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MASTER

Initiation of Detonation by the Interaction of Shocks with Density Discontinuities

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The basic processes in the shock initiation of inhomogeneous explosives have been investigated theoretically using the model of a cylinder of nitromethane containing a void or an aluminum pellet. The interaction of a shock with the density discontinuities, the resulting formation of a hot spot, and the buildup to propagating detonation were computed using two-dimensional numerical hydrodynamics of the "PIC" type with chemical reaction and accurate equations of state. The hot spots formed at aluminum pellets exhibit failure or propagation of detonation in approximately the same manner as the one-dimensional, hydrodynamic hot spots studied previously. The failure of hot spots formed at voids could be studied only in those cases in which the failure mechanism did not depend on details of the structure of the reaction zone, as this structure could not be reproduced in the calculation.

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INTRODUCTION

The mechanism of shock initiation of detonation has been considered, both experimentally and theoretically, by numerous investigators. Experiments which show many details of the initiation process have been performed with homogeneous explosives, such as liquid TNT or single crystal PETN, by Campbell, Davis, and Travis¹, and with inhomogeneous explosives, such as pressed TNT, by Campbell, Davis, Ramsay, and Travis². Detailed calculations of the shock initiation of homogeneous explosives³ show that initiation is by thermal explosion resulting from shock heating. The experiments^{1,2} indicate that initiation of inhomogeneous explosives cannot result only from uniform shock heating of the explosive, but rather that shock interactions with the density inhomogeneities produce numerous local hot spots in the explosive. The hot spots decompose and liberate energy which strengthens the shock so that, when it interacts with additional inhomogeneities, hotter hot spots are formed and more of the explosive is decomposed. The shock wave grows stronger and stronger, releasing more and more energy, until it becomes strong enough to produce temperatures at which all of the explosive reacts, and detonation begins. This initiation process is too complicated to describe with existing numerical computing techniques and cannot be reproduced with a one-dimensional model if one uses realistic rates of homogeneous decomposition of the explosive⁴.

To investigate the basic processes in inhomogeneous explosives, the experiments were simplified to an investigation of the interaction of a shock with a single inhomogeneity, such as an air bubble or a metal wire

in nitromethane¹. It was observed that a shock which was too weak for immediate initiation, interacting with a density discontinuity of sufficient size, produced a hot spot in the liquid explosive which would initiate propagating detonation.

The formation of a hot spot from a shock-bubble interaction was studied theoretically by Evans, Harlow, and Meixner⁵ for gases and for nitromethane. In the nitromethane case, calculational fluctuations precluded any detailed description of the hot spot. Boyer, Grandey, Schermerhorn, and Uyehara⁶ considered theoretically the collapse of an air bubble in a non-reactive solid, but did not obtain a detailed description of the hot spot.

Mader³ studied the one-dimensional reactive hydrodynamics of hot spots and concluded that two competing processes occur just outside the hot spot. The first process is the expansion resulting from the divergent flow of the heated fluid, which tends to cool it. The second process is chemical decomposition of the fluid, which tends to heat it. Propagating detonation occurs only if the second process dominates.

In order to increase our understanding of the basic processes involved in the shock initiation of inhomogeneous explosives we have used numerical two-dimensional hydrodynamics to study theoretically the formation of hot spots from shocks interacting with spherical, cylindrical, or biconical voids, and with cylinders and spheres of aluminum, in the belief that these interactions will exhibit approximately the same behavior as those resulting from real density discontinuities in heterogeneous explosives. We shall describe the results for two typical examples, the spherical void and the aluminum cylinder, which illustrate

the predominant features of the formation of hot spots and initiation of detonation. Additional examples are contained in references 4 and 7.

