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AUTHOR(S): Charles L. Mader

MASTER

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los alamos
scientific laboratory
of the University of California
LOS ALAMOS, NEW MEXICO 87545

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TWO DIMENSIONAL HOMOGENEOUS AND HETEROGENEOUS DETONATION WAVE PROPAGATION

Charles L. Mader
Los Alamos Scientific Laboratory
University of California
Los Alamos, New Mexico 87545

The process of detonation propagation of homogeneous explosives along surfaces may be described using resolved reaction zones, Arrhenius rate laws and two dimensional reactive hydrodynamic calculations. The wave curvature increases with increasing reaction zone thickness. The process of detonation propagation and failure of heterogeneous explosives along surfaces and around corners may be described if the decomposition that occurs from hot spots formed by shock interactions with density discontinuities is described by a burn rate determined from the experimentally measured distance of run to detonation as a function of shock pressure, the reactive and nonreactive Hugoniot and the assumption that the reaction rate derived near the front can be applied throughout the flow.

INTRODUCTION

The time-dependent behavior of detonations with resolved reaction zones in condensed homogeneous explosives has been described (1,2), using an Arrhenius rate law. The failure of a nitromethane detonation, resulting from a side rarefaction cooling the explosive inside its reaction zone, was calculated and the experimentally observed rarefaction velocity was reproduced. We shall extend the study to nitromethane detonations proceeding perpendicular to metal surfaces and examine wave curvature and failure as a function of reaction zone thickness.

Experimental observations (3) of detonation waves in heterogeneous explosives proceeding perpendicular to metal plates showed very little wave curvature after a large plane-wave-initiated cylindrical explosive charge had run several charge diameters. An empirical model with an unresolved explosive reaction zone and programmed to maintain a constant velocity, plane detonation front reproduced the experimental observations. Because the basic mechanism of heterogeneous shock initiation is shock interaction at density discontinuities producing local hot spots that decompose and add their energy to the flow, models such as the heterogeneous-sharp-shock-partial-reaction burn model, have been developed to model the flow (4). They have not been useful for solving two dimensional reactive flows because they did not respond to local state variables in a realistic manner. We used a new model called Forest Fire (5) to describe the hot spot reaction rate in the bulk of the heterogeneous explosive to detonations proceeding perpendicular to metal plates, to detonations turning corners and to detonations proceeding along free surfaces for shock sensitive and insensitive explosives.

HOMOGENEOUS DETONATIONS

Reference 1 shows that the reaction zone of nitromethane is ~2500 A long and that it is probably pulsating about the steady-state values if the usual activitation energies (E) and frequency factors (Z) are appropriate. It is impossible to make calculations with such small reaction zones being resolved for systems the size usually studied experimentally. We can study the effect the size of the reaction zone has on the flow by increasing the frequency factor to scale up the size of the reaction zone. We can also eliminate the pulsating nature of the reaction zone by choosing an activation energy that results in steady nonpulsating flow. As shown in Ref. 1, an activation energy of 30 kcal/mole results in steady flow. and by varying the frequency factor, we can have various thickness reaction zones. However, because such scaling results in unrealistically large reaction zones, care is required in extrapolating the calculated results to real experiments.

Experimental measurements of the detonation wave arrival of nitromethane across the surface of a charge have shown that there is remarkably little wave curvature even after the wave has run many charge diameters in a large plane-wave-initiated cylindrical charge. In our first study we investigated how a resolved reaction zone in nitromethane proceeds perpendicular to a copper surface. Figure 1 shows that the larger reaction zone resulted in an increased wave curvature. The calculations were performed using the 2DL reactive hydrodynamic code (6) with a mesh of 0.01 cm square. The equation-of-state parameters used for nitromethane are described in Ref. 7 and those for copper aluminum and Plexiglas are described in Ref. 8. The detonation wave was started using the same steady-state piston described in Ref. 6. The absolute value of pressure is plotted and the slight discontinuity at the nitromethane-copper interface is from the different amounts of artificial viscosity in the two materials.

