

AD-A119 262 ILLINOIS UNIV AT URBANA DEPT OF MECHANICAL AND INDUST--ETC F/G 19/1
MODELING OF DEFLAGRATION-TO-SHOCK-TO-DETONATION TRANSITION (DSD--ETC(U)
JUL 82 H W KRIER, P B BULTER, D COYNE AFOSR-81-0145
UNCLASSIFIED UIIU-ENG-82-4002 AFOSR-TR-82-0686 NL

1 OF 1
AD-A
119 262

END

DATE

FILED

10-82

DTIC

AD A119262

Department of Mechanical
and Industrial Engineering

University of Illinois at Urbana-Champaign
Urbana, IL 61801



9

Annual Report

MODELING OF DEFLAGRATION-TO-SHOCK-TO-DETONATION TRANSITION (DSDT) IN
POROUS HIGH ENERGY SOLID PROPELLANTS AND EXPLOSIVES

Prepared by:

Herman Krier, Principal Investigator
P. Barry Butler and Daniel W. Coyne,
Graduate Research Assistants

Department of Mechanical and Industrial Engineering
144 Mechanical Engineering Building
1206 West Green Street
University of Illinois at Urbana-Champaign
Urbana, IL 61801

Prepared for:

Air Force Office of Scientific Research
Aerospace Sciences Directorate
Bolling Air Force Base, DC 20332
Program Manager: Dr. Michael Strosio

For Research Performed under
Grant AFOSR 81-0145

During Period
1 June 1981 through 30 May 1982

Approved for Public Release;
Distribution Unlimited,
Grant AFOSR-81-0145, July 1982

FILE COPY

82 09 15 040

DTIC
SELECTED
SEP 16 1982

Annual Report*: UILU ENG 82-4002

MODELING OF DEFLAGRATION-TO-SHOCK-TO-DETONATION TRANSITION (DSDT)
IN POROUS HIGH ENERGY SOLID PROPELLANTS AND EXPLOSIVES

Prepared by:

Herman Krier, Principal Investigator
P. Barry Butler and Daniel W. Coyne, Graduate Research Assistants

Department of Mechanical and Industrial Engineering
144 Mechanical Engineering Building
1206 West Green Street
University of Illinois at Urbana-Champaign
Urbana, IL 61801

Prepared for:

Air Force Office of Scientific Research
Aerospace Sciences Directorate
Bolling Air Force Base, DC 20332
Program Manager: Dr. Michael Stroschio

For Research Performed under

Grant AFOSR 81-0145

During Period 1 June 1981 through 30 May 1982

* Approved for Public Release; Distribution Unlimited, Grant AFOSR-81-0145
July 1982

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH (AFOSR)
NOTED FOR DISTRIBUTION TO DTIC
This technical report is approved for release and is
approved for release under E.O. 11652-12.
Distribution is unlimited.
MATTHEW J. KATZ
Chief, Technical Information Division

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER AFOSR-TR- 82-0686	2. GOVT ACCESSION NO. AD-A119262	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) MODELING OF DEFLAGRATION-TO-SHOCK-TO-DETONATION TRANSITION (DSDT) IN POROUS HIGH ENERGY SOLID PROPELLANTS AND EXPLOSIVES		5. TYPE OF REPORT & PERIOD COVERED ANNUAL REPORT - July 1982
		6. PERFORMING ORG. REPORT NUMBER UILU-Eng-82-4002
7. AUTHOR(s) Herman Krier, P. Barry Bulter and Danial Coyne		8. CONTRACT OR GRANT NUMBER(s) AFOSR 81-0145
9. PERFORMING ORGANIZATION NAME AND ADDRESS University of Illinois at Urbana-Champaign Department of Mechanical and Industrial Engr. Urbana, Illinois 61801		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS 61102F 2301/A6
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Office of Scientific Research/NA Building 410; Attn: M. Stvoscio Bolling Air Force Base, DC 20332		12. REPORT DATE July 1982
		13. NUMBER OF PAGES 26
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) Approved for public release; distribution unlimited		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) Detonation Physics DDT Porous explosives		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) This annual report represents the summary of work done on the modeling of processes leading from deflagration to detonation in porous or granular high energy propellants. Particular attention is paid to the analysis of shock development from compression waves forming ahead of confined burning in the original material. It is surmized that if the shock is sufficiently strong, it will lead to <u>shock to detonation transition</u> (SDT).		

DD FORM 1 JAN 73 1473

EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE(When Data Entered)

During the development of the shock wave, the porous material may collapse into a solid plug of void free propellant because the speed at which the wave propagates increases as the material is compressed. The modeling effort presented indicates how two-phase unsteady combustion processes in granular material can couple to the solid mechanics of shock formation and eventually to a steady-state detonation.

Accession For	
NTIS GRA&I	☒
DTIC TAB	☐
Unannounced	☐
Justification	
By	
Distribution/	
Availability Codes	
Dist	Avail and/or Special
A	



UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE(When Data Entered)

ABSTRACT

This annual report represents the summary of work done on the modeling of processes leading from deflagration to detonation in porous or granular high energy propellants. Particular attention is paid to the analysis of shock development from compression waves forming ahead of confined burning in the original material. It is surmized that if the shock is sufficiently strong, it will lead to shock to detonation transition (SDT).

During the development of the shock wave, the porous material may collapse into a solid plug of void free propellant because the speed at which the wave propagates increases as the material is compressed. The modeling effort presented indicates how two-phase unsteady combustion proceses in granular material can couple to the solid mechanics of shock formation and eventually to a steady-state detonation.

ACKNOWLEDGEMENT

The authors wish to acknowledge the many helpful discussions about this research with scientists from Sandia National Laboratories, Albuquerque, NM, especially Dr. Jace Nunziato, Dr. Mel Baer, Dr. Dennis Hayes, Dr. John Taylor, and Dr. Phil Stanton. Their own work in this field has much application in our own reported here.

1. INTRODUCTION

The purpose of our work over the past year has been to assess the possibility of a detonation occurring in porous energetic materials. In years prior to this, we were able to show [1] that steady detonation characteristics (CJ pressure, CJ temperature, detonation velocity) were obtainable without the stress wave analysis applied to the solid phase. This meant that the rate of flame propagation through the bed was due entirely to the driving gas pressure and not to the shock initiation of the precursor wave. This was referred to by some as the "convective flame model."