COMPUTATION METHOD

The objective of the computation method was to obtain a complete solution to the three-dimensional, axially symmetric equations of fluid dynamics for a reactive material using the most accurate of the available equations of state and input data. The method of solution was numerical and was based on a modification^{4,7} of the "Particle-In-Cell" method of Harlow⁸; briefly, it can be described as follows: The partial differential equations for nonviscous, nonconducting, compressible fluid flow are written in conservative form in cylindrical coordinates. The equations are transformed to the finite-difference form appropriate to a fixed (Eulerian) mesh of cells (actually toroids of square cross section) which cover the domain of interest. In this form they are used to determine the dynamics of the fluid. The fluid itself is represented by a set of "particles". Each particle is actually a circular ring about the axis (or a point in cross-section) whose coordinates represent the position of a macroscopic amount of fluid. The movement of the particles through the mesh of cells then represents the dynamics. Starting from a given set of initial and boundary conditions, the calculation advances the configuration through time in a sequence of finite intervals. Accuracy in resolving the dynamics is dependent upon the number of cells and particles. For practical purposes the accuracy is limited by the size of the computer and the amount of machine time that is available. In the calculations

reported here, 2048 cells were used, with 32 cells along a radius and 64 cells along the axis. We used 16 particles per cell, or a total of 32,768 particles. A few calculations were performed with 64 particles per cell, or a total of 131,072 particles, and the results compared well with those obtained with 16 particles per cell.

The Fickett and Wood⁹ beta equation of state was chosen as the form for the detonation products off the C-J isentrope. The pressure, volume, temperature, and energy values along the C-J isentrope were computed using the Becker-Kistiakowsky-Wilson equation of state as calibrated by Mader¹⁰. The Grüneisen equation of state was chosen as the equation of state of the undetonated explosive off the experimental Hugoniot. Pressures and volumes on the Hugoniot are available from experimental data. Temperatures on the Hugoniot were calculated using the technique of Walsh and Christian¹¹ in a somewhat arbitrary manner¹² so as to obtain temperatures in agreement with the available experimental Hugoniot temperatures. The equation of state for mixtures of condensed explosive and detonation products was computed assuming pressure and temperature equilibrium. When two components were present in a cell separated by a boundary, the equation of state was computed assuming pressure equilibrium, with the difference between the total Hugoniot energy at the same specific volume and the total cell energy distributed between the components according to the ratio of the total Hugoniot energies of the components. This equation of state, although empirical, is believed to be accurate since it reproduces all the available experimental equation of state data.

The incorporation of chemical reaction into the Particle-In-Cell method was accomplished using Arrhenius kinetics and assuming that when a particle moves from an old cell to a new cell it carries the old cell mass fraction into the new cell and mixes homogeneously.

A detailed description of the hydrodynamic equations, the difference equations, and the values for the input parameters has been presented previously^{4,7}.

Accuracy of the results of this procedure was indicated by comparison with detonation processes for which solutions were already available. For example, the one-dimensional features³ of the shock initiation of nitromethane were successfully reproduced for nitromethane in cylindrical geometry⁷. Accuracy of the results was also indicated by their agreement with those of experiments such as "Phermex"¹³ radiographs of closure of a spherical air bubble in water by a shock⁴.

All calculations were performed using an IBM electronic data processing machine, type 7030 (the "STRETCH" computer). The results were plotted with a Stromberg-Carlson SC-4020 microfilm recorder.

SHOCK INTERACTION WITH A SPHERICAL VOID

The initial and boundary conditions of the calculation were chosen to match the model of a cylinder of nitromethane containing a spherical void centered on the axis. The axial symmetry of the system allows a complete description in two coordinates--the distance along the axis, and the distance from the axis.

The results of a nonreactive calculation are presented in Figure 1

in the form of pictures which show shapes, wave positions, and fluid element (particle) positions for a cylinder of nitromethane of 0.064 cm radius and 0.128 cm high, containing a 0.02 cm radius void. A piston is applied to the bottom of the cylinder, shocking the nitromethane to 85 kbar and 1200°K. The left half of each picture is a reflection of the right half, showing the location of the hot spot as it forms. The position of those cells whose temperature is greater than 1400°K is shown with an "x". The adiabatic explosion time of nitromethane at 1400°K is approximately 0.030 μ sec.

The following simplified analysis of the results shows the main features of the hot spot formation. The 85 kbar, 1200°K shock arrives at the lower surface of the void traveling with a shock velocity of 0.45 cm/ μ sec and a particle velocity of 0.171 cm/ μ sec. The free surface velocity of the surface fluid becomes 0.342 cm/ μ sec with a temperature of 530°K. Convergence and shocks increase the free surface velocity and temperature of this fluid until it has a free surface velocity of 0.52 cm/ μ sec and a temperature of 1200°K at the time of closure of the void. The first regions to become hotter than 1400°K are just above the equator of the void at the axis (from convergence) and at the outer rim of the void (from void closure). The two regions grow and form a single hot region at about the time complete closure of the void occurs. Upon closure of the void, a 170 kbar shock travels into the unshocked region above the initial position of the void, heating it to 2100°K, and back into the hotter fluid below, resulting in a temperature of 3000°K. The actual process is much more complex, with the velocities,

pressures, and temperatures varying about the values assigned to them in this simplified discussion. The size of the hot spot approximates the size of the original void, and the temperature varies from 1400 to 4000°K as shown in the isotherms at 0.2 and 0.24 μ sec in Figure 2. The hottest part of the hot spot begins to cool from expansion soon after closure of the void.