Because the detonation wave curvature decreases with decreasing reaction zone thickness, it is not surprising that nitromethane, with its very thin reaction zone, shows very little curvature. The reason for this result appears to be that although the head of the rarefaction goes into the reaction zone at the same speed regardless of the reaction zone thickness, the wave curvature depends upon how much the confining surface or wall moves out during passage of the reaction zone. Because lower density walls permit more outward motion than higher density walls, the lower density walls result in more curved fronts. Shortening the reaction zone keeps the wall from moving outward as much during transit which results in less shock curvature. The two critical parameters are the rarefaction speed and the reaction zone length.

Figure 2 shows that the increased divergence resulting from cylindrical geometry permits the outward moving surface to be more effective in increasing the wave curvature. The effect of changing the density of the confining wall is shown in Fig. 3, where the detonation wave proceeds along a copper and then an aluminum wall. Compared with the copper wall in Fig. 1, the curvature increases and the reaction zone becomes thicker as the reaction proceeds along the aluminum wall. These results qualitatively agree with the experimental observations.

Campbell, Malin and Holland (9) observed that thin foils of metal were as effective at confining the nitromethane detonation wave as were thick cylinders of the same metal. In Fig. 4 the thickness of the confining copper wall is decreased but the shockfront and reaction zone profile is the same as in Fig. 1. Other calculations showed that the reaction zone must be thick enough for the rarefaction from the outer copper surface to arrive back at the nitromethane-copper interface before passage of the reaction zone for the reaction zone and wave curvature to be effected by the thickness of the confining metal.

The detonation wave curvature increases with increasing reaction zone thickness. A thin metal cylinder may prevent detonation failure if the reaction zone is thin enough for the rarefaction from the outside metal surface to arrive in the detonation products after passage of the reaction zone. The observed failure and reignition of nitromethane detonation by holes in confining surfaces can be reproduced qualitatively by the Arrhenius kinetic model as shown in Ref. 5.

HETEROGENEOUS DETONATIONS

Heterogeneous explosives such as PBX-9404 or Composition B show a different behavior than homogeneous explosives when propagating along confining surfaces. A heterogeneous explosive can turn sharp corners and propagate outward. A heterogeneous explosive, depending upon its sensitivity, may exhibit either very little or a lot of curvature when propagating along a metal surface. The mechanism of initiation for heterogeneous explosives is different than the Arrhenius kinetic model found adequate for homogeneous explosives. Heterogeneous explosives are initiated and may propagate by the process of shock interaction with density discontinuities such as voids. These interactions result in hot regions that decompose and give increasing pressures that cause more and hotter decomposing regions. Some heterogeneous explosives may require hot spots even for the propagation of the detonation wave.

Because previous modeling of heterogeneous shock initiation of explosives has proved useful only for certain applications (4), a more general model for the bulk decomposition of a heterogeneous explosive has been developed. It may be used to reproduce the explosive behavior in many one- and two-dimensional situations for which data is available. It is called the Forest Fire model and is described in Ref. 5. The model gives the rate of explosive decomposition as a function of the local pressure (or any other state variable) in the explosive shown in Fig. 5. In this section we shall describe the results of applying the Forest Fire description of heterogeneous explosive detonation propagation to detonation propagation along surfaces and around corners.

The Los Alamos Scientific Laboratory radiographic facility, PHERMEX (10) was used to study the detonation wave profile in heterogeneous explosives as it proceeds up metal surfaces (3, 10). It has also been used to study the profiles when a detonation wave in Composition B or X0219 turns a corner (11, 12).

As described in Ref. 3, a radiographic study was made of a 10.16-cm cube of Composition B, with and without tantalum foils, initiated by

a plane wave lens confined by 2.54 cm-thick aluminum plates. The radiographs show a remarkably flat detonation front followed by a large decrease in density originating near the front of the wave as it intersects the metal plate.

A numerical calculation using Arrhenius kinetics results in considerable curvature of the detonating wave if realistic kinetic parameters are used. The Forest Fire model of heterogeneous shock initiation results in a calculated flow closely resembling that observed experimentally as shown in Fig. 6. This suggests that the observed detonation behavior is a result of the heterogeneous shock initiation processes. Therefore, the more insensitive explosives should give greater wave curvature and have larger failure diameters. Explosives initiated and burned with a heterogeneous shock initiation model, such as Forest Fire, do not exhibit scaling behavior and hence failure depends upon the pressure magnitude and how long it can be maintained. The Forest Fire model results agree with experimental observations for many explosives.

