T.&A.M. Report No. 495

Discrete Modeling of Beds of Propellant Exposed to Strong Stimulus*

D. Scott Stewart
Theoretical and Applied Mechanics
University of Illinois, Urbana, Illinois

Blaine W. Asay
Los Alamos National Laboratory
Los Alamos, New Mexico

Abstract

This paper is a description of experimental and theoretical modeling concepts that are being developed to describe the behavior of confined propellant beds made of discrete particles, when subjected to a strong stimulus such as the impact of a penetrating jet. A principal goal is to discover basic mechanisms within the bed that control a reactive wave that either fails and extinguishes, or propagates as a rapid burning or detonating wave. This paper is an extended version of a lecture given by D. S. Stewart at the Institute for Mathematics and its Application in November of 1989.

Introduction

In the Spring of 1987 at the "Workshop on High Mach Number Combustion" at the Cornell Mathematical Sciences Institute, Toshi Fujiwara (of the University of Nagoya Japan), described an experiment which he called, "Bubble Detonation", [1]. In this experiment, a series of bubbles filled with premixed Hydrogen-Air mixture, were generated in a vertical tube and rose due to buoyancy, with a characteristic separation distance.

*To appear in Dynamical Issues in combustion Theory, Volume 35 in the series IMA Volumes in Mathematics and Its Applications, Fife, Linan, Williams, eds., Springer Verlag.

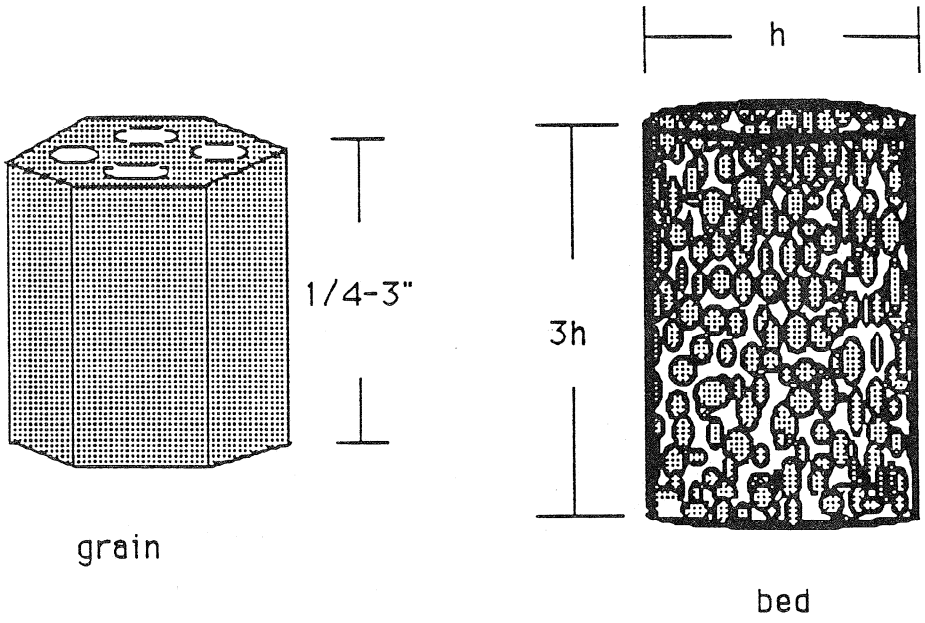

Figure 1: An example of a typical explosive grain and a propellant bed.

At some point a bottom bubble was ignited and its subsequent combustion generated a forward pressure wave that (presumably) had sufficient strength to develop into a shock, which in turn collided with the next bubble in the chain and caused its collapse and ignition. In this way, at least temporarily, a self-sustained chain reaction was created with an identifiable average velocity for the lead disturbance along the chain. This type of phenomena, when the detonation leaps from separated reactant sources is known in the explosives literature as *sympathetic detonation.*

Later that summer Blaine and his colleagues, John Ramsay and John McAfee at Los Alamos National Laboratory (LANL), introduced me to a problem of interest to the Army which involved a canister of large-grain gun propellant. Each grain of gun propellant is actually composed of a mixture of propellant ingredients (Nitramines, binders...) which is made into a paste, extruded, cut into chunks and solidified into pellets. The grains have an overall characteristic average dimension ranging from 3/4 to 3 inches and have small tubular openings throughout their interior. Propellants are specifically designed (empirically) to burn quickly at high pressure and temperature, and are difficult to detonate as individual grains.

A typical propellant bed, is formed by pouring the grains into a canister

with an aspect ratio of 3 to 1 and the grains are sized so that approximately 10 grains fit across the side. On the order of 10^3 to 10^4 grains may make up the entirety of the bed.

A safety issue for propellant use requires that the propellant and the bed be designed to avoid detonation in response to a high pressure, high temperature impact. Such low vulnerability propellant is called *LOVA*. It is difficult or nearly impossible to initiate a detonation in an individual grain of propellant. However, large collections of grains in a propellant bed can sustain a high order detonation, with pressures on the same order as a detonation in a homogenous explosive made from the propellant mixture.

A representative experiment carried out by Asay and his colleagues is shown in Figure 2. A copper or plexiglass tube, 2 inches in diameter, 10 inches long, (say) is loaded with propellant grains. A steel *witness* plate is placed at the bottom of the tube and a detonator is attached to a booster pad of PBX 9501 explosive at the top of the tube. A strong shock, (with pressures on the order of 100 Kilobar, (from the denotation in the PBX) is sent into the propellant bed. The sides of the tube are instrumented with shock pins so that the shock arrival time can be determined at the pins and $x - t$ records of the shock propagation along the tube length can be constructed. The witness plate is recovered and it shows that high order detonation has occurred when indentations of the propellant chunks, having been pushed into the steel, are found like the fossil marks of the Trilobites that perished in the preCambrian mud.

Initiation experiments on propellant beds also show that when detonations occur, they exhibit behavior that while, non-ideal, is more common to, purer, homogenous, condensed phase explosives. For example, a *diameter effect* curve can be found for the detonating propellant bed. The diameter effect measures how the steady detonation velocity varies with the radius of the tube. An explosive is said to be *ideal* if there is no variation of the detonation from its planar, Chapman-Jouguet value, with the radius of the tube. Although a well-defined and reproducible diameter effect curve is found, mimicking the performance of a homogeneous explosive, the beds exhibit extreme, non-ideal behavior, with the lowest recorded detonation velocity being as low as 30% to 40% of the highest, [2].