To obtain a description of the hot spot decomposition and the resulting initiation of propagating detonation, chemical reaction with an Arrhenius rate law was included in the calculation. The results of a reactive calculation are shown in Figure 3 for the same geometry and boundary conditions as in the nonreactive calculation shown in Figure 1. The left half of each is, as before, a reflection of the right half, and is used to show the location of the decomposition products. The position of those cells that have completely decomposed is shown with an "x".

Failure of propagating detonation from the divergent nature of the flow cannot be expected since the reaction is almost instantaneous in the time and space scale used in the calculations. With an appropriate time scale, all quantities are functions of the ratio of their radius to the hot spot radius because no other physical length scale (such as reaction zone thickness) enters into the problem.

Experimental evidence of Davis⁷ indicates that failure occurs primarily from side rarefactions cooling the explosive inside the reaction zone. The confinement of the detonating explosive controls the strength of the side rarefactions. The detonation wave formed from the hot spot is confined by hot, high-density, shocked explosive moving in the

direction of the detonation wave. The rarefaction that travels into the reaction zone from such confinement is of sufficient strength that the failure diameter of the detonation formed from the hot spots is of the same order of magnitude as the observed critical sizes of hot spots formed from void closure⁷. A more detailed numerical description of the process of failure of propagating detonation is not presently possible.

When a piston pressure that is considerably lower than 85 kbar is applied to nitromethane containing a void, the resulting hot spot will be cooler and chemical reaction ceases to be instantaneous in the time and space scale of the calculation. For example, a 25 kbar shock in nitromethane interacting with a 0.02 cm radius void results in a hot spot which decomposes but fails to initiate propagating detonation.

SHOCK INTERACTION WITH AN ALUMINUM CYLINDER

The initial and boundary conditions of the calculation were chosen to match the model of a cylinder of nitromethane containing a solid aluminum cylinder centered on the axis.

Figure 4 shows the shape of the aluminum cylinder and the location of the shock fronts at various times for a cylinder of aluminum of 0.032 cm radius and 0.032 cm height in a cylinder of nonreactive nitromethane of 0.064 cm radius and 0.128 cm high.

The following simplified analysis of the results shows the main features of the hot spot formation. The 85 kbar, 1200°K shock arrives at the lower surface of the aluminum cylinder traveling with a shock

velocity of 0.45 cm/ μ sec and a particle velocity of 0.171 cm/ μ sec. The matching conditions give a pressure of 170 kbar, a particle velocity of 0.093 cm/ μ sec, a temperature of 500°K, and a shock velocity of 0.66 cm/ μ sec in the aluminum. The pressure in the previously shocked nitromethane below the cylinder is also 170 kbar, the particle velocity is 0.093 cm/ μ sec, and the temperature is about 1500°K.

The shock wave in the aluminum is divergent and has fallen to about 100 kbar when it reaches the upper surface of the cylinder. The matching conditions give 30 kbar in the nitromethane above the cylinder. The main shock flows around the cylinder and overtakes the initial weaker shock. The actual process is much more complex with the velocities and pressure varying about the values assigned to them in this simplified discussion.

We did not observe failure of the hot spots formed from the interaction of an 85 kbar shock with a void because the hot spot was formed at the shock front and at a temperature so high (2000 to 3000°K) that the reaction was almost instantaneous in the time and space scale used. In the case of the cylinder of aluminum, the hot spot is formed behind the shock front and below the cylinder, and is at a sufficiently low temperature (1400 to 1500°K) that the reaction is not instantaneous in the time and space scale of interest. The subsequent development of the hot spot resembles that of the one-dimensional hydrodynamic hot spot³. The hot explosive decomposes, sending a shock wave into the undetonated, previously shocked explosive. Whether or not the hot spot propagates depends upon the initial strength of the shock wave and how well it is supported.

