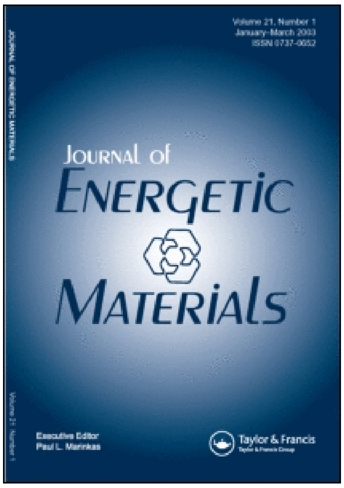

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NUMERICAL MODELING OF THE EFFECT OF TEMPERATURE AND PARTICLE SIZE ON SHOCK INITIATION PROPERTIES OF HMX AND TATB

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ABSTRACT

The three-dimensional Eulerian reactive hydrodynamic code 3DE has been used to investigate the effects of particle size (and the remaining void or hole size) and of initial temperature on the shock initiation of heterogeneous explosive charges of HMX and TATB.

Shocks interacting with HMX and TATB containing various hole sizes have been modeled. The void fraction was held at 0.5% while the spherical hole sizes were varied from 5.0- to 0.00005 mm radius. The shock pressure was also varied.

As the hole size in TATB was varied from 5.0 to 0.5 mm, the explosive became more sensitive to shock. Decreasing the hole size to 0.0005 mm resulted in failure of the shock wave to build toward a propagating detonation. This is similar to the results previously reported for TNT.

HMX became more sensitive to shock as the hole size was varied from 0.5 to 0.005 mm. The hole size had to be decreased to 0.0005 mm before the explosive became less shock sensitive. Smaller hole sizes (0.00005 mm) resulted in failure of the shock wave to build to detonation.

At the same density, the most shock-sensitive explosive is the one with particle sizes between coarse and fine material. The shock sensitivity of HMX continues to increase with decreasing hole sizes for hole sizes where TNT or TATB fail.

The shock sensitivity of TATB, TNT, and HMX increases with initial temperature. TATB at 250°C is as shock-sensitive as HMX at 25°C. This is in agreement with experimental observations. The shock sensitivity of HMX is less dependent on temperature than TATB or TNT.

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INTRODUCTION

The effects of particle size and the resulting hole or void size on the shock initiation properties of cast and pressed heterogeneous explosives have been studied using the wedge test and the gap test for many years. Studies have also been performed investigating the effect of temperature on shock initiation properties of explosives.

Cast TNT has been observed to be less shock-sensitive than pressed TNT at the same density. Cast TNT has fewer and larger holes than pressed TNT, resulting in fewer hot-spots that are too far apart to be as effective in supporting the reactive shock wave as pressed charges with more, although smaller, hot-spots. Campbell, Davis, Ramsay, and Travis[1] have used the wedge test to measure the distance of run to detonation as a function of shock pressure (the Pop plot) for pressed-TNT charges of coarse TNT (200-250 micrometer) and found that they are less shock-sensitive than pressed charges of finer TNT (20-25 micrometers).

Donna Price[2] has reviewed the effect of particle size on the shock sensitivity of pure porous explosives considering both gap test and wedge test data. She showed that in many gap tests, coarse porous explosive seems more shock-sensitive than fine, whereas in most wedge tests, the reverse is true. She concludes that the apparent reversal is actually a result of crossing

Pop plots and that the gap tests sense a lower pressure region than those usually available in wedge test data.

Moulard, Kury, and Delcos[3] studied two special monomodal RDX polyurethane cast PBX formulations of 70 wt% RDX (either 6 micrometer or 134-micrometer medium particle size) and 30 wt% polyurethane. The shock initiation properties of these formulations were measured in thin plate impact, projectile impact, and wedge tests. The formulations containing the fine RDX were significantly less sensitive than those with coarse RDX at the same density of 1.44 g/cc, at least up to 10.0-GPa shock pressure. From these studies we conclude that at the same density, the most shock-sensitive explosives are those with particle sizes between the coarse particles and the very fine particles.

Heterogeneous explosives are initiated and propagate by the process of shock interaction with density discontinuities such as voids. These interactions result in hot regions that decompose and produce increasing pressures, causing more and hotter decomposition regions. The shock wave increases in strength, releasing more and more energy, until it becomes strong enough that all the explosive reacts and detonation begins.

This process is described by the "Hydrodynamic Hot-Spot Model," which models the hot-spot formation from the shock interaction that occurs at density discontinuities and describes the decomposition using the

Arrhenius rate law and the temperatures from the HOM equation of state.[4]

The numerical modeling of the interaction of a shock wave with a single density discontinuity was reported in Ref. (4), where an 8.5-GPa shock interacting with a single spherical hole in nitromethane was studied. The study was extended to four rectangular holes.[4] It was determined that 0.0032-mm-radius cylindrical voids built toward detonation and 0.001-mm-radius voids formed hot-spots that failed to propagate because of rarefactions cooling the reactive wave.