In addition, it is possible through the use of flash radiographs, to visualize the detonating propellant bed. A ragged detonation shock front is observed and the organized reaction front is perhaps 5 to 10 grains deep as measured

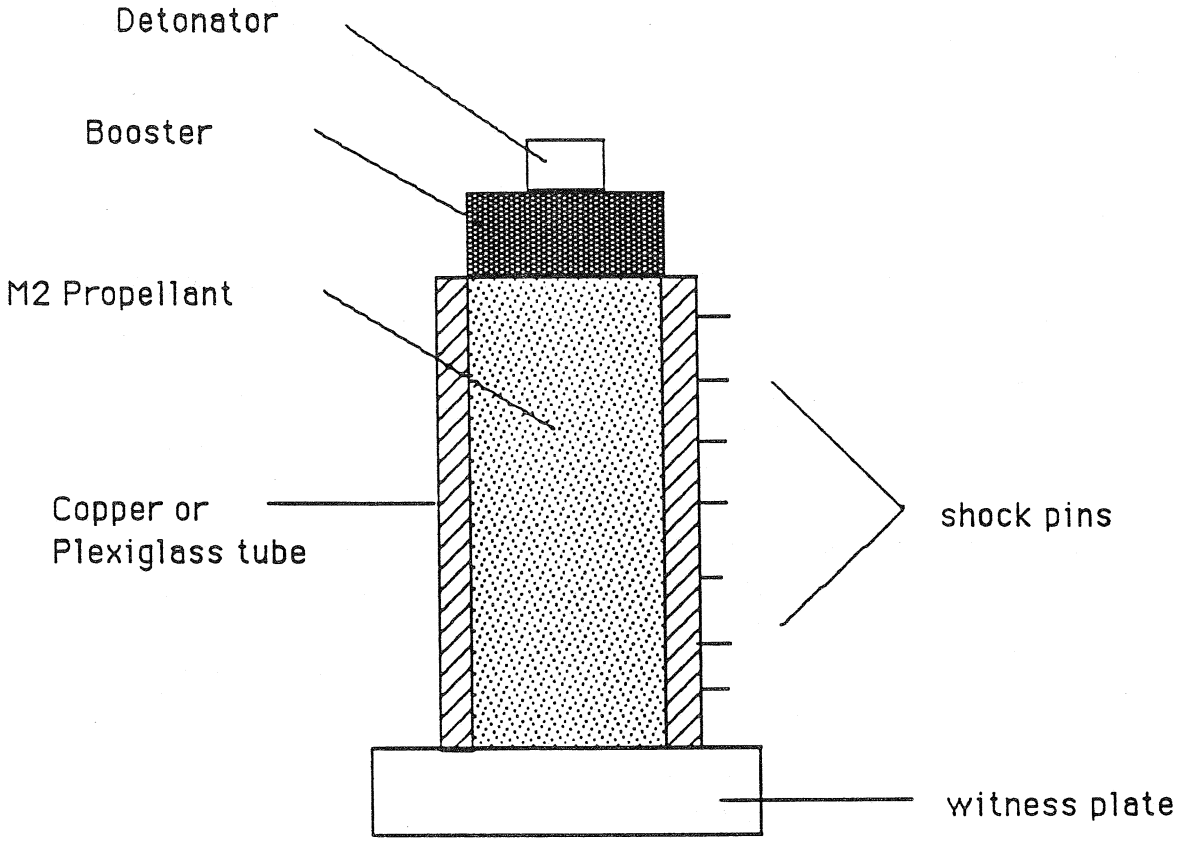

Figure 2: Schematic of a representative experiment.

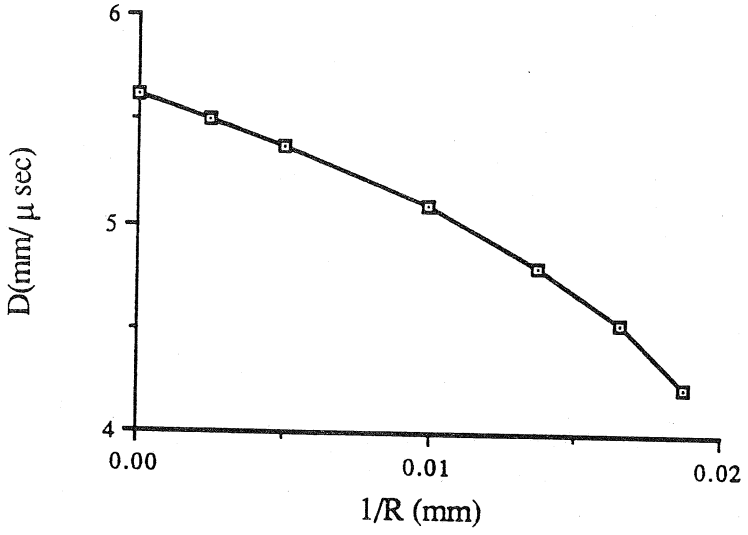

Figure 3: A representative diameter effect curve for a JA2 propellant bed.

from the lead front.

Thus our goal is to develop a systematic framework in which to model the interactions of a bed of propellant grains for specific experiments from a discrete viewpoint. The model of the bed should ultimately be two or three - dimensional and should have on the order of 10^3 to 10^4 grains within it. A particular question that we are trying to answer is, "What are the basic mechanisms that causes a reactive wave, within a discrete system, to propagate or fail?"

We have focused on the discrete character of the system, since we believe the phenomena of interest is the result of the interactions of the individual ignition, burning and expansion events at each grain. Since the events that can be measured are on the order of the scale of the grains and of the dimensions of the bed itself, use a of continuum mixture theory for this problem is not an entirely consistent approach. However, it may be a complementary approach and I will say more about this below.

There may be implications from the results of this kind of discrete study for a much larger class of explosive materials. For example a high grade explosive like PBX 9501 is pressed into macroscopic pieces, from fine powders. When a detonation occurs in this material, it has a relatively short reaction zone, with as few as a 10 to 100, 10-micron sized particles in the reaction zone. Thus on a very small scale, the reaction zone in these explosives is likely to be ragged and in some sense discrete. Presently, it is impossible to assess the discrete character of the detonation reaction zones in materials pressed from fine powders. Whereas the flash radiographs and other diagnostic techniques allow direct visualization and measurement on the scale of the individual grains in propellant beds, due in part to the large, macroscopic size of the grains.

On the most basic level, we believe that the energy release process from the reaction sites of energetic grains and their interaction is similar and that a study of a discrete propellant bed combined with scaling arguments, and later with averaging to obtain results for comparison with continuum mixture theories, [3], may provide the opportunity to develop understanding of other explosive materials.