In our present work we have developed a six-point outline which summarizes the work in progress and is a base for future research. This partitioning of the entire DSDT (Deflagration to Shock to Detonation Transition) process into six parts has made the more complex problem easier to understand and deal with. The logic followed in developing it was as follows. Compression waves of increasing strength are continually propagating ahead of the flame front and eventually coalesce into a discontinuous shock front. During the development of the shock wave, the porous material collapses into a solid plug of void free propellant. Because the speed at which the waves propagates increases as the material is compressed, the shock wave is at all times increasing in strength. If this shock grows to a large enough strength within the physical constraint (length) of the material being shocked, it may cause detonation by one of several methods to be discussed later in the report.

2. THE MODEL

Shown in Fig. 1 is a schematic representation of the six part DSDT. Superimposed on each figure is a line representing the gas porosity (gas volume/total volume) as a function of bed location. A value of ϕ equal to unity represents a zone of all gas while ϕ equal to zero indicates a homogeneous solid.

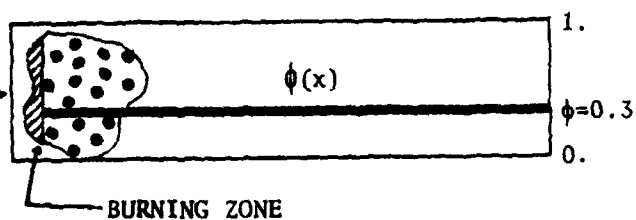
Part A represents the initial blast caused by the ignitor used to initiate DSDT in the bed. In the second portion, the convectively burning porous bed is shown to be pressurizing the region behind the ignition front. This is a result of the product gases being confined by the walls. The porosity variation for this time indicates an all gas makeup in this particular zone. Actually, there is a finite reaction zone where the propellant is decomposing into the product gases. Reference [1] showed that if the reactive material was made of large enough particles, this reaction zone may be very large. This results in a slower pressurization rate of the gas cavity. The significance of this on the shock development will be made clear in Section D.

Illustrated in the last four parts of Fig. 1 is what we refer to as the second possible branch of DSDT, the shock compression branch (also see Fig. 2). This will be expanded on in Sections C through F.

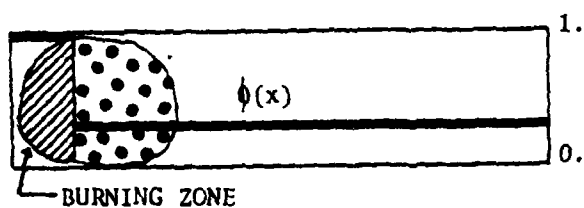
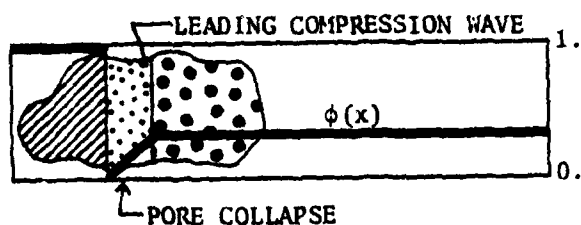
As indicated by Fig. 2, we believe that there may be mechanisms other than shock compression theory. Because we are dealing with a porous mixture, hot gases, as well as stress waves, may be propagated ahead of the flame front. This is untrue when analyzing the case of homogeneous solid where only stress waves can be propagation ahead.

What we refer to as Branch 1 in Fig. 2 could occur if the propellant grains are small enough and their chemical composition energetic enough. In

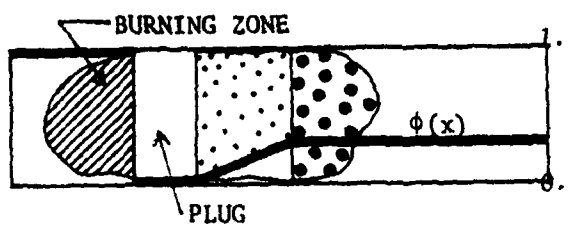
IGNITOR



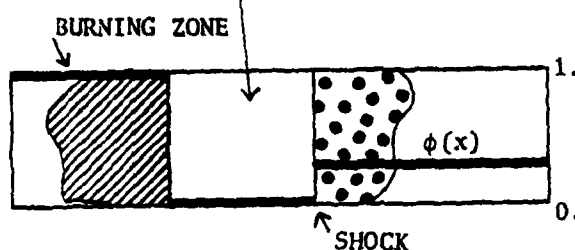
A. IGNITION OF POROUS MATERIAL

B. CONVECTIVE FLAME SPREADING WITH
PRESSURE RISE IN GAS ZONE

C. PORE COLLAPSE



D. PLUG FORMATION



E. SHOCK FORMATION

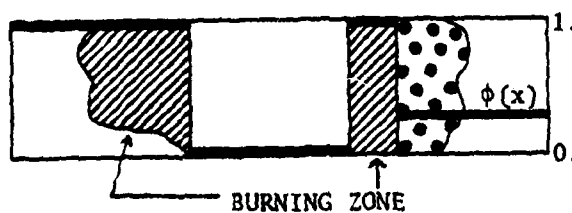
F. SHOCK INITIATION OF POROUS
MATERIAL

FIGURE 1. SIX-PART REPRESENTATION OF DSDT

TWO POSSIBLE MECHANISMS FOR DETONATION IN
POROUS EXPLOSIVES (PROPELLANTS)

UNIVERSITY OF ILLINOIS, URBANA-CHAMPAIGN

1. CONVECTIVELY DRIVEN UNSTEADY DEFLAGRATION

2a) BRANCH I -- STEADY STATE DETONATION

- I) CONVECTIVELY DRIVEN
 - II) HIGH GAS GENERATION
 - SMALL PARTICLES
 - HIGH BURNING RATE
 - III) HIGH ENERGY RELEASE
 - IV) TIGHTLY PACKED
 - MODERATELY LOW INITIAL POROSITY
 - V) NO SIGNIFICANT DEFORMATION OF SPHERICAL PARTICLES
- RESULTS REPORTED: BUTLER/FRIER, COMBUSTION AND FLAME,
Vol. 44, MARCH 1982.