Venable (11, 5) performed a radiographic study of a Baratol plane-wave-initiated Composition B slab detonation proceeding perpendicular to an aluminum block and up a 45 degree wedge. Calculations using the Forest Fire model reproduced the features of the radiographs as shown in Fig. 7. This was not a very significant test of the Forest Fire model because the C-J volume burn technique or programmed burn technique of burning explosives can give also similar profiles to those observed experimentally. An Arrhenius burn with a resolved reaction zone will not give detonation wave behavior such as observed experimentally.

Dick (12) performed a radiographic study of a detonation wave proceeding up a block of a very insensitive triamino trinitrobenzene (TATB) based explosive, called X0219 (90% TATB, 10% KelF, ρ_0 = 1.914), and its failure to propagate completely around a corner. Dick's experimental profiles and the calculated profiles using the Forest Fire model are shown in Fig. 8. The agreement shown is encouraging. However, the amount of explosive that remains undecomposed after passage of the shock wave depends primarily upon the curvature of the detonation wave before it turns the corner. If the wave is sufficiently curved, the detonation proceeds like a diverging detonation wave and little or no explosive remains undecomposed. If the wave is flat, or nearly so, when it arrives at the corner then much more partially decomposed explosive will remain after shock passage. The actual experiment was performed with air in the corner so the Lagrangian calculation which required some low density material in the corner (we used Plexiglas) underestimates the amount of explosive that remains undecomposed. An aluminum corner results in very little undecomposed explosive, and a lower density material slightly increases the amount of undecomposed explosive.

To study this system in a more realistic geometry, we used the Eulerian code 2DE (13) because it can handle large distortion problems such as an explosive-air interface. The calculated results using Forest Fire turn are similar to those calculated with the 2DL code in Fig. 8. Again, the results depend upon the detonation wave profile before it reaches the corner. An interesting aspect of the calculational study was that if the wave was started out flat, the explosive region near the explosive-air interface remained partially decomposed and the detonation wave never completely burned across the front until the wave became sufficiently curved at the front and near the interface. The failure process of a heterogeneous explosive must be a complicated interaction of the effective reaction zone thickness (presumably dependent upon the void and resulting hot spot size and decomposition rate) determining how flat the wave should be and the curvature required for decomposition to occur near the surface of the charge. Because the details of the hot spot reaction zone are missing from our calculation and model, much remains to be done before realistic calculations of failure radius can be achieved.

Calculations were performed using the Forest Fire burn in 2DL for 0.7- and 1.3-cm-radius cylinders of X0219 confined by Plexiglas and for half thickness slabs of 1.3 and 2.6 cm. The thinner charges developed greater curvature and the 0.7-cm-radius cylinder failed to propagate. Calculations were also performed using the Forest Fire burn in 2DE for 0.65 and 1.3-cm-radius cylinders of X0219 confined by air. The 0.65-cm-radius cylinder failed to propagate as shown in Fig. 9. The experimentally observed failure radius of X0219 is 0.75 cm. The results of similar calculations for 9404, Composition B, and X0290 are compared with the experimental failure radius of Campbell and Engelke (14) in Table I. These results are dependent upon the initiation method and the burn resolution. The dominate feature of failure in heterogeneous explosives appears to be the same hot spot decomposition reaction that determines the shock initiation behavior.

CONCLUSIONS

The process of detonation initiation and propagation of homogeneous explosives along surfaces may be qualitatively described using Arrhenius kinetics. Because the reaction zone scale is orders of magnitude smaller than the scale of the experiments of interest, quantitative calculations are difficult to achieve. The ability of thin metal cylinders to prevent detonation failure in nitromethane and the observed failure and reignition of nitromethane by changes in confinement geometry may be qualitatively reproduced by numerical reactive fluid dynamics with Arrhenius kinetics.