A theory of discrete interactions

First I would like to give an overview of how our modeling is being developed. Each grain (later referred to as a particle) in the bed is assigned a set of numbers associated with its characteristics. These will include but not be limited to: the initial position, orientation, stored chemical energy, other thermal characteristics, the aspect ratio of the propellant grain etc.. Thus the original state of the propellant bed will be associated with a matrix in which each entry contains the initial characteristics of the grains within the bed.

Secondly, a set of *interaction rules* between grains will be developed from a list of assumptions defining the model. These rules, the prescription of the initial stimulus (by a shock or penetrating jet) and the initial state of the bed, will determine the propagation of the wave in the bed. The interaction rules are based on the basic shock physics known about explosive materials and later we hope to include the results of detailed models for the combustion of individual grains. These interaction rules might be thought of as similar to the interaction rules that conserve mass, momentum and energy during the collision of molecules in the kinetic theory of gases.

The model assumptions and interaction rules should be as simple as possible and use as much information based on experimental observation of the beds as possible. Also we hope to carry out experiments designed to test the individual particle behavior as it relates to interactions with other propellant particles. From these experiments we expect further constraints and modification of the rules, as given below, will be made.

Care and experience, specific to the experiment being modeled, is required in choosing physically based interaction models. And certain otherwise, unassignable parameters will be calibrated to the experiments. In fact in a state-variable theory, one must think of these parameters as experimentally determined constitutive functions or constants. The hope is that our modeling will predict measurable behavior that is *not sensitive* to changes in the assumptions that form the microstructural model, otherwise the model assumptions and approach are ill-posed. In addition, if the mathematical framework is simple enough, it will be possible to test the sensitivity of the results to changes in the modeling assumptions.

To illustrate the concepts, we have developed a simple linear chain model of a propellant bed, similar to Fujiwara's "Bubble Detonation" experiment.

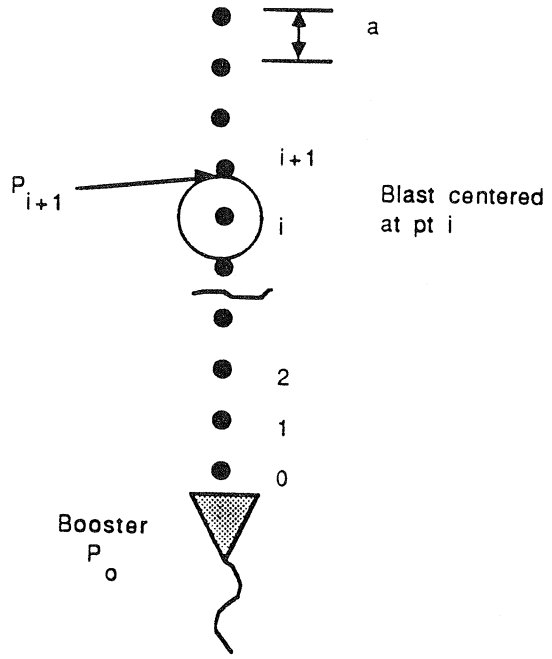

Figure 4: The linear chain of propellant particles (grains).

A detailed derivation is given in the next section.

The linear chain has equal spacing between the center of each particle and are unconfined so that the combustion products expand laterally. A 3-dimensional blast wave solution is used to signal disturbances moving from one particle to the next. Thus the geometry is not strictly 1-dimensional, since lateral pressure waves will propagate away from the chain and will not reinforce the signals and stimulus moving along the chain. Figure 4. shows a representative diagram. Note that experiments quite similar to the chain shown in Figure 4. have already been carried out at LANL.

The booster provides an initial stimulus at the bottom of the chain to the first particle and thus provides an initial condition. The subsequent shock passes through, and the combustion (or detonation) and the expansion of the products of the first particle provides the stimulus to the second particle and so on.

The other modeling assumptions (which lead to the interaction rules) for this experiment are:

- It is only necessary to track the forward pressure wave that initiates each particle. (Pressure is taken as the main variable in the theory. Note that it is possible to measure or estimate pressure in these experiments.)
- Particles are only affected by pressure waves.
- Particles are discrete sites with no shape.
- Particles emit signals symmetrically and radially.
- Particles burn instantaneously, but may release different amounts of energy according to the initiating pressure.
- Particles release their energy by a point blast explosion.
- The motion of the particles can be neglected. (Lead wrapped particles in experiments show little motion compared to the distances traveled by the shocks in the beds).
- If no energy is released, then the lead pressure disturbance decays.

Clearly, the assumptions are crude and far from perfect, but they embody essential aspects of both detonation and slower combustion of discrete particles. Note that the blast wave solution is quite simple (algebraic) in mathematical form and describes the natural geometric decay of a discrete pressure pulse with respect to time which is centered on a discrete reaction site.

Not surprisingly, as we will show, this list of assumptions leads to a *nonlinear recursion relation* for the pressure in fowardmost particle along the chain. This recursion relation for the pressure at the $i-th$ particle can be summarized as

$$P_{i+1} = h(P_i; C, \epsilon, P_c, g), \text{ with } P_0 = 1. \tag{1}$$

The pressure has been scaled so that the initial pressure generated by the booster is one. Note that the parameters C, ϵ, P_c and g appear. The parameter C is the dimensionless energy available for combustion in a propellant particle. The dimensional particle spacing a, (say) appears in the definition of C, and C decreases as the spacing increases. The parameters ϵ and P_c

are related to a very simple combustion model that assumes that all of the energy in the particle is released to the next blast wave if the initiating pressure is above P_c and that if the pressure is below P_c, the parameter ϵ governs the fraction of the total that is released. The parameter g is related to the dissipative processes in the bed. Simple arguments requiring a pressure pulse to decay along an inert chain show $0 < g < 1$.

The recursion relation is solved simply by successive evaluation. The modeling assumptions also lead to formulas that evaluate the time and distance required for the leading pressure disturbance to travel from particle to particle. Namely,

$$\triangle t_{i+1} = f(P_i; C, \epsilon, P_c, g) \quad \text{and} \quad x_i = i. \tag{2}$$

The recursion relation, shows criticality in that the wave can either propagate as a high speed, high pressure wave or as a low speed, low pressure wave and that this criticality is found for specific values of parameters defined by the model. Figure 5. shows representative examples of these calculations where P_c is varied and the other parameters are held fixed. When P_c is sufficiently low, a high speed wave results, when P_c is higher, a low speed wave results. Note that i represents the $i - th$ particle along the string. Figure 5a. shows the initiating pressure of the leading particle in the string as a function of time. Figure 5b. shows the plot of the leading disturbance in an $x - t$ plane.