2b) BRANCH II -- WORK IN PROGRESS: AFOSR 81-0145

- I) PARTICLE DEFORMATION AND BREAKUP
- II) PORE COLLAPSE - LIMIT OF ZERO PERMEABILITY
- III) PRESSURE BUILD-UP BEHIND PLUG
- IV) STRESS HEATING OF SOLID MATERIAL BY COALESCING SHOCKS AND HOT SPOT GENERATION
- V) DETONATION BY SHOCK INITIATION

FIGURE 2. DSDT FLOW CHART

this branch, the rate at which the flame burns or regresses through the open propellant structure may have detonation characteristics.

This rapid deflagration is not the same as the steady-state open ended deflagration described in textbooks dealing with reactive gas dynamics. But because the ends of the chamber are closed and the energetic propellant provides for a rapid enough pressure rise, the flame accelerates through the first portion of the bed.

The above paragraphs have given a brief description of the DSDT phenomenon as we interpret it. The following sections will expand upon our knowledge in each of the six steps in more detail. A short discussion on the different mechanisms causing heating at a shock front will then be presented. The final topic will be the governing equations and how they are modified for each of the six different parts.

2.A IGNITION PROCESS

Our model is a one-dimensional analysis of a porous propellant bed of a constant cross-sectional area and variable length, which attempts to model the apparatus of some experiments [2,3]. A uniform initial porosity (gas volume/total volume) of 0.2 to 0.3 is used to represent a packed sphere configuration. Except at the ignitor face, pressures and temperatures are at atmospheric levels throughout the bed. For our present work, the ignition is assumed to occur at the plane located at $x = 0$ where the gas and particle temperatures are increased to appropriate levels. In our future work, we plan to investigate initial pressure disturbances created by the ignitor blast and the effect they have on the DSDT process.

2.B CONVECTIVE FLAME SPREADING

Once the ignition process is analysed, the next logical step is to study the convective flame spreading through the energetic material. For this part, the past work of Butler, Lembeck, and Krier is used [1].

Once ignited, the decomposition of individual particles is modeled as a pressure-dependent regressive burn. Conservation of mass requires the mass of solid burning to be transferred into the gas phase and conserved throughout the entire control volume. The confined product gases cause the local gas pressure to rapidly increase behind the ignition front and as a result of the pressure gradients developed, hot gases are driven forward through the unreacted porous material. The voids in the propellant allow this to happen where in a homogeneous material it would act to only further compress the product gases.

Convective heat transfer from the product gases to the unreacted propellant causes ignition of the energized propellant; the process repeats itself as the gas pressure continues to increase. It is this high pressure gas zone which acts as a driving force for the stress waves being propagated into the solid ahead.

The effect of the compression wave is shown in Fig. 1C. At this time the leading compression wave has traveled into the porous solid a distance, Δx . In the region between the leading compression wave and the flame front the porosity decreases because of the increasing strength of the compression waves. It will be shown in the next section that the porosity is directly related to the local stress by a pore collapse model or a pressure-solids fraction ($P - \alpha$ where $\alpha = [1 - \phi]^{-1}$) law.

The analysis of a nonhomogeneous flow problem involves the introduction of a new unknown into the problem, the porosity (or mass fraction). The

porosity of the mixture can have any value between unity (all gas) and zero (all solid). To form closure to the system, an additional independent equation is necessary. A possible equation to fulfill this requirement would be a porosity-pressure relation, one particular equation was the pore closure model of Carroll and Holt [4]. The next section will outline this relation.

2.C PORE COLLAPSE

The compression of the porous matrix was modeled by Carroll and Holt as a hollow sphere where the inner and outer radii are such that the pore diameter and the overall void fraction are those of the porous mixture [4]. The use of such a model to represent a granulated bed of propellant spheres (the inverse problem) has not been clearly justified and the possible errors associated with it should be considered.

Pore collapse occurs in three distinct phases. Phase 1 is the elastic region, Phase 2 is the elastic-plastic region, and Phase 3 is the plastic region. Phase 1 applies until the pressure has become large enough to cause plastic deformation at the inner radius. The change in porosity is very small during this stage. The second phase or the elastic-plastic region occurs as plastic deformation begins at the inner radius and propagates outward to the outer radius. As in the elastic region, the porosity change in the elastic-plastic region is very small. It is during Phase 3, where plastic deformation occurs throughout the solid material, that significant porosity changes occur.

The $P - \alpha$ (pressure- α) relations were derived by Carroll and Holt by solving the momentum equation with an imposed time-dependent hydrostatic pressure $P(t)$ at the outer radius and a zero pressure condition at the inner radius [4]. A volume preserving deformation assumption is also used. This requires the solid to be incompressible during the pore collapse.

Modifications were made by Kooker and Anderson [5] to include a porosity dependent yield stress (i.e., strain hardening) and a rate dependent resistance to pore collapse due to material viscosity. The equations for each of the three phases for this dynamic model can be found in Ref. [5].

When the spherical pore experiences a rate of pressurization less than 10 kbar/ μ sec, a much simpler static pore collapse model can be used. This was also presented by Carroll and Holt [4]. For this model, the inertia and viscous terms in the governing equations are removed and the remaining equation is,

$$P(t) = P_{eq}(\alpha) + P_{vo} \left[\frac{(\alpha_0 - 1)}{(\alpha - 1)} \right]^\gamma. \quad (1)$$

The left side of Eq. (1) represents the pressure applied externally to the sphere. The term $P_{eq}(\alpha)$ is the equilibrium stress field for the material and is different for each of the three phases of compaction. The last term is an internal resistance due to isentropic compression of the trapped gases. Gamma (γ) is the specific heat ratio of the trapped gas.

A further assumption is made that no change in porosity occurs during the elastic phase or the elastic-plastic phase. This was shown to be true when the ratio of yield strength to shear modulus is small and the initial alpha, α_0 , is not close to that of all solid ($\alpha = 1.0$).

With this assumption, the P - α relation reduces to a single equation for the plastic phase:

$$P(t) = 2/3 \gamma \ln \left(\frac{\alpha}{\alpha_0} \right) + P_{vo} \left[\frac{(\alpha_0 - 1)}{(\alpha - 1)} \right]^\gamma \quad (2)$$

where the transition pressure is approximated to be:

$$P_{crit} = 2/3 Y \ln \left(\frac{\alpha_0}{\alpha_0 - 1} \right) + P_{vo} \quad (3)$$

and Y = yield stress, α = total volume/solid volume = $(1 - \phi)^{-1}$.