The process of shock initiation of heterogeneous explosives has been analyzed numerically[5] by studying the interaction of shock waves with a cube of nitromethane containing 91 holes. An 8.5-GPa shock interacting with a single 0.002-mm hole did not build toward detonation. When the shock wave interacted with a matrix of 0.002-mm holes, it became strong enough to build toward detonation. When the size of the holes was reduced to 0.00004 mm, a marginal amount of the explosive decomposed to compensate for the energy loss to the flow caused by the shock wave interacting with the holes. The shock wave slowly grew stronger, but it did not build to detonation in the time of the calculation. A 5.5-GPa shock wave interacting with a matrix of 0.002-mm holes resulted in insufficient heating of the resulting hot spots to cause significant decomposition. Desensitization by preshocking resulted when holes were closed by the low-pressure 5.5-GPa shock wave. A higher pressure 8.5-GPa shock wave that arrived later had no holes with which to interact and behaved like a shock wave in a homogeneous explosive until it caught up with the lower pressure preshock wave.

The interaction of a shock wave with a single air hole and a matrix of air holes in PETN, HMX, and TATB was modeled in Ref. (6). The basic differences between shock-sensitive explosives (PETN or HMX) and shock-insensitive explosives (TATB or Nitroguanidine) were described by the hydrodynamic hot-spot model. The desensitization of TATB and resulting quenching of a propagating detonation were also modeled using the hydrodynamic hot-spot model.

The hydrodynamic hot-spot model has been used to model the basic processes in the shock initiation of heterogeneous explosives. Interaction of a shock wave with density discontinuities, the resulting hot-spot formation, interaction, and the build up toward detonation or failure have been modeled. The hydrodynamic hot-spot model has been used to investigate the basic differences between shock-sensitive and shock-insensitive explosives. The hydrodynamic hot-spot model has been used to model the basic processes that occur when a heterogeneous explosive has been shocked with a pressure too low to cause propagating detonation in the time of interest. The explosive is desensitized by the preshock, and a propagating detonation wave can be quenched when the detonation front arrives at the previously shocked explosive.

From the hydrodynamic hot-spot model,[4-8] we can postulate that the coarse particle explosives have fewer holes or voids per unit volume than the fine-particle explosives, resulting in fewer but larger hot-spots. As the explosive particles become finer, the number of hot-spots formed by a shock wave increases while the hot-spot size decreases. When the explosive becomes very fine, the hot-spot size can become so small that the hot-spots cool from side rarefactions before appreciable decomposition can occur. This results in a less shock-sensitive explosive if the explosive has very fine particle sizes. A three-dimensional study[7] of the effect of particle size and the resulting void or hole size on the shock initiation of heterogeneous charges of TNT showed that at the same density, the most shock-sensitive explosive was one with particle sizes between coarse and extremely fine material.

Another result of the hydrodynamic hot-spot model is that explosives with faster Arrhenius kinetics form hot-spots that decompose faster and are less effected by side rarefactions before appreciable decomposition occurs. Explosives with faster Arrhenius kinetics exhibit increasing shock sensitivity with decreasing particle size for smaller particle sizes than explosives with slower kinetics. The effect of increasing the initial temperature of an explosive in the hydrodynamic hot-spot model is to increase the temperature of the hot spots resulting from shock interactions with voids. The hotter hot-spots decompose more and result in faster build up to detonation. Thus, increasing the initial temperature of an explosive without significantly changing the density or density discontinuities results in a more shock-sensitive explosive.

It is known that low temperatures decrease the reliability of marginal boosters to initiate detonation in explosives such as Composition B, PBX-9404, and TNT. The reliability increases at elevated temperatures.

Urizar[9] studied the impact sensitivity of RDX, HMX, and PETN using a Type-12 impact tool and showed a decrease in the 50% point from 27 cm at 20°C to 15 cm at 160°C for RDX. Similar behavior was observed for HMX and PETN. He found that the violence of the explosion increased with increasing temperature. Schwarz[10] showed that a less energetic flyer plate is required to initiate a pellet of TATB when the initial temperature is 260°C compared to that required when the temperature is 25°C. The failure diameter of explosives has been found to decrease with increasing temperatures[11] and since the failure diameter is directly related to the Pop Plot[4] the explosives are more shock-sensitive with increasing temperature.

Ramsay, Craig and Dick[12] performed wedge tests for PBX-9501 (95/2.5/2.5 HMX/Estane/nitroplasticizer), DATB (95/5 DATB/Viton) and TNT at temperatures between 25° and 150°C. A decrease in the distance-to-detonation of approximately 30% for the same input pressure was found for DATB and PBX-9501 at 150°C. A small decrease in distance-to-detonation was found for cast TNT between 24 and 73°C.

The shock initiation of LX-17 (92.5/7.5 TATB/Kel-F) at temperatures between -54°C and 88°C was studied using embedded gauges in Ref. (13). The shock sensitivity increased with increasing temperature.

Recently Dallman[14] performed wedge tests for PBX-9502 (95/5 TATB/ Kel-F) explosive at 75° and 250°C. The PBX-9502 shock sensitivity increased with increasing temperature until at 250°C it was as shock sensitive as PBX-9501 (95/5 HMX/Estane) at pressures greater than 5.0-GPa.

In this paper, we will describe a three-dimensional study of the effect of particle size and the resulting void or hole size on the shock sensitivity of an explosive with slow Arrhenius kinetics (TATB) and an explosive with fast Arrhenius kinetics (HMX). We will also describe a study of the effect of initial temperature and attempt to quantify its expected effect on shock sensitivity.