Explicit dependencies of the discrete model's response on the bed and grain properties can be determined, like that of the particle energy, the booster pressure and the interparticulate distance, which are controllable by manufacture or experiment in a real propellant bed. We hope to test these dependencies directly by experiment.

There may be distinct mathematical and physical advantages in our approach over continuum modeling. By retaining as simple a structure as necessary, in our theoretical modeling, recursion relations are obtained. These are simpler to solve than the complex, nonlinear (often hyperbolic) partial differential equations of two-phase mixture theory that are often associated with propellant bed problems, [4].

By adopting this approach we have a more detailed handle on the effect of the microstructure of the bed (by essentially defining it apriori) and

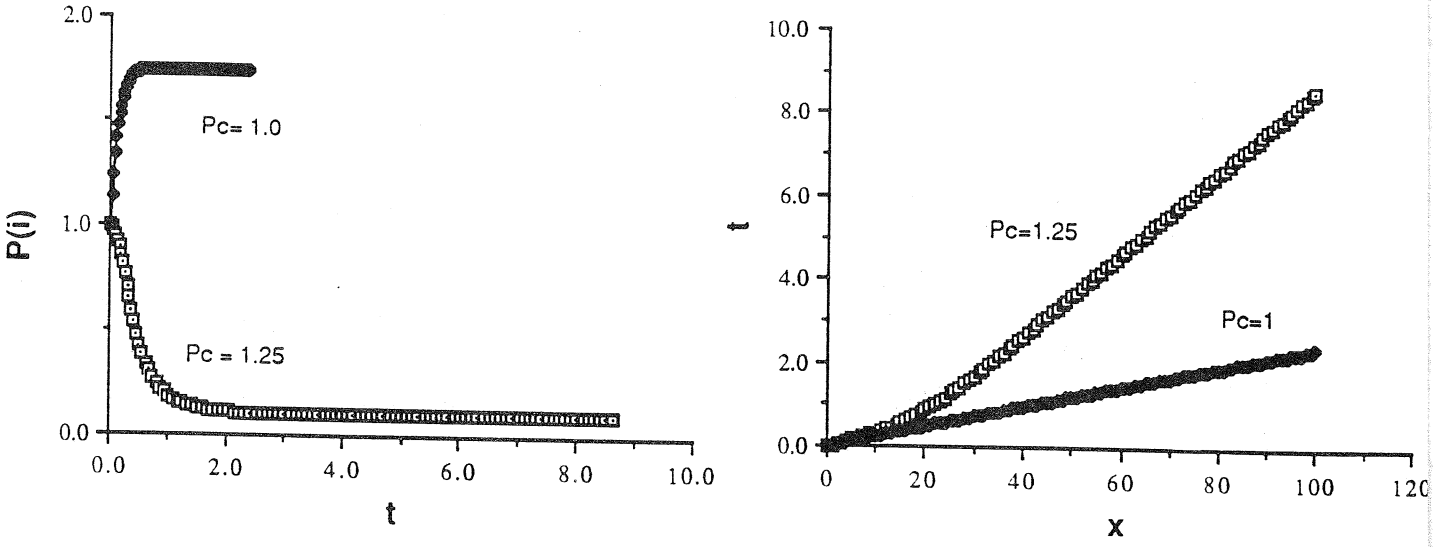

Figure 5: Pressure-time and position-times initiation transients, for $C = .25, g = .8, \epsilon = 1$.

the importance of certain mechanics and assumptions in our modeling. In contrast, the parameters and interaction terms of two-phase continuum mixture theory are often only fit parametrically to certain experiments and not directly related to the microstructural mechanisms within the bed. There are substantial ambiguities in the microstructural origins of the different functional forms used in the continuum two-phase mixture theories. The modeling adopted here, can be designed to complement continuum mixture theory by suitably averaging over large enough control volumes. Indeed, it is important to relate the results of our modeling to two-phase, continuum mixture theory.

Derivation of the chain model

Review of the blast wave solution

The starting point for our interaction model is a representative blast wave solution in spherical coordinates. From dimensional arguments, Taylor showed

that for a polytropic fluid, with initial blast energy E, the pressure and radius of the blast wave shock varies as

$$R(t) = k\left(\frac{E}{\rho}\right)^{1/5} t^{2/5}, P(t) = \frac{8}{25}\frac{k^2\rho}{\gamma+1}\left(\frac{E}{\rho}\right)^{2/5} t^{-6/5}. \tag{3}$$

Since these relations are derived from dimensional arguments, it is easy to generalize to a more general equation of state for the fluid. Note that k is a constant that is fixed by the total energy. For our purposes we note that $R(t)$ and $P(t)$ are not independently related, (due to the requirement of conservation of mass, momentum, energy) and can be assumed to take the generic form

$$R(t) = At^{\alpha}, P(t) = Bt^{-\beta}, A = eB^{\delta}, \tag{4}$$

with $\alpha, \beta, \delta, e > 0$, and specified. For example, for the polytropic equation of state

$$\alpha = \frac{2}{5}, \beta = \frac{6}{5}, \delta = \frac{1}{2}, e = \left[\frac{8}{25}\frac{\rho}{\gamma+1}\right]^{-1/2}. \tag{5}$$

Relations (4) embody the physics of a combusting or detonating particle that generates a pressure wave, which radiates roughly, from a central point, with the pressure generated by that particle dropping off with increasing time and distance.

Derivation of the recursion relation

Now consider the discrete linear chain shown in Figure 4. For convenience, the particles are assumed to be equally spaced with their centers at a distance a apart. Measured from the booster particle at $x = 0$, the particles are located at $x = i\,a$, where i corresponds to the $i - th$ particle as measured from the bottom. The *booster* particle provides the initiating pressure P_0.

We assume that it is sufficient to keep track of the pressure. Let P_{i+1} be the initiating pressure for the $i + 1 - th$ particle. Thus P_{i+1} represents the (shock) pressure just prior to collision with the $i + 1 - th$ particle and thus the position of the front is at $x = (i + 1)a$. Let $\triangle t_{i+1}$ be the time increment

required for the (shock) pressure wave to travel to the $i+1-th$ particle, from a disturbance originally centered at the $i-th$ particle.