In summary, $\alpha = \alpha_0$ for $(0 < P < P_{crit})$, $\alpha = f(P(t))$, by Eq. (2) for $(P > P_{crit})$ with the following assumptions,

- (1) A porous bed can be modeled by hollow spheres;
- (2) The solid material is incompressible during the pore collapse;
- (3) Very little porosity changes occur during the elastic and elastic-plastic phases; and
- (4) Dynamic effects can be neglected.

Figure 3 shows the static model for the pore-collapse with initial alphas of 1.2, 1.4, 1.6, and 1.8. The elastic and elastic-plastic transition pressures are shown with the dashed lines.

The pressure required for complete collapse can be seen from Fig. 3 to be relatively small compared to the pressure generated in the burning zone; thus, it is anticipated that complete pore collapse will occur when the compression waves reach a moderate strength (1 to 2 kbar). This leads to our fourth step, Plug Formation.

2.D PLUG FORMATION

As stated in Section 2.C, the particle stress to fully compact the explosive, HMX, is of the order of several thousand atmospheres. A gas pressure of this magnitude will be attained in a very short time in the confined zone behind the flame front. This critical stress is transferred to the solid (constant pressure boundary condition) and transmitted through the bed at the local sound velocity plus particle velocity. The bed then

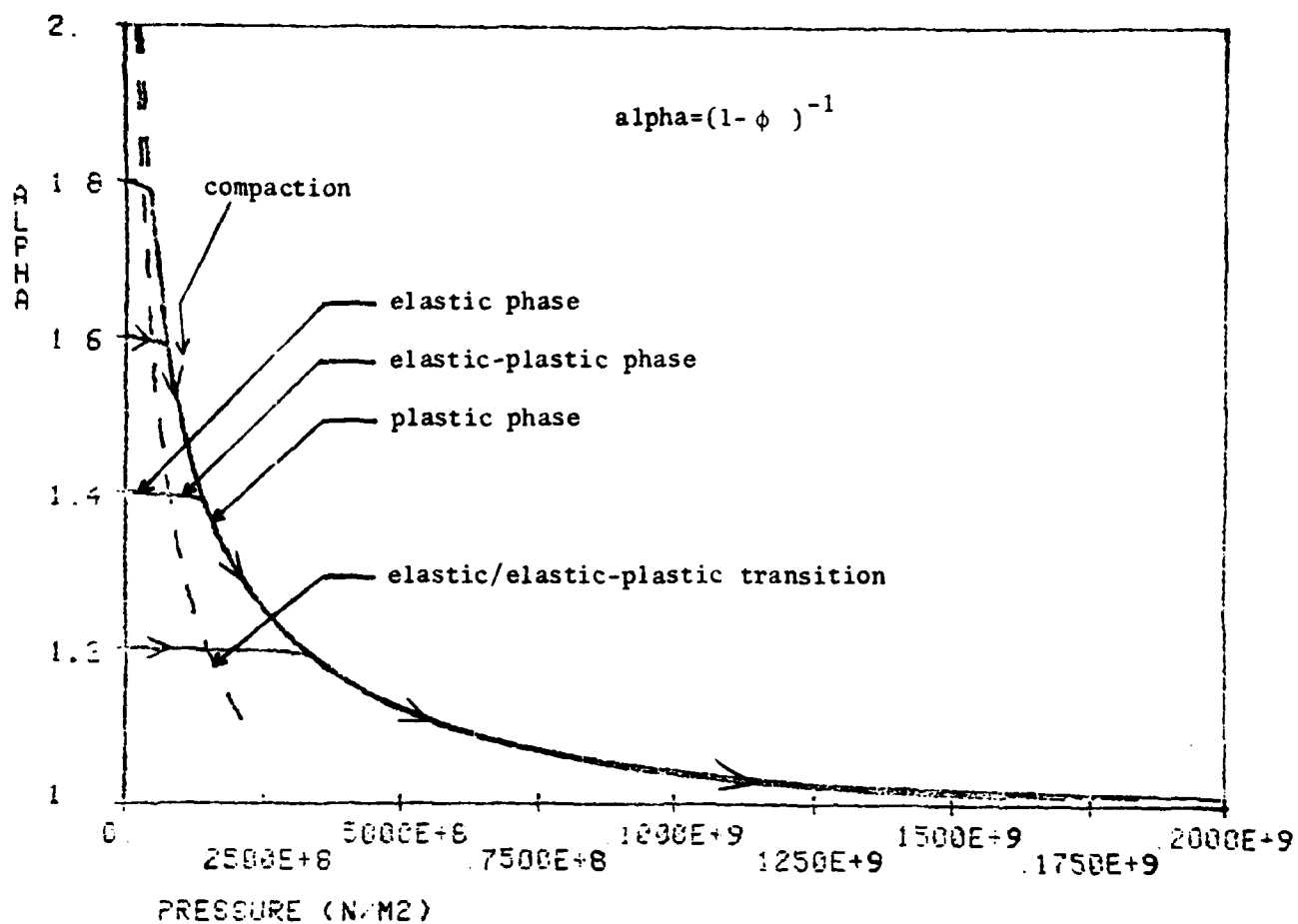


FIGURE 3 : Porosity (ALPHA = VOL.TOTAL/VOL.SOLID) versus pressure from the static "pore collapse" model, including the three phases of compaction (elastic, elastic-plastic, plastic), for HMX ($\rho_0 = 1.9$ g/cc, $Y_0 = .517$ kBar, $G_0 = 35.16$ kBar).

collapses as the wave passes over, starting at the flame front and progressing forward (away from the products zone), forming the solid plug. This was shown in Fig. 1d. Since the high pressure gas zone can no longer drive hot gases through the permeable solid, it pressurizes at even a higher rate.

For our present analysis, the solid material is assumed incompressible during the pore collapse process. In addition, we do not treat any type of frictional heating associated with the pore-collapse. Shear heating may be an important aspect and we intend to investigate it in the year ahead. When we do, it will probably yield a rate of pressurization dependency.

2.E SHOCK FORMATION

At this point, the stress waves which formed the solid plug have coalesced into a shock front traveling through the porous medium. This is analagous to the piston problem where stress waves sent out by a piston traveling in a closed tube eventually overtake the lead wave and develop a discontinuity or shock front.

The shock in the porous bed forms a boundary between two distinct zones. In front of the shock, the material is undisturbed from its initial state. Behind the shock, the pores have collapsed and the solid matrix is compressed to some final state (P_B, v_B). The pore collapse and solid compression occur within the thickness of the shock wave and are, therefore, assumed to occur instantaneously. This process is discussed below.