NUMERICAL MODELING

The three-dimensional Eulerian reactive hydrodynamic code 3DE is described in detail in Ref. (15). It uses techniques identical to those described in Ref. (4) and used successfully for describing two-dimensional Eulerian flow with mixed cells and multicomponent equations of state for modeling reactive flow. It has been used to study the interaction of multiple detonation waves,[16] the basic processes of shock initiation of heterogeneous explosives,[4–8] the reactive hydrodynamics of a matrix of tungsten particles in HMX,[17] and the reaction zone of heterogeneous explosives.[18,19]

The Arrhenius reactive rate law was used with the constants determined experimentally by Raymond N. Rogers and described in Ref. (4). The constants are listed in Table I.

TABLE I

Explosive	Activation Energy (kcal/mole)	Frequency Factor (microseconds^{-1})
HMX	52.7	5.0×10^{13}
TATB	59.9	3.18×10^{13}
TNT	34.4	2.51×10^{5}

The HOM equation-of-state constants used for HMX, TATB and TNT are described in Refs. 7 and 8. The equation of state for the detonation products were described using the BKW equation of state described in Refs. 4 and 20.

A constant velocity piston was applied to the bottom of a explosive cube, shocking the explosive initially to the desired pressure. When the shock wave interacts with a hole, a hot-spot with temperatures several hundred degrees hotter than the surrounding explosive is formed in the region above the hole after it is collapsed by the shock wave. The hot region decomposes and contributes energy to the shock wave, which has been degraded by the hole interaction. Whether this energy is sufficient to compensate for the loss from the hole interaction depends on the magnitude of the initial shock wave, the hole size, and the interaction with the flow from its nearest neighbor hot-spots.

SINGLE HOLE STUDY

The interaction of a shock wave with a single rectangular air hole in HMX and TATB was modeled using the 3DE code. The calculations were performed with 15 x 15 x 22 (i, j, k) cells. The air hole was 5 x 5 x 5 cells located in the center of the i-j plane and the bottom of the hole was 5 cells above the piston. The results of the calculations were classified according to the amount of burn caused by the hot-spot. If the initial burned region was not expanding at the end of the calculation, it was classified as failed. If the initial burn region was expanding along with the front of the shock wave the hot spot was classified as propagating. Intermediate cases where the burn region was expanding, but was behind the shock front were classified as marginal. A summary of the 51 cases modeled is presented in Table II.

By comparing the initiation characteristics as a function of particle size at fixed pressures, we can determine approximate shock sensitivity equivalency. For example we observe from Table II the following:

TATB at 250°C and 50 kbar ≅
TATB at 75°C and 100 kbar ≅
TATB at 27°C and 125 kbar ≅
HMX at 27°C and 75 kbar

or

TATB at 27°C and 150 kbar ≅
TATB at 75°C and 125 kbar ≅
TATB at 250°C and 75 kbar ≅
HMX at 27°C and between
75 and 100 kbar

The hydrodynamic hot spot model can be used to theoretically determine the relative effect of explosive sensitivity as a function of composition, pressure and temperature in a realistic manner using only the HOM equation of state and Arrhenius constants to describe the explosive.

From these results we chose the conditions for the more realistic multiple hole model. Pressures modeled were for cases where the single hole hot-spots decomposed but failed to expand appreciably. For HMX the pressure chosen for the multiple hole model study was 5.0-GPa and for TATB it was 7.5-GPa. The pressure chosen for TNT was 12.5-GPa as described in Ref. 7.

MULTIPLE HOLE STUDY

The interaction of a shock wave with matrix of spherical air holes in HMX, TATB and TNT was modeled with the void fraction held at 0.5% and the hole size varied from 5.0 to 0.00005 mm radius.

Calculations were performed using 22 x 20 x 111 (i, j, k) or 48,840 cells with a hole diameter of at least two cells. The spherical air holes were placed on a hexagonal close-packed lattice. Five layers of cells above the piston did not contain any holes. With 2 cells per sphere diameter, the matrix contains a maximum of 60 holes.

The densities used for HMX were 1.90 at 27°C, 1.8864 at 75°C, and 1.8385 at 250°C. The densities used for TATB were 1.937 at 27°C, 1.9245 at 75°C and 1.8756 at 250°C.

A summary of the multiple air hole calculations is given in TABLE III.

The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for TATB with a matrix of 0.05-mm-radius holes at 27°C in Figure 1, and at 75°C in Figure 2. The amount of decomposition increases with temperature with propagation of detonation occurring at 75°C. The detonation occurs quicker at 250°C than 75°C.

The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for HMX with a matrix of 0.05 mm air holes at 27°C in Figure 3, which is marginal, and for 0.005 mm air holes in Figure 4 which propagates. In Figures 5 and 6 the air holes are 0.00005 mm radius at 27°C in Figure 5 and 250°C in Figure 6. The matrix of holes fails to form a propagating detonation at 27°C and propagates at 250°C.

The most sensitive HMX explosive is the one with particle sizes between coarse and very fine explosive. The hole size for a matrix of HMX with maximum sensitivity is two orders of magnitude smaller than for TATB as are the hole size for failure to occur.

CONCLUSIONS

The hydrodynamic hot-spot model describes the basic differences between the shock-sensitive and shock insensitive explosives. The interaction of a shock wave with air holes in HMX, TATB and TNT, the resulting hot-spot formation, interaction and the build up toward detonation or failure have been modeled. An increase in hole size results in larger hot-spots that decompose more of the explosive, add their energy to the shock wave, and result in increased sensitivity to shock. An increase in number of holes also results in more hots spots that decompose more explosive and increase the sensitivity of the explosive to shock. The interaction between hole size and number of holes is complicated and requires numerical modeling for adequate evaluation of specific cases. The hole size can become sufficiently small that the hot spot is cooled by side rarefaction before appreciable decomposition can occur. Since increasing the number of holes, while holding the percentage of voids present constant, results in smaller holes, we have competing processes that may result in either a more or less shock sensitive explosive. If the hole size is below the critical hole size, then the explosive will become less sensitive with increasing number of holes of decreasing diameter.