Since formulas (4) hold for each point explosion or origin of blast energy, then for equally-spaced particles

$$a = A_i(\Delta t_{i+1})^{\alpha}, P_{i+1} = B_i(\Delta t_{i+1})^{-\beta}, A_i = eB_i^{\delta}, \tag{6}$$

where A_i, B_i depend on energy of origin of the $i-th$ blast wave and are not independent. The energy at the origin of the $i-th$ blast wave should depend on the energy release provided by the $i-th$ particle, but it should also be affected by the energy transmitted to the $i-th$ center from the $i-1-th$ blast. Indeed, the total energy available at the $i-th$ point may well be affected by all the previous blasts, $i-1, i-2, i-3, \ldots$ etc. .

One may also consider the case that no additional energy is released by the particles, in which case the particle-shock interactions should serve to decrease the energy of the original blast, thus decreasing the energy and pressure transmitted along the chain. This energy presumably is absorbed by the particles as they become damaged by the passing shock.

If we take B as fundamental (corresponding to the blast energy centered at the particle site), with A determined, then we complete the model by giving an interaction rule for B that includes (say) dissipative losses and chemical energy release. A very simple model that contains these basic effects is

$$B_i = gB_{i-1} + fB_0. \tag{7}$$

In the above formula, g is constant and depends possibly on the particle shape, orientation etc. The constant B_0 is related to the maximum explosive energy that can be released by a single particle and f is a function, $0 \leq f \leq 1$ that should depend on the initiating pressure of the $i-th$ particle and possibly on previous interactions as well. Thus to complete the model specification, we need to specify g, B_0 and f.

In the absence of reaction, $f = 0$, and one solves for Δt_{i+1}, eliminates B_i and uses the rule (7) to obtain the recursion formula for P_i,

$$P_{i+1} = g^k P_i, k \equiv (1 + \beta\delta/\alpha). \tag{8}$$

A pressure wave that decays in amplitude along the chain is possible only if

$$0 \leq g < 1. \tag{9}$$

The reaction model for f could be as complex as we like, but in the interest of simplicity one might consider that f only depends (monotonically) on the initiating pressure P_i. Presumably, above a critical pressure, P_c , the particle releases all of its energy. Below P_c only some fraction of the total chemical energy is released. Thus a simple form such as

$$f = \begin{cases} e^{\epsilon(P_i - P_c)}, & P_i < P_c, \\ 1, & P_i \geq P_c, \end{cases} \tag{10}$$

can be suggested. Note that ϵ and P_c play the role of chemical kinetic parameters in the sense that their specification describes the quantity of energy release and the sensitivity of the energy release to changes in the initiating pressure.

In summary, a simple, discrete model for the initiation of the chain is posed as

$$P_{i+1} = \left(\frac{e}{a}\right)^{\beta/\alpha} {B_i}^k, \tag{11}$$

$$B_i = gB_{i-1} + B_0 f_i, \tag{12}$$

$$f = \begin{cases} e^{\epsilon(P - P_c)}, & P_i < P_c, \\ 1, & P_i \geq P_c, \end{cases} \tag{13}$$

$$\triangle t_{i+1} = \left(\frac{a}{A_i}\right)^{1/\alpha} = \left(\frac{a}{e}\right) {B_i}^{-\delta/\alpha}, \tag{14}$$

$$x_i = i\, a, \tag{15}$$

$$P = P_0, \text{ at } i = 0. \tag{16}$$

Elimination of B_i, in favor of its definition in terms of P_i leads to the recursion formulas,

$$P_{i+1} = \left[g {P_i}^{1/k} + B_0 \left(\frac{e}{a}\right)^{\beta/(k\alpha)} f_i \right]^k, \text{ with } P_{i=0} = P_0, \tag{17}$$

$$\triangle t_{i+1} = \left(\frac{a}{e}\right)^{1/(k\alpha)} {P_{i+1}}^{-\delta/(k\alpha)}, \tag{18}$$

$$x_i = i\,a. \tag{19}$$

The interpretation and the development of guidelines for the experiments, ultimately require a dimensional analysis and the choice of characteristic scales. Tilde quantities now to refer to dimensional quantities and plain variables refer to dimensionless quantities. For a length scale we choose the interparticle length $\tilde{a}$. The characteristic pressure is chosen to be the booster pressure $\tilde{P}_0$. The characteristic time is chosen to be the transit time required for the blast to travel across a distance $\tilde{a}$, given the release of all the chemical energy,

$$\triangle \tilde{t} = \left(\frac{\tilde{a}}{\tilde{e}}\right)^{1/\alpha} {\tilde{B}_0}^{-\delta/\alpha}. \tag{20}$$

This time is different than the time that would be identified from the booster pressure.

Based on this scaling we are led to the following dimensionless formulation.

$$P_{i+1} = \left[g {P_i}^{1/k} + C f_i\right]^k, \text{ with } P_{i=0} = 1, \tag{21}$$

$$\triangle t_{i+1} = C^{1/\alpha} {P_i}^{-\delta/(k\alpha)}, \tag{22}$$

$$x_i = i. \tag{23}$$

where

$$C = \frac{\tilde{B}_0(\tilde{e}/\tilde{a})^{\beta/(k\alpha)}}{{\tilde{P}_0}^{1/k}}, \epsilon = \frac{\tilde{\epsilon}}{\tilde{P}_0}, P_c = \frac{\tilde{P}_c}{\tilde{P}_0}, \tag{24}$$

and f is still given by (10).