In addition to the two zones mentioned above, there is still the third (product gas) zone immediately behind the plugged zone. Since the product gases are now completely confined (due to the wall and solid plug) they continually transmit stronger stress waves over time, which act to reinforce the already developed shock wave traveling ahead of it. The reason for the

reinforcement of the shock wave, as in the piston problem, is the property of the medium to increase the local sound velocity as it is compressed. Because of this, each successive stress wave travels at a faster speed than the one prior to it, and eventually, they reach the shock and strengthen it.

2.F.1 SHOCK INITIATION OF POROUS MATERIALS

Past experiments have shown that most solids obey a linear shock velocity-particle velocity (U_S, u) relation for the shock strengths of interest to us. That is, the relation,

$$U_S = A + Bu \quad (4)$$

is a fairly good description of experimental data available for most materials. Here, A and B are constants dependent on the material being shocked. In the limit of an infinitesimal pressure disturbance (sound wave), the particle velocity (u) approaches zero and the constant A is then found to be the adiabatic sound velocity, c_0 . The constant B has no physical significance other than the slope in the $U_S - u$ plane.

The linear form of Eq. (4) makes it convenient for developing other important relations. Using it in conjunction with the shock Hugoniot jump conditions, one obtains an equation relating Hugoniot pressure, P_H , to specific volume, v , namely,

$$P_H = \frac{A^2 R}{v_0 (1 - AR)^2} \quad (5)$$

where $R = 1 - v/v_0$. In Eq. (5), the subscript H is in reference to the end states along the Hugoniot and the subscript o represents the initial conditions, also on the Hugoniot line.

Reference [6] is a compilation of shock data for numerous inert and reactive solids. In this reference, the U_S - u data for each material is fit with a straight line, i.e. Eq. (4). It should be noted that while the curve fits for the inert solids and liquids involve many data points, some of the highly reactive explosives (HMX,RDX) have only two or three scattered points through which a straight line is fit.

Figure 4 shows the effect that a 20 percent change in the slope of a U_S - u line has on the P - v and T - v relations, the method for determining $T = T(v)$ will be discussed shortly.

Equation (5) represents only the end states obtained through a shock process. In other words, only those states with the pair (P,v) on the Hugoniot. In order to represent all states possible rather than just the jump conditions, a more general Mie-Gruneissen state equation is used, i.e.,

$$P(v,E) = \frac{\Gamma}{v} e + \frac{A^2}{v_0} \frac{(1 - \frac{\Gamma}{2v} (v_0 - v))}{(1 - BR)^2}. \quad (6)$$

One can see by substitution that if the general state equation (Eq. (6)) is evaluated along the Hugoniot ($e = e_H = 0.5 * P_H * (v_0 - v)$), then Eq. (6) becomes the same expression as Eq. (5).

In Eq. (6), Γ is the Gruneissen coefficient defined as $\Gamma(v) \equiv (\partial P / \partial e)_v$. Using $\Gamma/v = \text{constant}$ appears to be a reasonable assumption for shock compressions valid up to $v_0/v = 1.50$. This will be important in determining the temperature rise due to shocking a material.

The process of shock initiating a homogeneous solid will be described with the aid of Fig. 5. Here, the solid material is initially at rest, represented as state o. As the shock fully traverses, a point on the material, it is compressed to state B. The path process between states o and

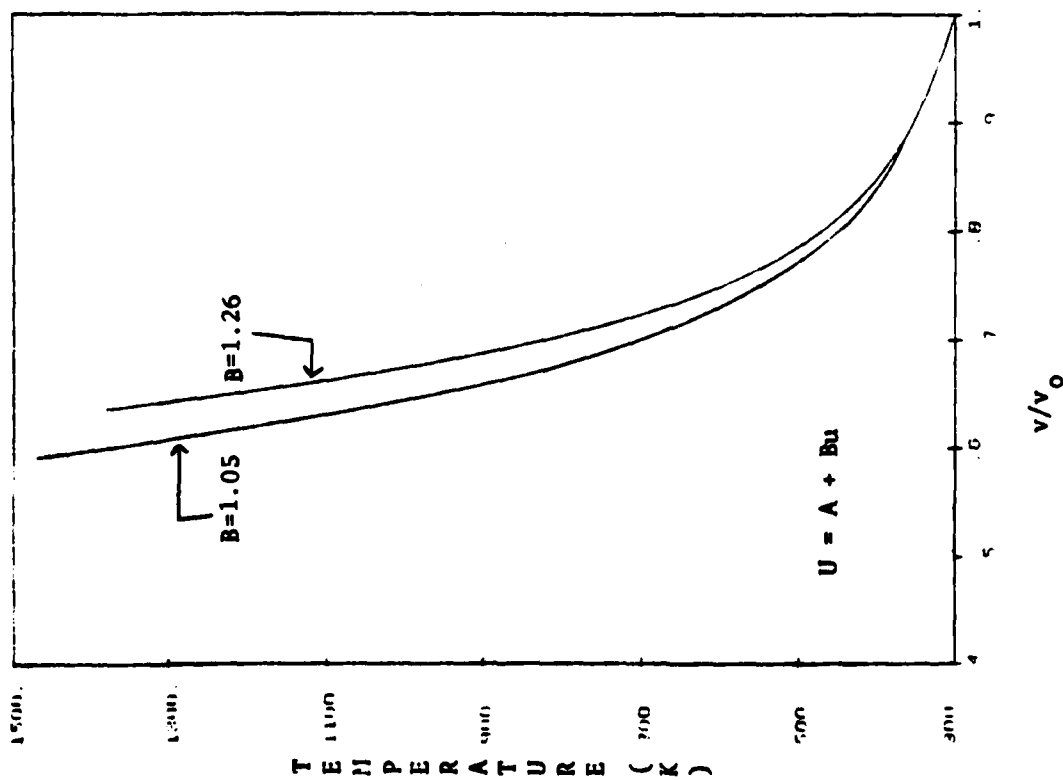


FIGURE 4a. Temperature-Specific Volume for HIX.