TABLE I

Experimental and Calculated Failure Radii

	Experimental Failure Radius (cm)	Calculated Results
X0219	0.75 ± .05	1.3 propagated 0.7 failed
X0290	0.45 ± .05	0.50 propagated 0.30 failed
Comp B	0.214 ± .03	0.30 propagated 0.20 failed
940[4]	0.06 ± .01	0.10 propagated 0.05 failed

Detonation initiation and propagation of heterogeneous explosives cannot be described adequately using Arrhenius kinetics. A new model can describe the decomposition that occurs from hot spots formed by shock interactions with density discontinuities in heterogeneous explosives and can also describe the passage of heterogeneous detonation waves around corners and along surfaces. Failure or propagation of a heterogeneous detonation wave depends upon the interrelated effects of the wave curvature and the shock sensitivity of the explosive. Some of the basic differences have been established between homogeneous and heterogeneous explosive propagation and failure.

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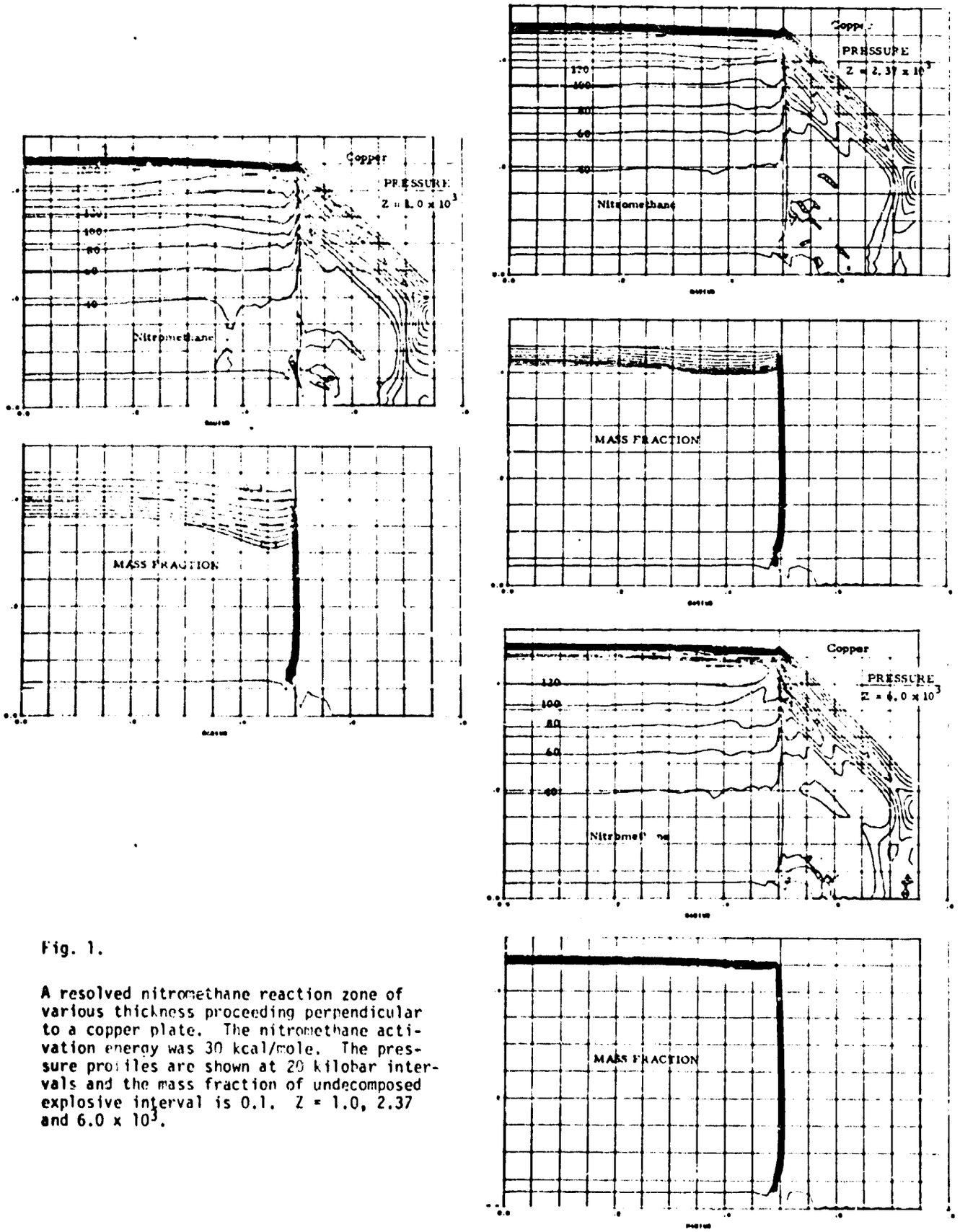
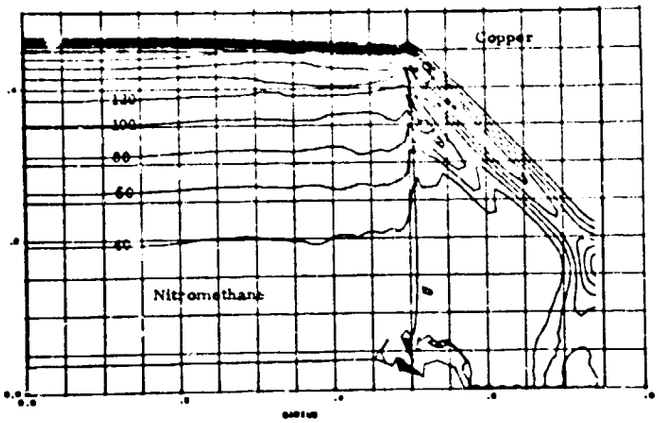


