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Effect of thermal pressure in converging detonation waves

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Abstract. Propagation of converging detonation waves in various explosives is studied using the equation of state, which considers both the thermal and elastic pressures. It is seen that the rate of increase of thermal pressure is higher than that of the elastic pressure during convergence. The present equation of state is better since it also gives the variation of temperature, whereas the polytropic form of the equation of state is independent of temperature. It is seen that the total detonation pressure is slightly greater than the elastic pressure. Results are compared with those reported elsewhere.

Keywords. Converging detonations; thermal pressures in detonation.

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1. Introduction

Convergence of detonation waves in solid explosives is of immense importance, when very high pressures and temperatures are required. The problem of converging detonation waves in solid and gaseous explosives was studied by various authors (Abarbanel 1967; Lee 1967; Singh 1978, 1983), using the polytropic equation of state. Mader (1979) used BKW equation of state and studied the convergence of detonation waves in solid explosives by numerical methods. It was shown by Singh (1981) that BKW equation of state gives much lower pressures than that given by the polytropic equation of state (Singh 1978, hereafter to be referred as paper I). It is known that explosive products are not purely solids but have dual character—that of solids as well as gases. For such types of media, Hornberg (1978) suggested an equation of state, where thermal as well as elastic pressures were considered. Such an equation was first suggested by Zeldovich and Kompaneets (1960) which Hornberg called Zeldovich's generalised equation of state of solid explosives.

We have studied the convergence of detonation waves in solid explosives using Zeldovich's generalised equation of state. Jump conditions for over-driven detonation waves are derived in § 2. Variations of pressure and temperature as the detonation wave converges are studied in § 3. The results are discussed in § 4.

2. Formulation of the problem

Let us assume that a spherical detonation wave travels from the surface of a solid explosive charge, towards its centre. At any time t, let R be the position of the detonation front, where R is measured from the centre of convergence. Let p, ρ, U and u

be the pressure, density, over-driven detonation velocity and particle velocity of detonation products respectively. The quantities behind the detonation front are related with those ahead of it by

$$\rho(U-u)=\rho_0 U, \tag{1}$$

$$\rho(U-u)^2+p=\rho_0 U^2, \tag{2}$$

$$\tfrac{1}{2}(U-u)^2+E+\frac{p}{\rho}=\tfrac{1}{2}U^2+Q, \tag{3}$$

where E is the internal energy and ρ_0 is the density of the unexploded charge. It is assumed that the heat of detonation Q remains constant during the process of convergence, and is given by (Hornberg 1978)

$$Q=[n+(1+\Gamma)y]\left[\frac{1}{(n-1)}+\frac{y}{\Gamma}-\frac{(1+y)^2}{2[n+(1+\Gamma)y]}\right]D^2, \tag{4}$$

where Q is measured per unit mass and y is a function of temperature T and is given by

$$y=\left[\frac{p/\rho}{c_v\Gamma T}-1\right]. \tag{5}$$

In the above relation c_v, Γ and T are respectively the specific heat at constant volume, the Grüneisen constant and the temperature of detonation products. y is defined as the ratio of thermal pressure to elastic pressure (Hornberg 1978)

$$y=\frac{c_v\Gamma v^{n-1}T}{\bar{C}}, \tag{6}$$

where $\bar{C}$ is defined in (7). Total pressure of detonation products is defined as the sum of elastic and thermal pressures and is given as follows

$$p=\bar{C}\rho^n+\frac{c_v\Gamma T}{v}, \tag{7}$$

where the first term gives the elastic pressure and the second term the thermal pressure and v is inverse of density ρ. Internal energy E is given by

$$E=\frac{p}{(n-1)\rho}\left[1+\frac{(n-1)}{\Gamma}y\right]. \tag{8}$$

Equations (1)–(8) show that there are seven unknown quantities p, U, u, ρ, E, y and T, to solve which we have six equations (1)–(3), (5), (6) and (8). Solving these equations using (4) and taking z and y as independent parameters, one gets

$$u=\frac{(1+\bar{y})DF}{(n+1)\bar{f}_1} \tag{9}$$

$$U=Dz/F \tag{10}$$

$$\rho/\rho_0=\frac{(n+1)\bar{f}_1 z}{n\bar{f}_4 G^2 z_0}, \tag{11}$$

where

$$z = \frac{(n+1)\bar{f}_1 p}{(1+\bar{y})\rho_0 D^2},$$

$$\left.\begin{aligned} f_1 &= \left[1 + \left(\frac{2+\Gamma}{n+1}\right) y\right] \\ f_2 &= \left[1 + \frac{(n-1)(2+\Gamma)}{\Gamma(n+1)} y\right] \\ f_3 &= \left[1 + \frac{(n-1)}{\Gamma} y\right] \\ f_4 &= \left[1 + \frac{(1+\Gamma)}{n} y\right]. \end{aligned}\right\} \tag{12}$$