Increasing the temperature of an explosive causes a small decrease in density which results in slightly lower pressure hot-spots; however the resulting hot spot is hotter for the higher temperature explosives. More of the hot-spot explosive decomposes resulting in an increasing shock sensitivity with increasing temperature. The hydrodynamic hot-spot model indicates that the effect of temperature is greatest for the explosives with slower Arrhenius decomposition rates. The model gives about the same shock sensitivity for TATB at 250°C as for HMX at 25°C, which is in agreement with the experimental observations[14].

The hydrodynamic hot-spot model can be used to evaluate the relative effect of explosive shock sensitivity as a function of composition, pressure, temperature, and density (as represented by the number and sizes of the holes present for hot-spot generation).

A higher decomposition rate results in explosives that exhibit a decrease in sensitivity with particle size at smaller particle sizes than explosives with slow rates. The faster decomposition rate results is less time for the hot spot to be cooled before complete decomposition has occurred.

The hydrodynamic hot-spot model has resulted in an increased understanding of the effect of hole size, number of holes, explosive Arrhenius decomposition rate, initial temperature and shock pressure on shock initiation of heterogeneous explosives. The hydrodynamic hot-spot model reproduces the observed shock initiation behavior. This indicates that the dominate features are shock heating by hydrodynamic hot spot formation, cooling by rarefactions and the Arrhenius decomposition rate as a function of temperature.

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TABLE II
Single Air Hole

Explosive	Hole Size mm	Temperature Deg K	Pressure GPa	Result
TATB	0.5	300	7.5	failed
TATB	0.5	300	10.0	marginal
TATB	0.5	300	12.5	propagated
TATB	0.05	300	12.5	marginal
TATB	0.005	300	12.5	failed
TATB	0.0005	300	12.5	failed
TATB	0.5	300	15.0	propagated
TATB	0.05	300	15.0	propagated
TATB	0.005	300	15.0	marginal
TATB	0.0005	300	15.0	failed
TATB	0.5	348	7.5	marginal
TATB	0.05	348	7.5	failed
TATB	0.005	348	7.5	failed
TATB	0.0005	348	7.5	failed
TATB	0.5	348	10.0	propagated
TATB	0.05	348	10.0	marginal
TATB	0.005	348	10.0	failed
TATB	0.0005	348	10.0	failed
TATB	0.5	348	12.5	propagated
TATB	0.05	348	12.5	propagated
TATB	0.005	348	12.5	marginal
TATB	0.0005	348	12.5	failed
TATB	0.5	523	5.0	propagated
TATB	0.05	523	5.0	marginal
TATB	0.005	523	5.0	failed
TATB	0.0005	523	5.0	failed
TATB	0.5	523	7.5	propagated
TATB	0.05	523	7.5	propagated
TATB	0.005	523	7.5	marginal
TATB	0.0005	523	7.5	failed

TABLE II
(Continued)

Explosive	Hole Size mm	Temperature Deg K	Pressure GPa	Result
HMX	0.5	300	5.0	failed
HMX	0.5	300	7.5	propagated
HMX	0.05	300	7.5	marginal
HMX	0.005	300	7.5	failed
HMX	0.0005	300	7.5	failed
HMX	0.5	300	10.0	propagated
HMX	0.05	300	10.0	propagated
HMX	0.005	300	10.0	propagated
HMX	0.0005	300	10.0	marginal
HMX	0.5	300	12.5	propagated
HMX	0.05	300	12.5	propagated
HMX	0.005	300	12.5	propagated
HMX	0.0005	300	12.5	marginal
HMX	0.5	348	5.0	failed
HMX	0.05	348	5.0	failed
HMX	0.005	348	5.0	failed
HMX	0.0005	348	5.0	failed
HMX	0.5	348	7.5	propagated
HMX	0.05	348	7.5	propagated
HMX	0.005	348	7.5	marginal
HMX	0.0005	348	7.5	failed

TABLE III
Multiple Air Holes

Explosive	Hole Size mm	Temperature Deg K	Pressure GPa	Result
TATB	5.0	300	7.5	Propagates
TATB	0.5	300	7.5	Propagates
TATB	0.05	300	7.5	Marginal
TATB	0.005	300	7.5	Marginal
TATB	0.05	348	7.5	Propagates
TATB	0.05	523	7.5	Propagates
TATB	0.05	523	5.0	Propagates
TNT	5.0	300	12.5	Propagates
TNT	0.5	300	12.5	Propagates
TNT	0.05	300	12.5	Marginal
TNT	0.005	300	12.5	Fails
HMX	0.05	300	5.0	Marginal
HMX	0.005	300	5.0	Propagates
HMX	0.0005	300	5.0	Marginal
HMX	0.00005	300	5.0	Fails
HMX	0.00005	348	5.0	Fails
HMX	0.00005	523	5.0	Propagates