Fig. 1.

A resolved nitromethane reaction zone of various thickness proceeding perpendicular to a copper plate. The nitromethane activation energy was 30 kcal/mole. The pressure profiles are shown at 20 kilobar intervals and the mass fraction of undecomposed explosive interval is 0.1. $Z = 1.0$, 2.37 and 6.0×10^3.



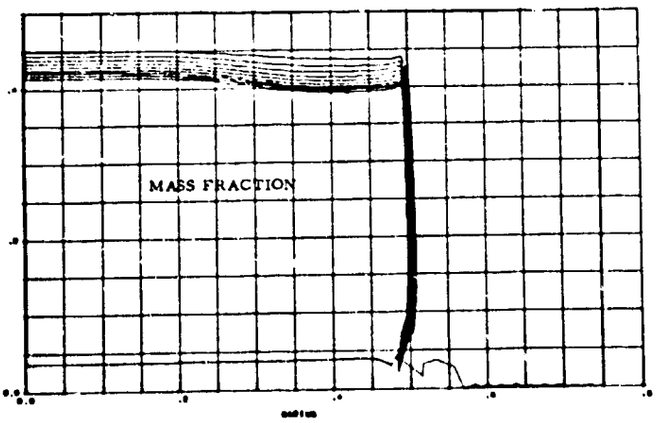
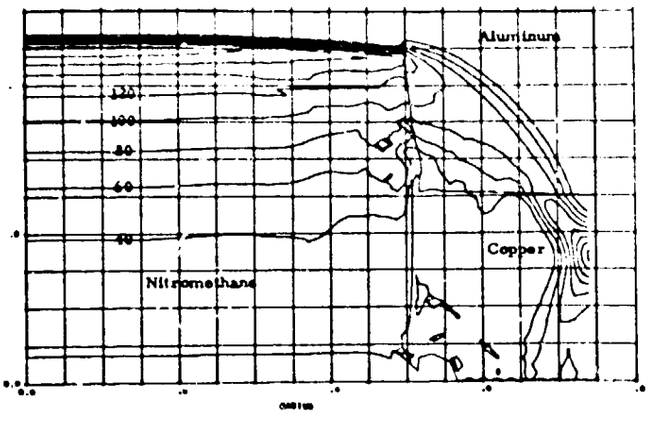


Fig. 2. A resolved nitromethane zone proceeding perpendicular to a copper cylinder. $Z = 2.37 \times 10^3$, $E = 30$.