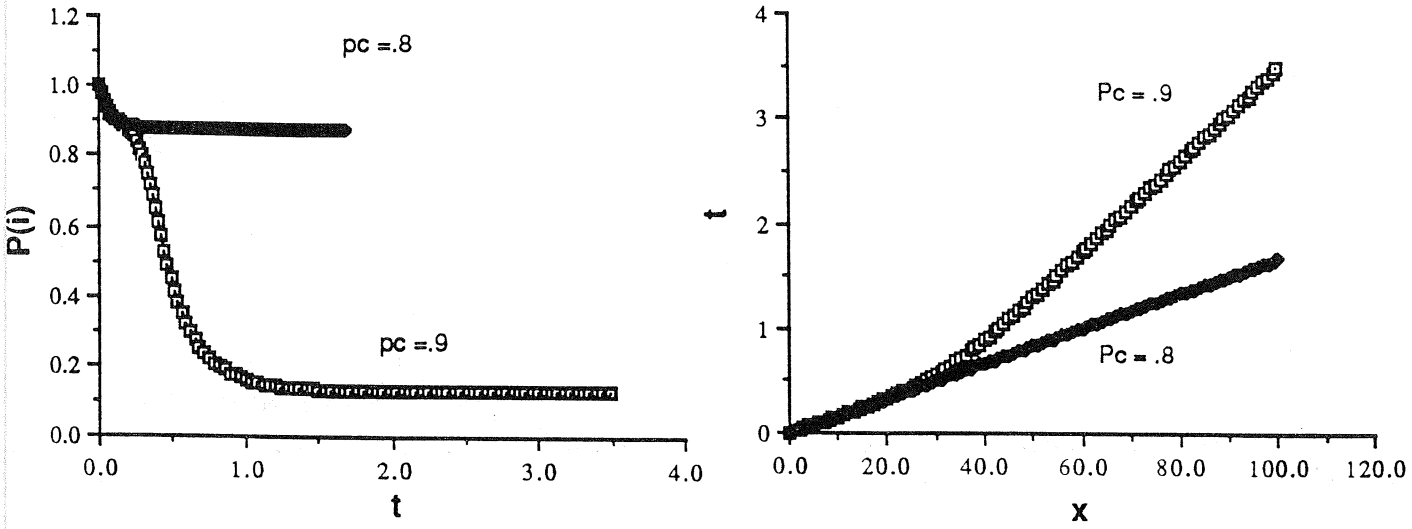

Figure 6: Pressure-time and position-times initiation transients for values of P_c near failure,for $C = .19, g = .8, \epsilon = 1$.

Properties of the recursion relation

Initiation behavior

Next we show some representative results showing the initiation behavior for this chain model. Figure 6. shows typical initiation behavior when the booster pressure is above the steady, high pressure response of the chain. Figure 6a. shows the pressure time history of the shock front, Figure 6b. shows the location of the front. During the transient, the front pressure experiences a decay to the final pressure. Various values of P_c were chosen to illustrate that the initiation transient develops into a high or low pressure, steady wave, depending on the value of P_c, (say). Thus a critical value of P_c exists and can be thought of as an initiation criterion.

Figure 5. shows the behavior when the booster pressure is below the steady, high pressure response of the chain.

By adjusting the parameters we can get more or less dramatic results near the critical values that select the high pressure over the low pressure, steady response. Figure 7. shows dramatic pressure differences for the high

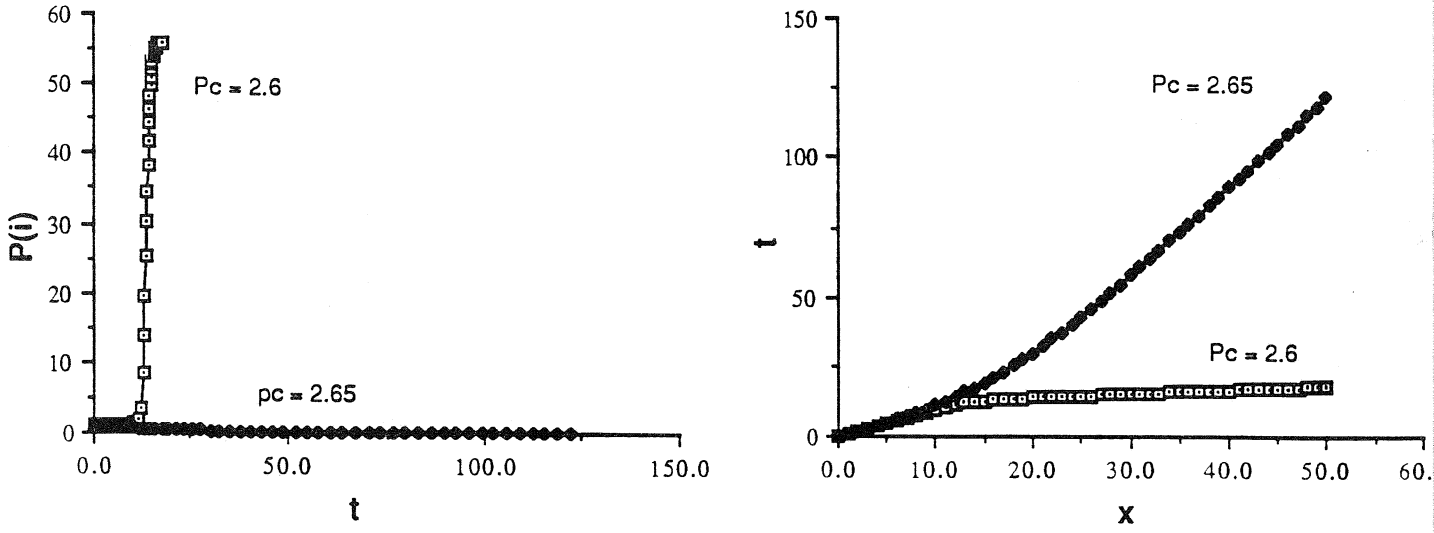

Figure 7: Pressure-time and position-times initiation transients, for $C = 1, g = .8, \epsilon = 1$.

pressure and the low pressure wave for small changes in the parameter P_c.

Steady solutions

Steady solutions are found easily by setting $P_{i+1} = P_i \equiv P_s$, and imply that the reactive wave in the chain is self-sustained. For the choice of f that we made earlier, it is easy to solve explicitly for P_s in terms of the parameters C, g, e, and P_c . We find that

$$\begin{aligned} P_c &= P_s - \frac{1}{\epsilon} \ln \left[\frac{(1-g){P_s}^{2/5}}{C} \right], \text{ for } P_s < P_c, \\ P_s &= \left[\frac{C}{1-g} \right]^{5/2}, \text{ for } P_s \geq P_c. \end{aligned} \tag{25}$$

Depending on C, g, e and P_c it is easy to show, that there may be single or multiple steady states. Clearly, if multiple steady states are possible, then the dynamic stability of those steady states is an issue. With the assumption that each iterate is a perturbation from the steady state,

$$P_i = P_s + P_i', \text{ where, } |P_i'| << 1, \tag{26}$$

substitution of (26) into (212) shows that to a linear approximation, P_i' satisfies the recursion relation

$$P_{i+1}' = \left[g + kCP_s^{1-1/k} \frac{df(P_s)}{dP_i} \right] P_i'. \tag{27}$$

Stability of the steady state depends on the inequality

$$\left[g + kCP_s^{1-1/k} \frac{df(P_s)}{dP_i} \right] < 1. \tag{28}$$

For our choice of f,

$$\frac{df(P_s)}{dP_i} = \begin{cases} \epsilon f(P_s), & P_s < P_c, \\ 0, & P_s \geq P_c. \end{cases} \tag{29}$$

In particular, when $P_s > P_c$, since $g < 1$, (28) is always satisfied and the inequality shows stability. Thus the high pressure branch is stable by this argument. For the lower pressure branch, $P_s < P_c$ and it is easy to show that (28) reduces to the simpler inequality,

$$k\epsilon P_s < 1, \text{ when, } P_s < P_c. \tag{30}$$

When ϵ, or the steady state pressure P_s is sufficiently small, then stable solutions are also possible. The intermediate values of the steady state pressures are found to be unstable.