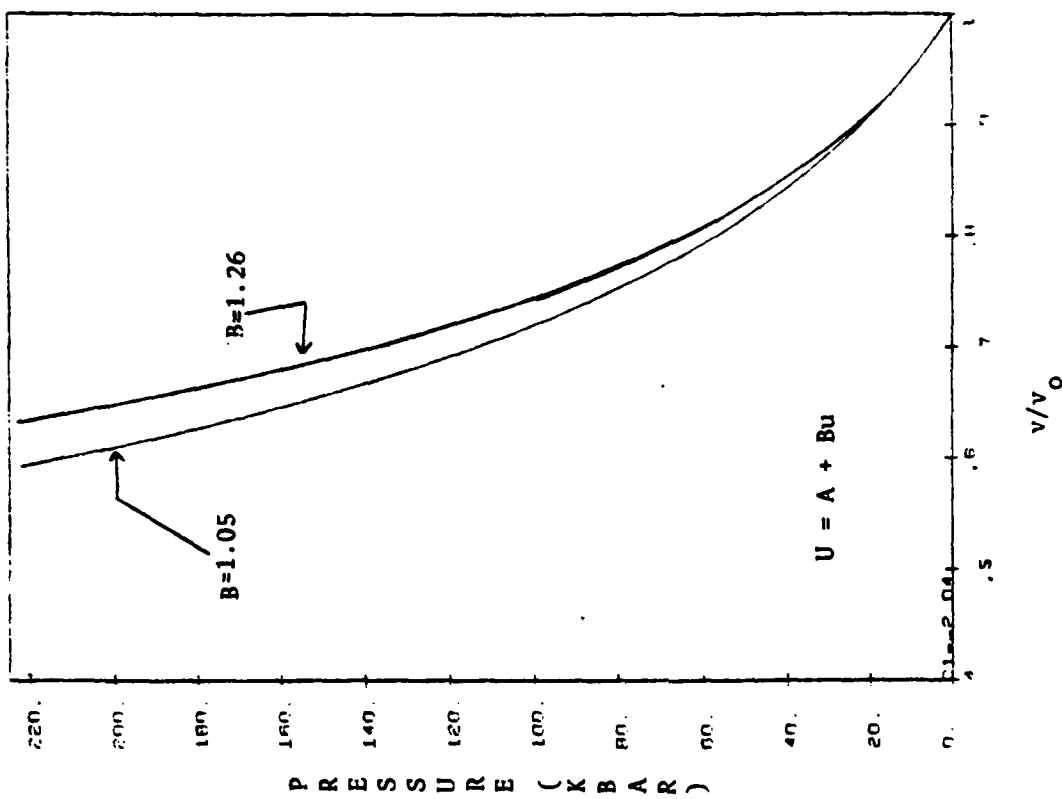


FIGURE 4b. Pressure-Specific Volume for HIX

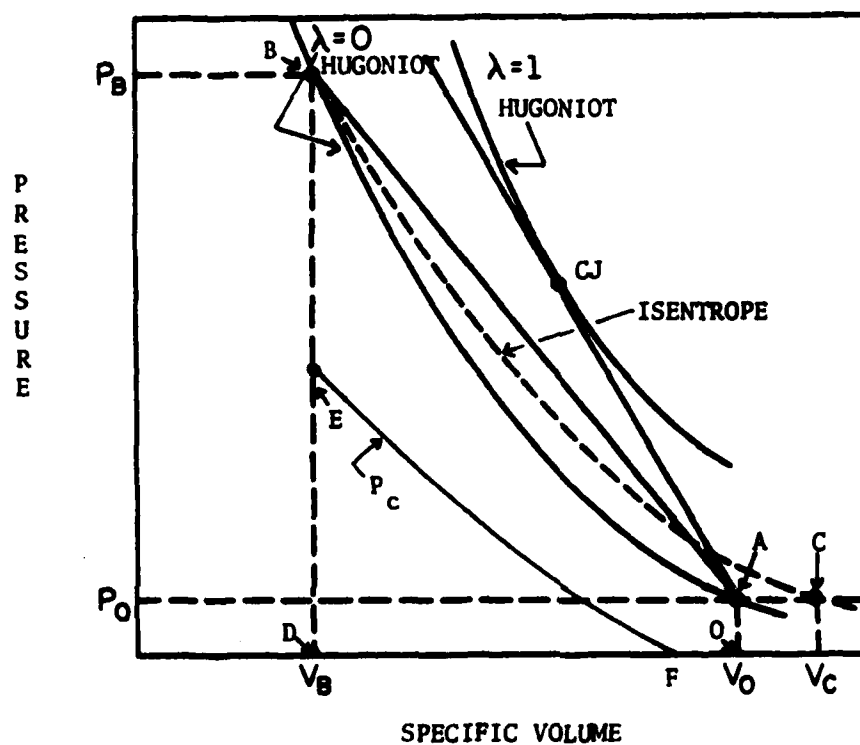


FIGURE 5. Hugoniot for unreacted($\lambda=0$) and fully reacted($\lambda=1$) explosives

B is not necessarily along the Hugoniot. The Hugoniot is only a locus of end points and not a path.

If the material was an inert solid or liquid and the shock wave was only a short pulse, followed by an expansion wave, the shocked inert material (state B) would expand back to the original pressure, P_0 , along the isentrope shown and have the end state (c). However, when a reactive material is shocked to state B, the energy increase associated with the shock wave will cause some degree of chemical decomposition. If the amount of energy is sufficient to support the full decomposition, the products will reach equilibrium at state CJ, the Chapman-Jouget point. Here, λ , the degree of reaction is unity representing complete reaction. The process of increasing the energy of a homogeneous solid through the shock wave will be discussed in the next section, followed by a description for treating porous materials.

2.F.2 TEMPERATURE INCREASE DUE TO SHOCK WAVES

The method used for determining temperature increases due to shock waves is that of Zel'dovich and Raizer [7] and involves the partitioning of energy and pressure into three separate components.

The first component of pressure is due to the interatomic potential and is referred to as the elastic or cold term. At zero degrees Kelvin and one atmosphere pressure, the atoms neither repel or attract one another and at this point the elastic pressure is zero. The volume occupied by the solid at this point, V_{0c} , is slightly less than the volume occupied by the same mass of material at room temperature. Because the solid thermally expands when heated from 0°K to 300°K, the solid actually has a negative pressure (attractive interatomic force) at ambient conditions. As the material is compressed, either isentropically or irreversibly in a shock-like process, the atoms repel

one another and therefore contribute to the elastic pressure in a positive sense. The elastic component of the total energy is related to the elastic pressure through the work-energy relation,

$$P_c dv = -de_c \quad (7)$$

where the subscript c is in reference to the elastic or cold component of the total internal energy, e, or total pressure, P. The name cold energy or pressure has significance in that the elastic pressure-volume relation can be shown to be the 0°K isotherm and also the S = 0 isentrope.