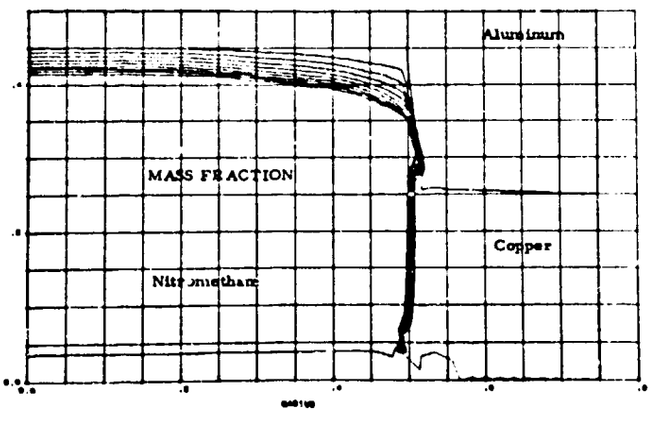
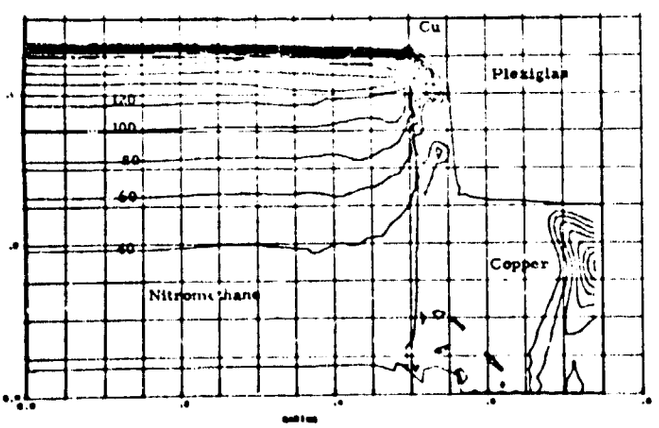


Fig. 3. A resolved nitromethane zone proceeding perpendicular to wall of copper and aluminum. $Z = 2.37 \times 10^3$, $E = 30$.



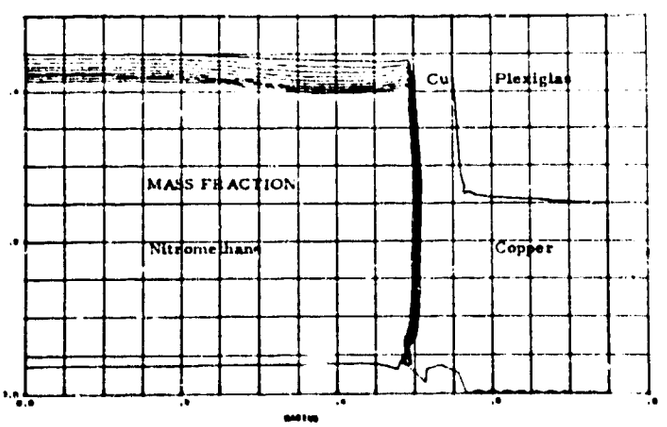


Fig. 4. A resolved nitromethane reaction zone proceeding perpendicular to a copper plate that becomes about as thin as the reaction zone thickness. $Z = 2.37 \times 10^3$, $E = 30$.

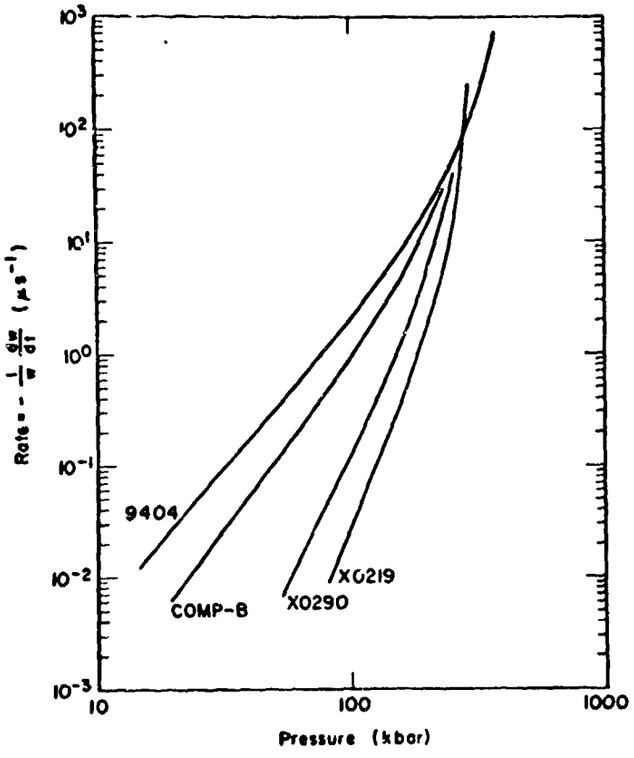


Fig. 5. The rate of decomposition as a function of the pressure from the Forest Fire model.