Figure 8. shows an example indicating how the stability of the steady states varies with the total energy release parameter, P_c. The steady pressure on the high pressure branch of the steady response is above the initiating pressure. The steady high pressure response and the very low pressure response are stable. The intermediate pressure responses change their stability at a critical value of P_c. When the $P_s - P_c$ steady response curve is single-valued, it is composed of a constant, high pressure branch connected to a monotonically decreasing branch as P_c is varied from zero to higher values. This case is not shown.

A final comment on this simple linear chain model is that, if we modify our model but stay within the context of difference equations, then rich

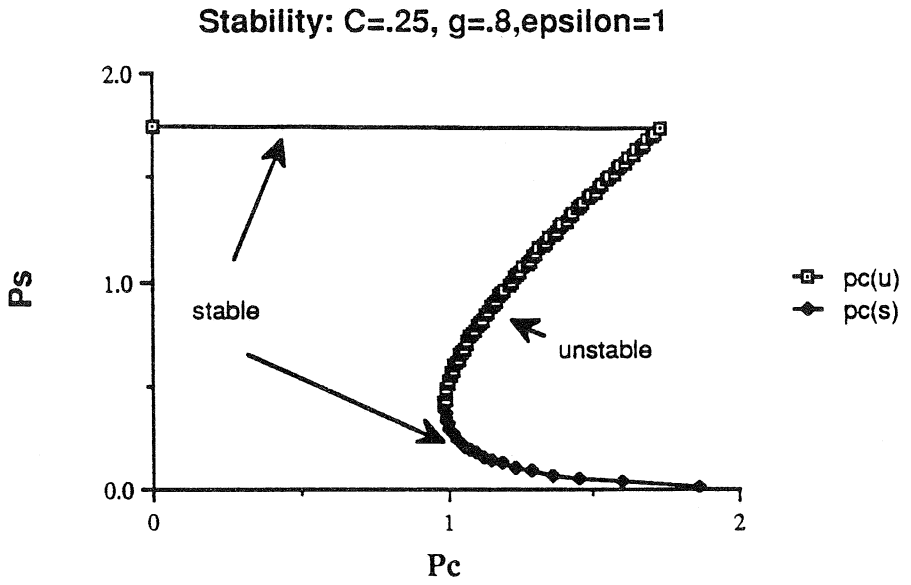

Figure 8: The steady response curve, P_s versus P_c showing stability or instability for $C = .25, g = .8, \epsilon = 1$.

dynamics are possible. For example, it is well known that bifurcation to chaos is contained in the simple *Logistic map*,

$$P_{i+1} = cP_i(1 - P_i), \text{ for } 0 < P_i \leq 1. \tag{31}$$

as the parameter c is changed. Whether chaotic dynamics are relevant or are an appropriate description for our propellant bed model, is yet to be determined.

Multi-D propellant bed models

There are certain transport mechanisms of the bed problem that cannot be adequately incorporated in the simple chain model due to lateral interactions between particles. Here we explain the basic design of a Multi - D model.

First each particle will be associated with an ordered array of numbers (a vector) that describes its current state, characterizing its position, initial energy, thermal properties, aspect ratio, etc and its state of burning. If there are 1,000 particles in the bed (say), then there would be 1,000 such ordered pairs. Note that for finite size charges, perhaps no more than 10,000 propellant particles are required.

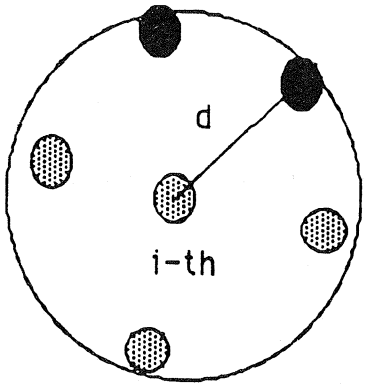

Figure 9: A collection of particles within a Multi - D bed.

A *nearest neighbor* assumption is that each particle is at most influenced by its nearest neighbor found within some radius d from the center of the particle. The coordinates of the nearest neighbors can be included in the vector describing each particle. The arrangement of particles will be similar to that shown in Figure 9. with the $i-th$ particle shown at the center.

Like the linear chain model, the interactions between particles will be governed by a set of modeling assumptions. The main difference is that each particle will necessarily be influenced by more than one particle, with disturbances arriving from lateral directions instead of just from behind. (Indeed it is easy to add more complexity from additional influences from behind, in the linear chain model if this is required.) Once a critical state is reached in the particle, it releases its energy and produces a pressure pulse as before.

The calculation in the bed advances by calculating each interaction as a pressure pulse traverses from one particle to the next. If the nearest neighbor assumption is used, then the number of calculations needed to advance the bed will be limited and be related to the number of particles in the width of the charge (say) times the average number of nearest neighbors in the bed.

The initial stimulus required to start the burning in the bed will come

from an assumption that some particle or collection of particles is shocked or burnt, according to an assumed stimulus. This stimulus could be a plane shock or from the impact of a concentrated jet.

The state of each particle will be known at each interaction time. The interaction times will be calculated from applying the interaction rules and by sweeping the beds at each particle interaction. The state of the particle will be stored in a vector. The computational task of simulating a reacting wave through the bed is roughly equivalent to solving the heat equation in one dimension with 10,000 spatial nodes.

The confinement of the bed due to a metal tube (say), will also be easy to model by giving special interaction rules for particles adjacent to the boundary. The boundary rules will be based on the physics of shock reflection, similar to the use of the simple blast wave solutions in the interior.

Figure 10. gives a sense of some of the modeling concepts explained here and results that such a multi- D model will generate. The leading pressure disturbance in a discrete bed of propellant which is detonating or burning is experimentally found to be quite ragged. The figure schematically shows the pressure disturbances emitted radially and propagating from a collection, 4 particles deep in the bed. Black particles are unburned and grey particles are burnt. The vertical lines indicate a metal tube. For comparison, Figure 11. is an radiograph of a bed of detonating propellant taken by Blaine Asay at LANL.