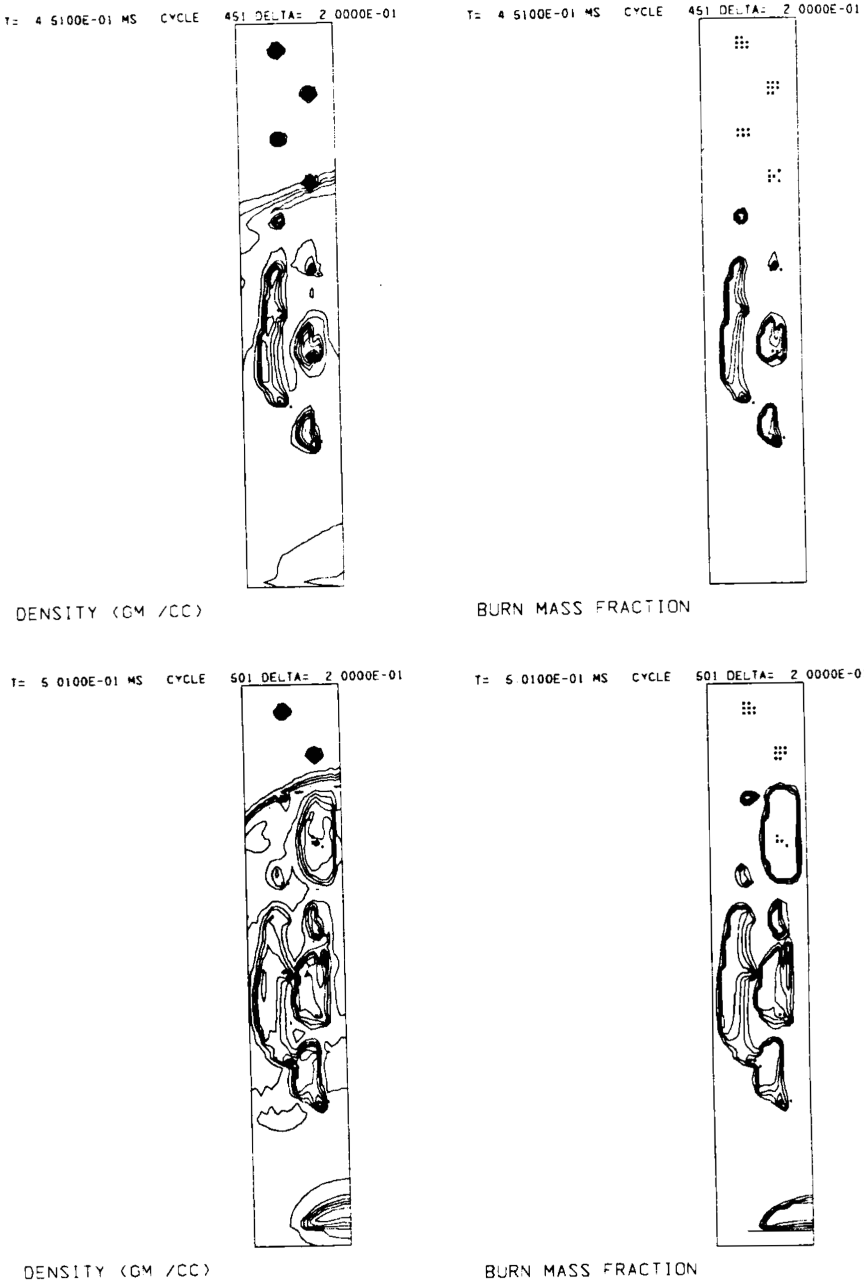

Figure 1. The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for TATB with a matrix of 0.05 mm radius holes at 27°C. The density contour interval is 0.2 gm/cc and the mass fraction contour interval is 0.2. The shock pressure is 7.5 GPa. The initiation is marginal.