Results of reactive calculations for a shock interacting with an aluminum cylinder in nitromethane show buildup to propagating detonation from a shock interacting with a 0.032 by 0.032 cm radius cylinder and show failure to buildup to propagating detonation from a shock interacting with a 0.002 cm radius cylinder of aluminum in nitromethane.

Travis¹⁴ has determined experimentally that the critical radius of an aluminum rod in nitromethane shocked initially to 85 kbar is greater than 0.005 cm and less than 0.04 cm. His observations are in good agreement with the computed results just described.

CONCLUSIONS

Two-dimensional numerical hydrodynamics of the Particle-In-Cell type with accurate equations of state can be used to compute the interaction of a shock with a density discontinuity, the formation of a hot spot, and buildup to propagating detonation.

The failure of the resulting hot spot to initiate propagating detonation may be described in those cases in which the failure mechanism does not depend on the details of the structure of the reaction zone, such as the hot spot formed from the interaction of an 85 kbar shock with an aluminum sphere or cylinder in nitromethane, and the hot spot formed from the interaction of a 25 kbar shock with a spherical void in nitromethane. The two-dimensional calculations show failure and propagation in approximately the same manner as the one-dimensional hydrodynamic hot spot model.

Increased understanding of the basic processes involved in the shock initiation of inhomogeneous explosives has been obtained by studying the formation of hot spots from shocks interacting with single density discontinuities. The problem of failure of propagating detonation from side rarefactions cooling the explosive inside the reaction zone is probably the next problem that must be solved before further progress can be made in understanding the basic processes involved in the shock initiation of inhomogeneous explosives. Studies of the time dependent reaction zone and of the phenomenon of failure diameter of explosives may yield further insight into the problems of shock initiation of explosives and are under active investigation at this laboratory.

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LITERATURE CITED

1. A. W. Campbell, W. C. Davis, and J. R. Travis, Phys. Fluids 4, 498 (1961).
2. A. W. Campbell, W. C. Davis, J. B. Ramsay, and J. R. Travis, Phys. Fluids 4, 511 (1961).
3. C. L. Mader, Phys. Fluids 6, 375 (1963).
4. C. L. Mader, Los Alamos Scientific Laboratory report LA-3235 (1965).
5. M. W. Evans, F. H. Harlow, and B. D. Meixner, Phys. Fluids 5, 651 (1962).
6. M. H. Boyer, R. A. Grandey, D. A. Schermerhorn, and H. Uyehara, Aeromutronic Division, Ford Motor Company, report N-1764 (1962).
7. C. L. Mader, Los Alamos Scientific Laboratory report LA-3077 (1964).
8. F. H. Harlow, Methods in Computational Physics 3, 319-343, Academic Press, New York (1964).
9. W. Fickett and W. W. Wood, Phys. Fluids 1, 528 (1958).
10. C. L. Mader, Los Alamos Scientific Laboratory report LA-2900 (1963).
11. J. M. Walsh and R. H. Christian, Phys. Rev. 97, 1544 (1955).
12. C. L. Mader, Phys. Fluids 8, 777 (1964).
13. D. Venable, Phys. Today 17, No. 12 (1964).
14. J. R. Travis, private communication.

Figure 1 - Sequence of particle configurations for a shock interacting with a 0.02 cm radius spherical void in a cylinder of nonreactive nitromethane. A piston is applied to the bottom of the cylinder shocking the nitromethane to 85 kbar and 1200°K. The position of those cells with a temperature greater than 1400°K is shown on the left half of the picture with an "x".

Figure 2 - Isotherm plots for the hot spot formed when a shock interacts with a spherical void in a cylinder of nonreactive nitromethane. Cylindrical axis is to the right. Dashed lines show the current interface position.

Figure 3 - Sequence of particle configurations for a shock interacting with a 0.02 cm radius spherical void in a cylinder of reactive nitromethane and the resulting initiation of propagating detonation. The position of those cells that have completely decomposed is shown on the left of the picture with an "x".

Figure 4 - The shape of an aluminum cylinder at various times after a shock in nonreactive nitromethane has interacted with it. The shape of the aluminum cylinder is shown with solid lines and the shape of the shock front is shown with dashed lines.

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