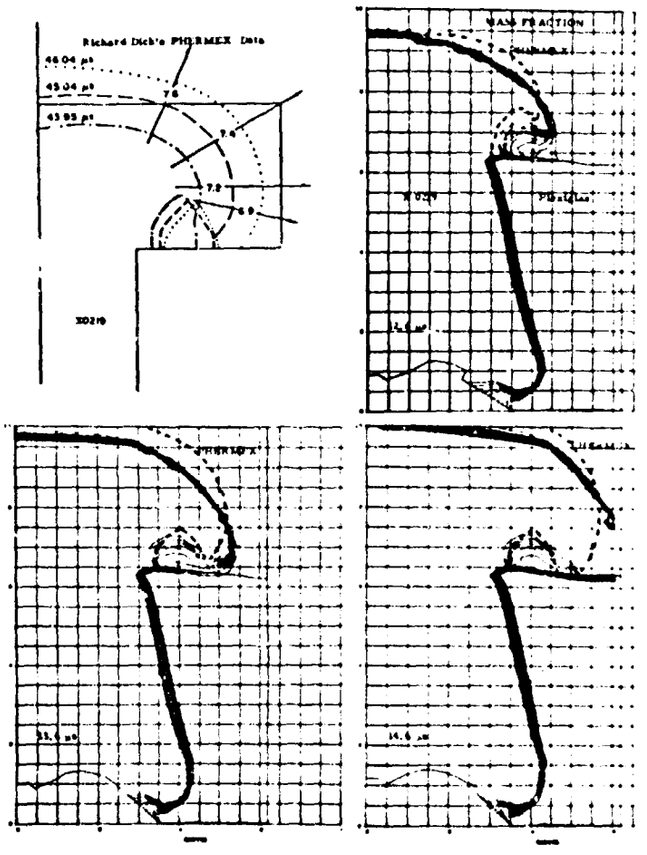


Fig. 8.

The radiographic and calculated 2 DL profiles of a detonation wave propagating around a corner of insensitive explosive X0219. The corner is filled with air in the experiment and with Plexiglax in the calculation.

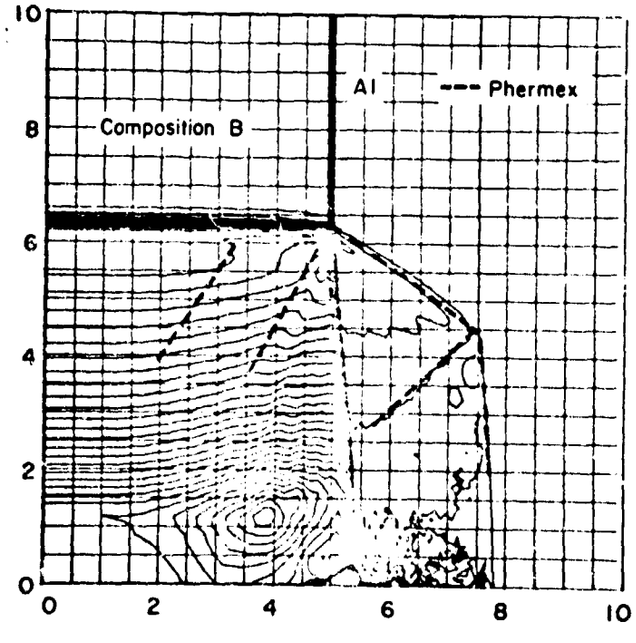


Fig. 6.

The constant density profiles at 8 μsec for a 5-cm-half-thickness slab of Composition B detonating by the Forest Fire model up an aluminum plate 2.5-cm-thick. The prominent features of a radiograph of the flow are shown with dashed lines.