Conclusion

From discrete modeling and simulations we expect to be able to get a good qualitative sense of the mechanics of many interactions found in the propagation of reactive waves in beds of propellant. We hope that our work will have implications for an extended class of explosive materials with finer scales such as pressed explosives. The goal is to look systematically for organized behavior that develops within the front when a successful detonation begins to emerge. Our approach will hopefully yield unexpected insights into the mechanics of failure and propagation of reactive waves within the bed and give a microstructural framework from which to rationally verify continuum mixture theory that has been developed previously for these materials.

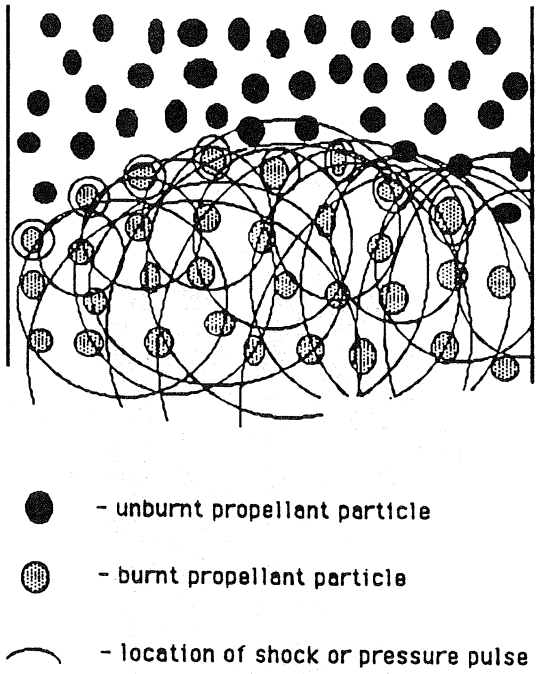

Figure 10: A schematic diagram of reactive wave propagation through a discrete Multi-D bed

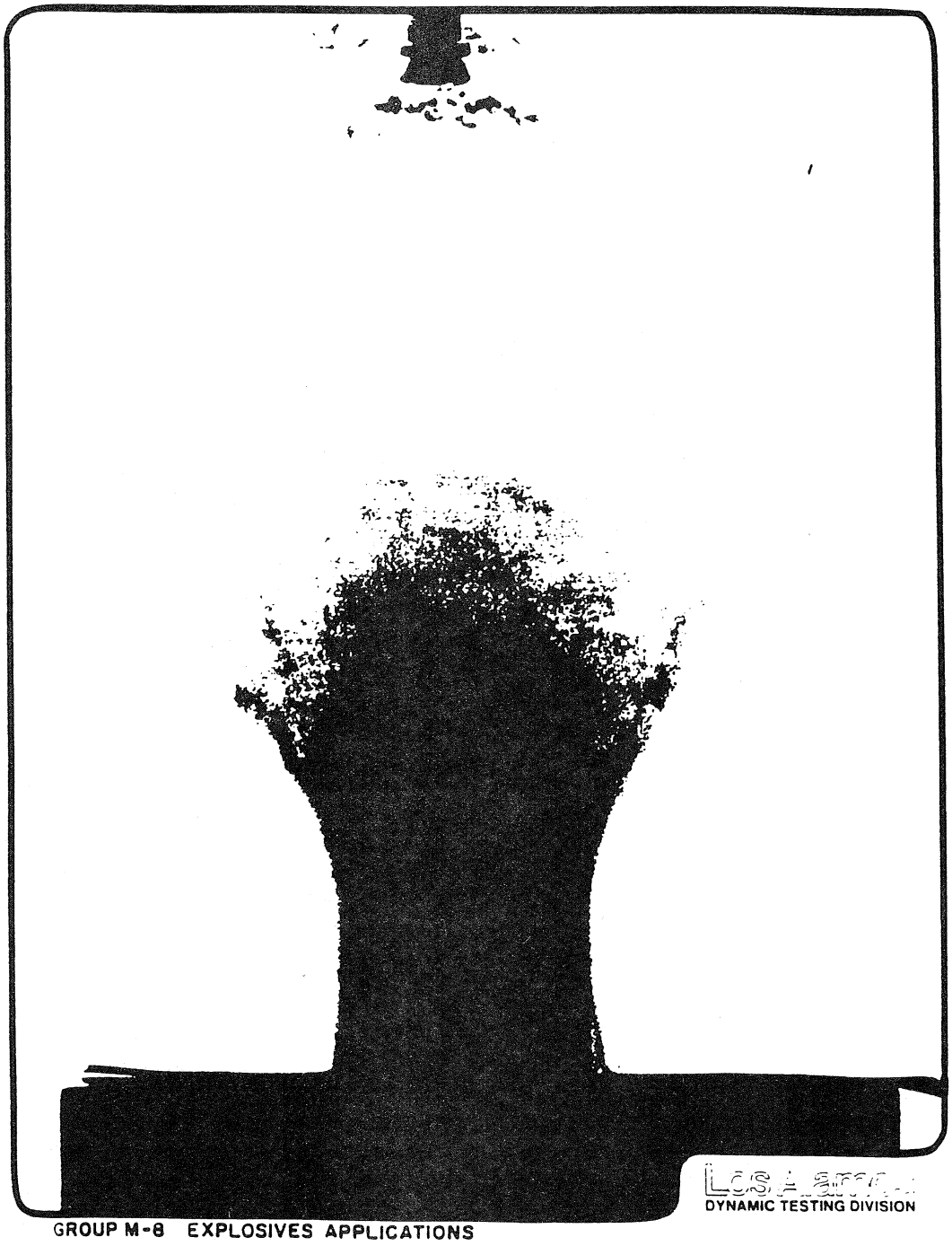

Figure 11: A radiograph of a bed of detonation propellant (B. W. Asay, LANL).

Acknowledgements

This work has been supported by Los Alamos National Laboratory, and contract DOE-LANL-9XG83931-P1.

References

1. Fujiwara, T. , A presentation at the High Mach Number Workshop, May 3-6, 1987 at the Mathematical Sciences Institute of Cornell University, Ithaca, New York.
2. Asay, B. W., Campbell, A. W., Ginsberg, M. J., and Ramsay, J. B., Detonation characteristics of gun propellant, 9th Symposium (International) on Detonation, August 1989, Portland Oregon.
3. Baer, M., R. and Nunziato, J. W. 1986, "A two-phase mixture theory for deflagration to detonation transition (DDT) in reacting granular material", Int. J. Multiphase Flow, Vol 12, No. 6., pp 861-889.
4. Powers, J. M., Stewart, D. S. and Krier, H. K. "Theory of two-phase detonation", to appear in Combustion and Flame.