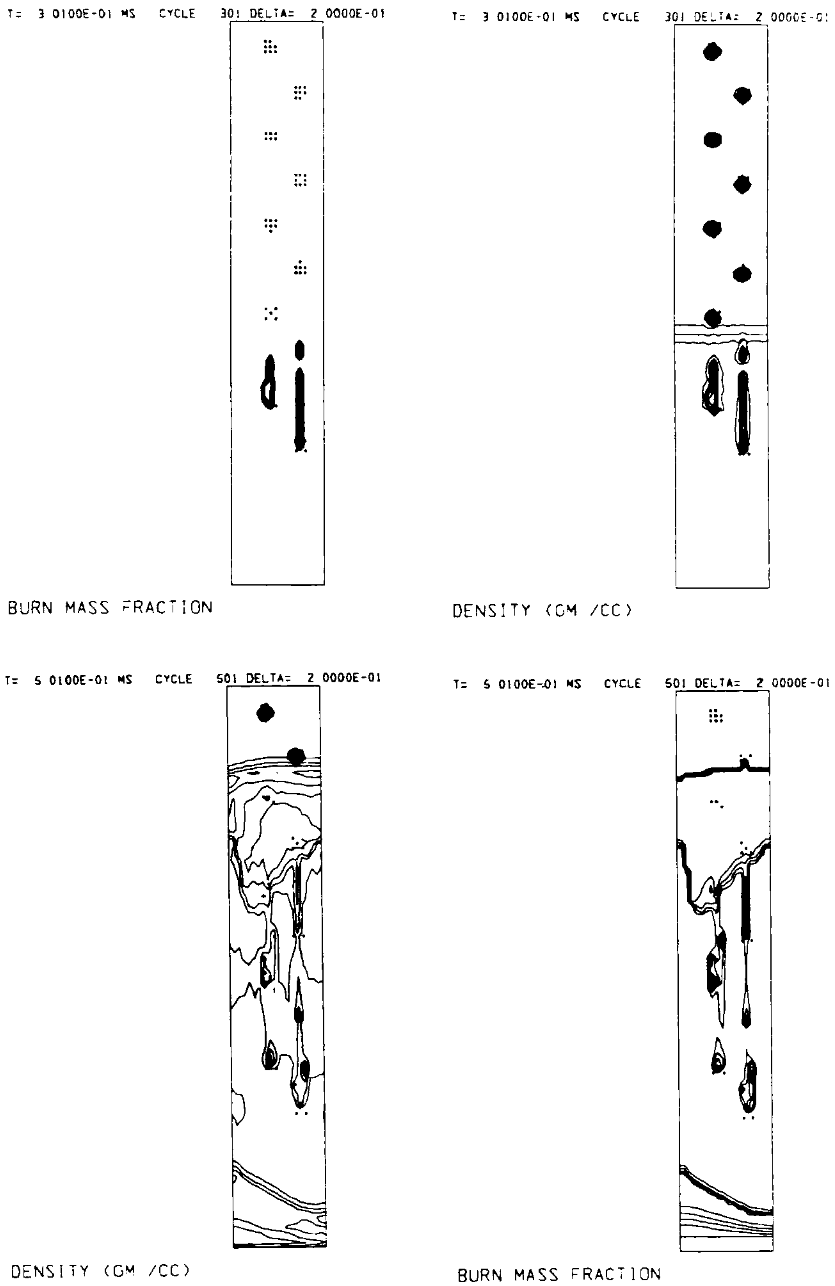

Figure 2. The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for TATB with a matrix of 0.05 mm radius holes at 75°C. The density contour interval is 0.2 gm/cc and the mass fraction contour interval is 0.2. The shock pressure is 7.5 GPa. The initiation propagates a detonation.

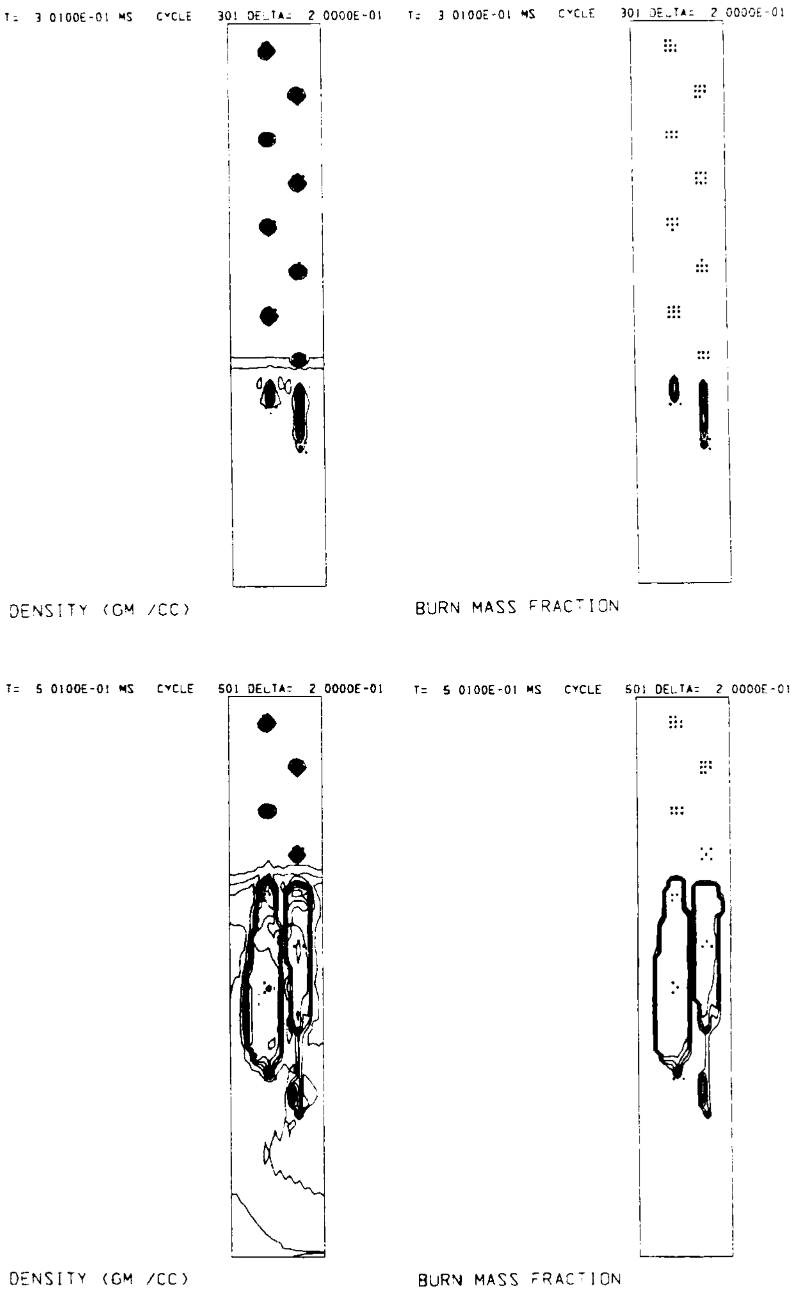

Figure 3. The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for HMX with a matrix of 0.05 mm radius holes at 27°C. The density contour interval is 0.2 gm/cc and the mass fraction contour interval is 0.2. The shock pressure is 5.0 GPa. The initiation is marginal.