The second and third components of the energy are due to the atomic and electronic motions, respectively. The electronic terms, e_e and P_e , are only of significance above approximately 10,000°K and hence outside the regime of the processes encountered here.

The thermal component of energy represents the harmonic oscillations of the atoms and is expressed as

$$e_T = C_v (T - T_0) + e_0. \quad (8)$$

To determine the thermal pressure from the thermal energy, e_T , the first law of thermodynamics and a Maxwell relation are used to obtain

$$\left(\frac{\partial e}{\partial v}\right)_T = T \left(\frac{\partial P}{\partial T}\right)_v - P. \quad (9)$$

This is a general equation applicable to both components, elastic and thermal. Since the cold pressure is only a function of volume (or more specifically interatomic distance, then $P_c = P_c(v)$ and Eq. (9) gives

$$P_c = - \frac{de_c}{dv}$$

the same expression as given prior to this, Eq. (7), in the work-energy analysis. For the thermal component,

$$P_T \equiv C_v T \left(\frac{\partial P_T}{\partial e_T} \right)_v. \quad (10)$$

Equation (10) can be expressed in terms of the thermodynamic derivative $\Gamma(v)$ (the Grüneisen coefficient) as

$$P_T = \Gamma(v) \frac{C_v T}{v} \quad (11)$$

where, as stated earlier, $\Gamma(v) = v \left(\frac{\partial P}{\partial e} \right)_v$. The Grüneisen coefficient, as expressed here, is a measure of the change in thermal pressure to thermal energy.

Equations (7), (9) and (11) are solved in addition to the algebraic component relations,

$$e = e_c + e_T \quad (12)$$

$$P = P_c + P_T \quad (13)$$

and the Hugoniot jump conditions,

$$e = e_H = \frac{1}{2} P_H (v_0 - v) \quad (14)$$

to generate the cold compression curve shown in Fig. 5. For this particular case, the ratio Γ/v is assumed to be constant. Figure 5 shows graphically how each component of energy is represented. The area $ABDOA$ is the total increase in internal energy due to shock pressure, P_B . Of the energy deposited by the shock, the area under the curve FED goes into the potential or elastic energy. The remaining area $ABEFOA$ is the contribution to the thermal component and therefore determines the temperature rise associated with the shock.

3. POROUS MATERIALS

The analysis for determining the temperature rise in a shocked porous material is somewhat similar to that discussed in Section 2.F.2 except the initial volume is now V_{00} , larger than the homogeneous initial volume, V_0 . The additional initial volume is occupied by the gases internal to the pores, usually assumed to be air or more simply a vacuum.

Since the shock energy is essentially the product of one-half the change in volume of the material times the shock pressure, a porous material shocked to the same final volume as a homogeneous material will have more energy deposited to it than the homogeneous solid. The elastic curve is the same for both cases, so the material which was initially porous will be shocked to a greater thermal energy, and thus higher temperature than the homogeneous solid.

4. COMPRESSIVE WAVES

In investigating the possibility of shock formation in a porous bed due to coalescence of compression waves, we have extended Macek's concepts and application of the method of characteristics [9]. The requirement of a high pressurization rate or the need to justify a proposed method to increase surface area is not needed when considering porous propellants, as was required to explain the large exponential pressure rise (used by Macek) in order for shock formation to occur in a homogeneous solid. Large surface area is present due to the nature of a porous material and the high pressurization rates required to form shock waves in a solid are not needed to form a shock wave in a porous material.

The first phase of this work is a mathematical model of a porous bed subjected to an imposed pressure gradient at one end. The method of characteristics is used (as Macek utilized) to determine if shock formation from the coalescence of compression waves is possible in a porous mixture. If shock formation is found to be possible, the rate of pressurization required to cause shock formation within reasonable distances is determined. Figures 6a and 6b show a sample case run for aluminum. A second phase of this study will then be to assess whether such a pressure rise is possible within the burning zone.

In addition to employing the method of characteristics, work is in progress on a numerical solution of the full hydrodynamic equations governing the stress wave build-up. The system of equations governing the flow is solved by utilizing a Lagrangian finite difference technique with the necessary artificial viscosity to handle the severe gradients associated with the shock development.

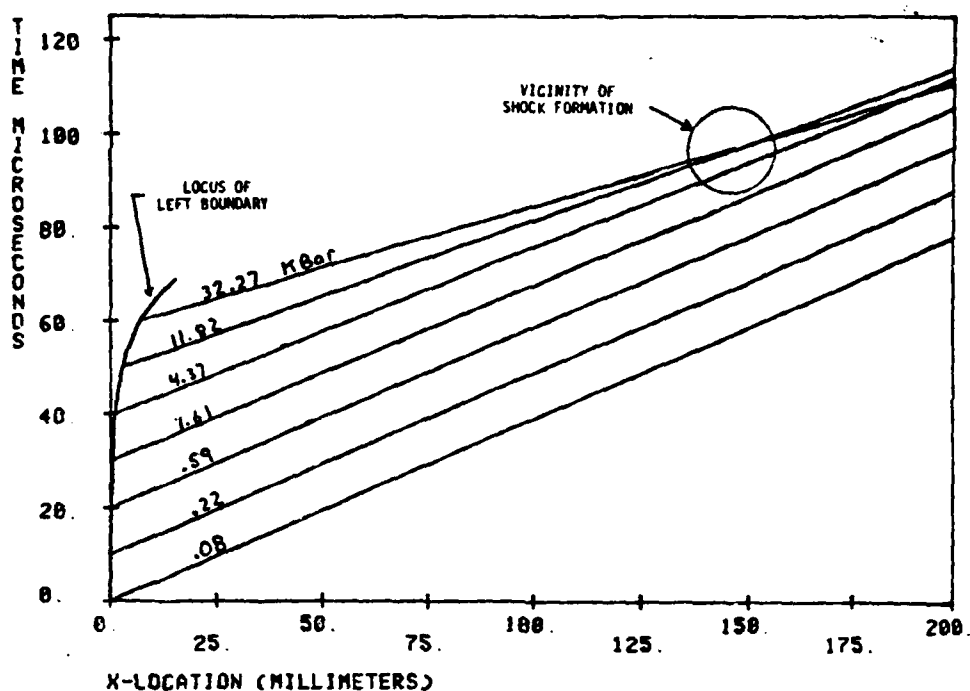


Figure 6a. Characteristics diagram demonstrating the shock formation in a solid (Aluminum, $\rho_0 = 1.6 \text{ g/cc}$, $C_0 = 2.56 \text{ mm}/\mu\text{sec}$) due to compression waves generated by an exponential pressure rise ($P = .08e^{.1t}$).