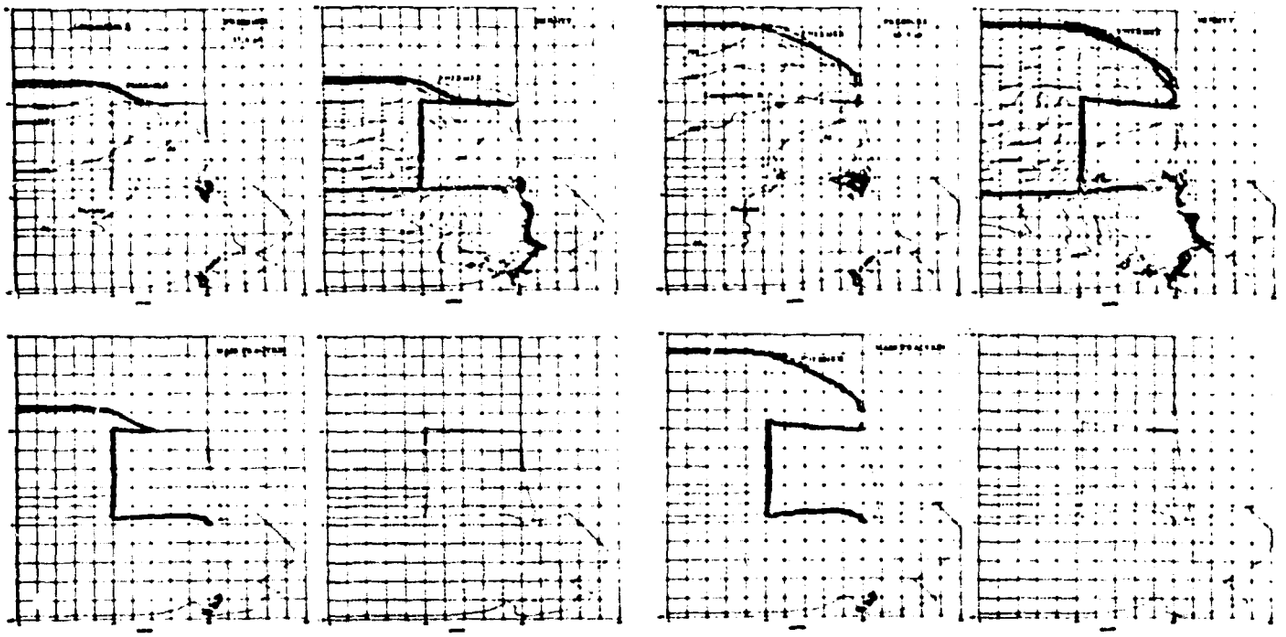


Fig. 7. Calculated profiles of a Composition B Forest Fire detonation proceeding around a 90° corner formed by an aluminum block. The pressure profile interval is 50 kbar, the density profile is 0.02 cc/gm, the mass fraction interval is 0.1 and the last figure is the mesh used in the calculation. The PHERMEX profiles are shown by dashed lines.

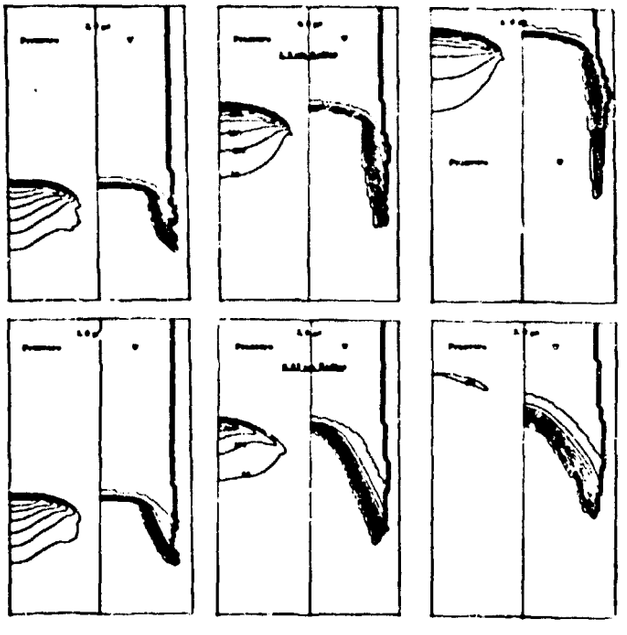


Fig. 9. The pressure and mass fraction profiles for a 0.65 and a 1.3-cm-radius cylinder of X0219 in air calculated using the 2DE code with the Forest Fire burn model.