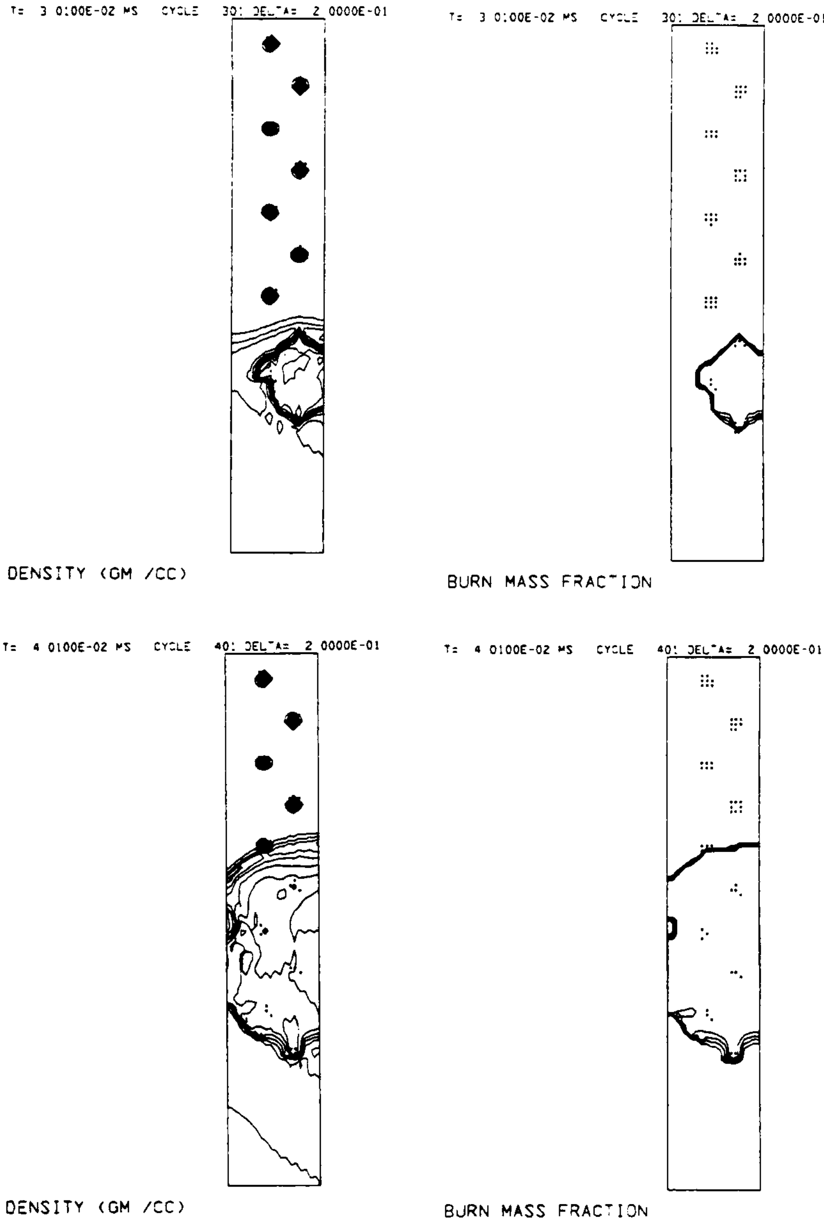

Figure 4. The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for HMX with a matrix of 0.005 mm radius holes at 27°C. The density contour interval is 0.2 gm/cc and the mass fraction contour interval is 0.2. The shock pressure is 5.0 GPa. The initiation propagates.