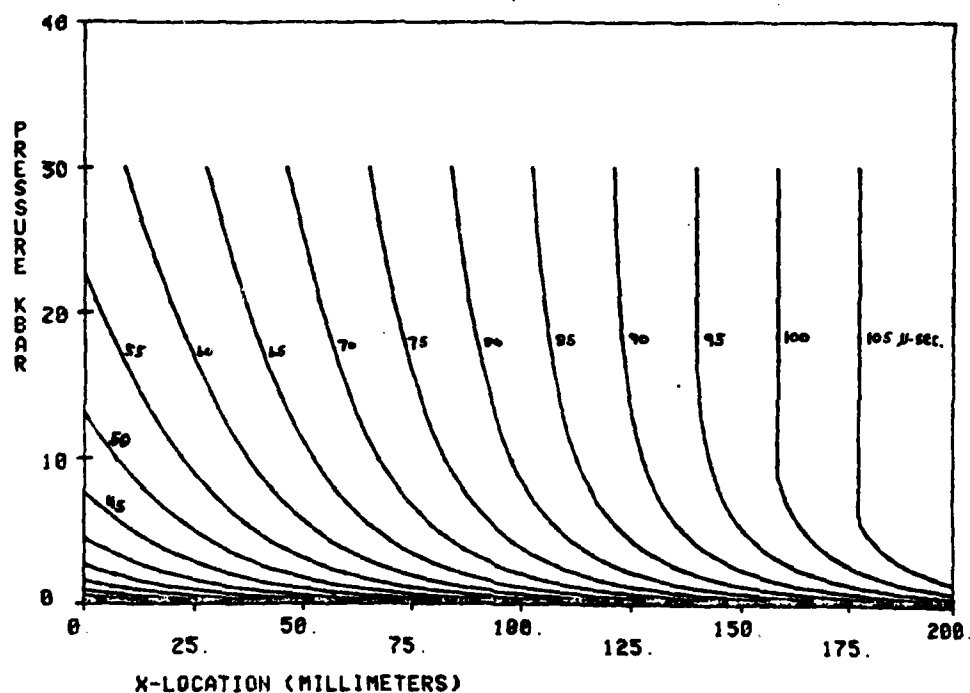


Figure 6b. Development of shock wave (calculated from the characteristics).

5. HOT SPOTS AND FRICTIONAL HEATING

Section 2.F showed by using classical shock hydrodynamics how the temperature rise due to a shock was calculated for a homogeneous and non-homogeneous material. Here, the energy associated with the shock wave was balanced by the interatomic potential and thermal energy of the solid. The porous material was shown to have a greater increase in temperature for a given shock strength.

Since experiments have shown that explosives with internal voids shock initiate at lower impact velocities (lower shock pressures) than homogeneous explosives, the idea of localized heating or "hot spots" is a topic of current interest. This means that there may be additional mechanisms to explain the initiation of porous explosives beyond the rise in bulk temperature due to its porous nature.

Hayes [8] presents a model for preferentially depositing a fraction of the shock energy to a certain portion of the material (proportional to the initial void fraction) and depositing the remaining energy to the bulk material. The bulk material is assumed to be compressed isentropically while the hot spots are compressed irreversibly. This leads to two distinct temperatures in the material.

Frey [10] focuses on the heating of porous materials due to friction of particular interest to us in his extension of the work by Carroll and Holt to determine the temperature rise at the interior of the pores at different pressure rise times. This analysis is important in determining whether or not a reactive material will ignite upon pore closure.

6. CONCLUDING COMMENTS

This brief report has provided information on the inter-connected, fluid and solid mechanical processes that must be described if one is to understand the mechanism for deflagration to detonation transition (DDT) in porous propellant explosives. It is clear that there remains considerable work to be done, not the least of which is to solve the unsteady shock reactive flow conservation equations. An extensive "hydro-code" is being developed to numerically solve the battery of equations which contains the system.

Whenever possible, information from the latest reported data is utilized to formulate the many constitutive relations required for closure. We expect to present useful predictions for DDT (and DSDT) in porous reactive solids based on work continuing on our continued AFOSR supported work.

7. REFERENCES

1. Butler, P. B., M. L. Lembeck, and H. Krier, "Modeling of Shock Development and Transition to Detonation Initiated by Burning in Porous Propellant Beds," Combustion and Flame, 46: 75-93 (1982).
2. Bernecker, R. R., and D. Price, Combustion and Flame, 22:111 (1974).
3. Campbell, A. W., "Deflagration-to-Detonation Transition in Granular HMX," 1980 JANNAF Propulsion Systems Hazard Subcommittee Meeting, pp. 105-130, Monterey, CA, October 29-30, 1980 (P/A Publication).
4. Carroll, M. M., and A. C. Holt, "Static and Dynamic Pore-Collapse Relations for Ductile Porous Materials," J. Appl. Physics, Vol. 43, No. 4, pp. 1627-1636 (1972).
5. Kooker, D. E., and R. D. Anderson, "A Mechanism for the Burning Rate of High Density, Porous, Energetic Materials," Seventh Int. Symp. on Detonation, Annapolis, Maryland, June 16-19 (1981).
6. Marsh, S. P., LASL Shock Hugoniot Data, University of California Press, Berkeley, California (1980).
7. Zel'dovich, Ya., B., and Yu. P. Raizer, Physics of Shock Waves and High-Temperature Hydrodynamic Phenomena, Academic Press, New York and London (1966).
8. Hayes, D. B., "Shock Induced Hot-Spot Formation and Subsequent Decomposition in Granular, Porous Hexanitrostiblene Explosive," Detonation Physics Symposium, Minsk, Russia.
9. Macek, A., "Transition from Deflagration to Detonation," J. Chem. Phys., 31, 162-167 (1959).
10. Frey, R., "The Initiation of Explosive Charges by Rapid Shear," Proc., 1980 JANNAF Propulsion Systems Hazard Meeting, CPIA No. 330, Vol. II (Dec. 1980).

Last Page