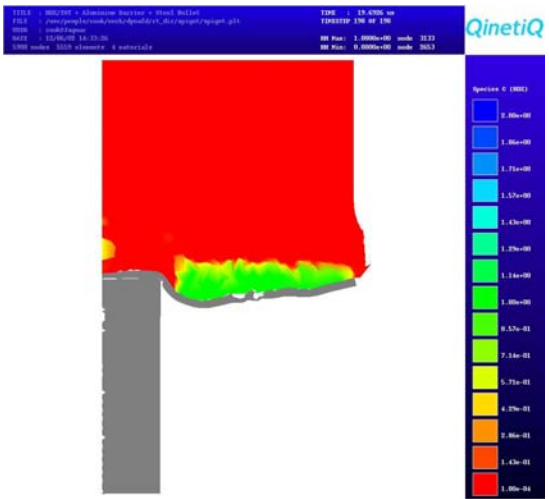


FIGURE 2. DYNA2D MESH OF A FRAGMENT IMPACT SIMULATION.

We have previously parameterised our Arrhenius ignition and growth model for RDX/TNT 60:40 against fragment impact data[10]. This parameterisation has included gas filled pores, the propensity of which has been estimated from the density, and the size was assumed to be 1μm in diameter. The preliminary fit obtained along with the experimental data is shown in figure 1. The axisymetric mesh used for these calculations is shown in figure 2. The flat-nosed fragment is shown at the bottom of the figure impacting a 3mm aluminium barrier plate behind which is a block of explosive. Using this as a baseline, a test was performed to examine how the additional shear hot spot model can affect the outcome of a run. The input deck was adapted so that it was compatible with the latest burn model. A velocity was chosen such that it does not detonate under normal conditions (i.e. without shear heating).

With the shear model disabled from the input deck, the run behaves as previously, with no detonation occurring. However, when the shear model is turned on, the extra heat being dumped into the explosive shell causes the energetic material to detonate.

Analysis of the run has shown that without shear heating (energy terms of zero in the look-up table), there is a spike in the strain rate which reaches about 4.5×10^8 s^{-1} at its maximum. The energy contributions into the shell from existing sources peak at



around 3.5×10^{-6} in any given timestep. The number of pores in each element is 2×10^{9}. Knowing this information, the data in the look-up table was chosen so that the shear heating made a significant contribution at the maximum strain rate that the material would reach. An energy of 2×10^{-14}J at a strain rate of 1×10^{8} s^{-1} was necessary to just initiate SDT in these runs.

FIGURE 3. LOW VELOCITY IMPACT SIMULATION OF AN RDX/TNT 60:40 CHARGE PROTECTED WITH AN ALUMINIUM BARRIER. THE SCALE REPRESENTS THE AMOUNT OF PRODUCT GAS PRODUCED.

A further series of simulations were carried out to investigate the effect of the model at lower strain rates. The same parameterised model was used in these calculations with the shear table look-up adjusted so that an energy of 2×10^{-14}J was produced at a strain rate of 1×10^{4} s^{-1} . In these simulations the fragment velocity was reduced to 25m/s (a velocity typical of free fall conditions). The results of these calculations showed that reaction occurred where the cover plate began to buckle in a ring to the periphery of the fragment (see figure 3). This is similar to experimental observation. Moreover, this modified model did not appear to affect the fragment impact predictions at the higher velocities. This demonstrates that this new hot spot model can act successful in parallel to the pore collapse hot spot model to extend the predictive capability.

CONCLUSIONS

The hot spot model specified in this report has been designed to operate either with the existing pore collapse hot spot model or with a particle burn model. Only the pore collapse implementation has been considered in this work. The hot spot model is based on the idea of cumulative damage that can be estimated from knowledge of the hysterisis of the material. This gives the energy deposited in the energetic material as a result of the work done in terms of a temperature rise. The additional internal energy created by the work done is then added to a thin shell of energetic material surrounding the outer edge of the pore or particle that has already been heated by bulk effects. Although the model is strictly applicable only to low strain rates, it appears capable of being used as a generic hot spot model even at high strain rates. In this case, the parameterisation can be obtained by matching to specific calibration data such as flyer or bullet impact, wedge test, and run distance data. The model can then be tested and/or validated against real weapon system results.

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