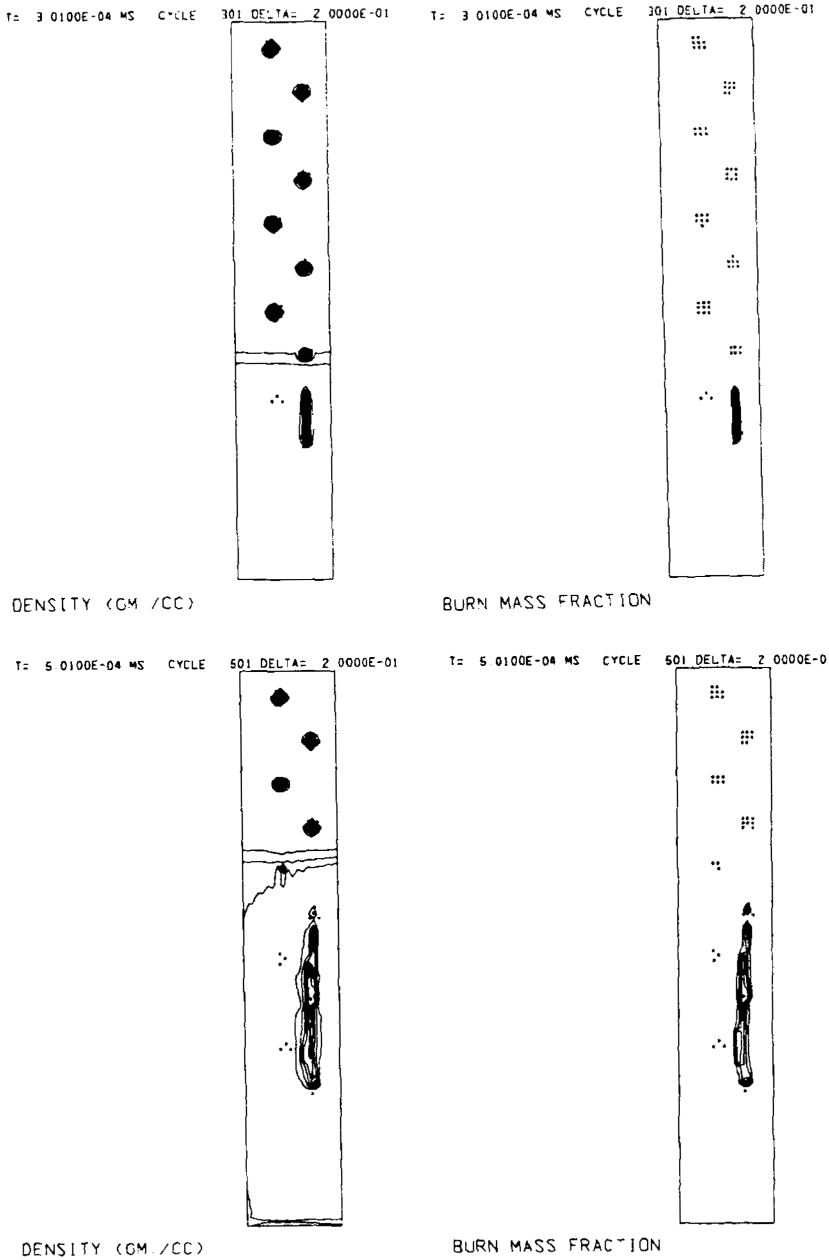

Figure 5. The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for HMX with a matrix of 0.00005 mm radius holes at 27°C. The density contour interval is 0.2 gm/cc and the mass fraction contour interval is 0.2. The shock pressure is 5.0 GPa. The hot spots fail to initiate the explosive.

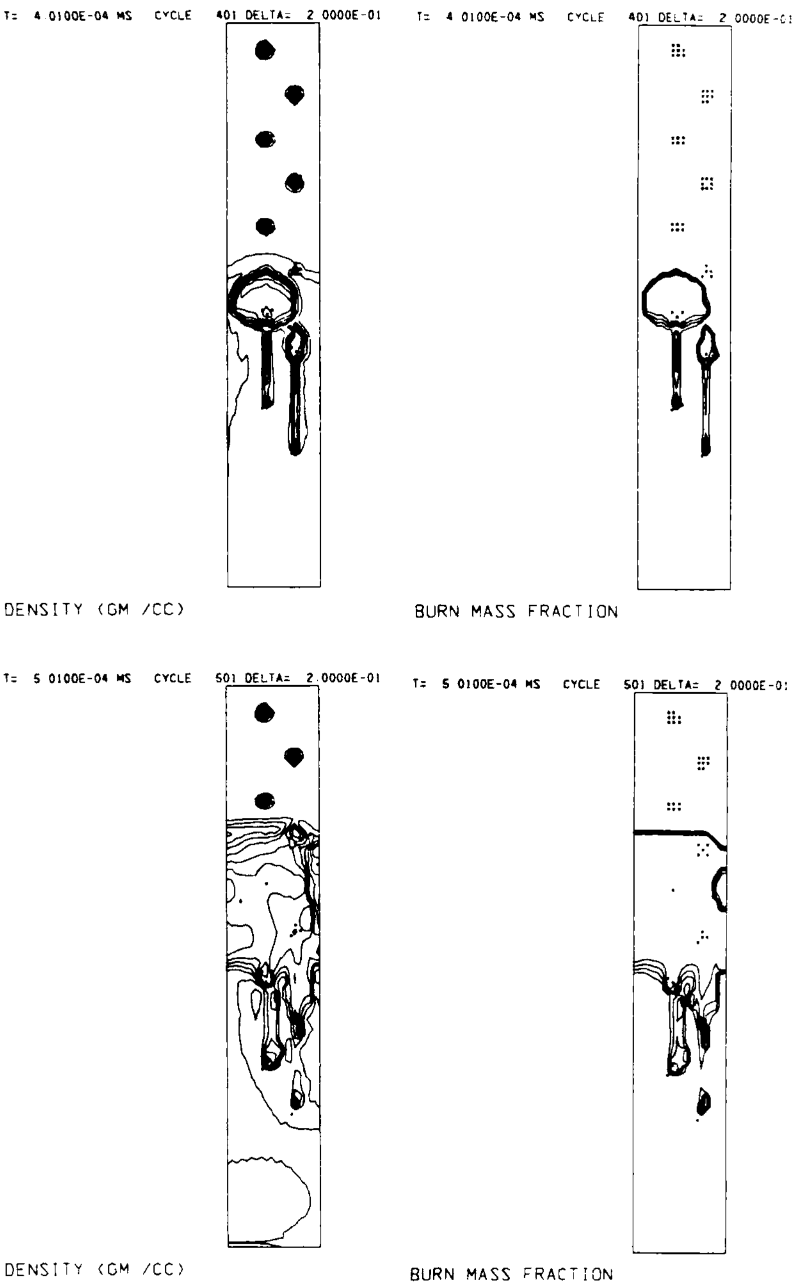

Figure 6. The density and mass fraction of undecomposed explosive cross sections through i=11 are shown at various times for HMX with a matrix of 0.00005 mm radius holes at 250°C. The density contour interval is 0.2 gm/cc and the mass fraction contour interval is 0.2. The shock pressure is 5.0 GPa. The initiation propagates.

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