$$\left.\begin{aligned} F &= \left[1 + \frac{2f_3}{(n+1)f_2}\left\{\frac{(n+1)\bar{f}_1}{(1+\bar{y})}(z-z_0) - 1 + z_0\right\}\right]^{1/2} \\ G &= \left[1 + \frac{(n-1)(1+y)\bar{f}_1(z-z_0)}{n f_2 \bar{f}_4 z_0} \right. \\ &\quad \left. + \frac{(1+y)(1+\bar{y})(n-1)}{n(n+1)f_2\bar{f}_4}\left(\frac{z_0-1}{z_0}\right)\right]^{1/2} \\ z_0 &= \left[\frac{(1+y)\bar{f}_3}{(1+\bar{y})f_3}\right] \end{aligned}\right\} \tag{13}$$

The sound velocity c is given by

$$c = \frac{n}{(n+1)} \frac{DG\bar{f}_4}{\bar{f}_1}\left(\frac{\bar{f}_3 f_4}{f_3 \bar{f}_4}\right)^{1/2}. \tag{14}$$

In relation (9)–(13), the bar above the symbols denotes the value of the functions at the Chapman-Jouguet (abreviated as C-J plane) surface. At the C-J plane $z = 1$ and (1)–(3) reduce to (21) of Hornberg (1978) for non-overdriven detonation waves.

Equations (9)–(11) are the generalised form of jump conditions for the equation of state (7). If we put $y = 0$ these equations reduce to equations (1)–(4) of paper I.

Equations (9) to (11) relate U, u and ρ/ρ_0 with y and z which are still unknown. It is our aim to express them as a function of the radius of convergence. Thus we require two extra relations to express all detonation parameters in terms of the radius of convergence R. Once y is determined, temperature T can be evaluated from (6). One extra relation is obtained by the Whitham's method of characteristics (Whitham 1958), which is discussed in §3.

3. Variation of pressure with the ratio of convergence

Following paper I, we use the equation of motion along the positive characteristic axis as the extra relation relating detonation parameters. The characteristic form of the equation of motion is

$$\mathrm{d}p+\rho u\,\mathrm{d}u+\frac{2\rho c^2 u}{(u+c)}\frac{\mathrm{d}R}{R}=0 \tag{15}$$

where c is the sound velocity behind the detonation front. Substituting for p, ρ, c and u from (9)–(14) in (15), one gets after simplifications,

$$H_1(\mathrm{d}y/\mathrm{d}R)+H_2(\mathrm{d}z/\mathrm{d}R)+H_3=0 \tag{16}$$

where

$$H_1=\frac{z}{FGz_0}\left(\frac{\overline{f}_3 f_4}{f_3\overline{f}_4}\right)^{1/2}\left(\frac{n-1-\Gamma}{\Gamma}\right)\left(\frac{n-1}{\Gamma}\right)\left[\frac{2(z-z_0)(n-1)\overline{f}_1}{(n+1)(1+\overline{y})f_2^2}-\frac{2(n-1)(1-z_0)}{(n+1)^2 f_2^2}+\frac{2n\overline{f}_3\overline{f}_4}{(n+1)(1+\overline{y})f_2 f_3}\right] \tag{17}$$

$$H_2=\left[1+\overline{y}+\frac{\overline{f}_1 f_3 z}{f_2 F G z_0}\left(\frac{\overline{f}_3 f_4}{f_3\overline{f}_4}\right)^{1/2}\right] \tag{18}$$

$$H_3=\frac{2nz}{R}\left[\frac{(1+y)F f_4}{(1+\overline{y})F+nG\overline{f}_4(\overline{f}_3 f_4/f_3\overline{f}_4)^{1/2}}\right] \tag{19}$$

Equation (16) is a non-linear differential equation in y and z. In order to solve this equation, we require one more relation in $\mathrm{d}y/\mathrm{d}R$ and $\mathrm{d}z/\mathrm{d}R$ which is obtained from (6) and (7) with the help of (11) as

$$G_1(\mathrm{d}z/\mathrm{d}R)=G_2(\mathrm{d}y/\mathrm{d}R) \tag{20}$$

where

$$G_1=\left[\frac{n-1}{z}-n\left(\frac{G^2-1}{G^2}\right)\frac{\overline{f}_1}{f_5}\right], \tag{21}$$

$$G_2=\left[\left(\frac{n-1}{1+y}\right)-\frac{n(n-1)}{\Gamma f_3}+n\left(\frac{G^2-1}{G^2}\right)\left\{\left(\frac{n-1}{\Gamma}\right)\left(\frac{n-1-\Gamma}{(n+1)f_2 f_3}\right)+\frac{nf_4 z_0(n-1-\Gamma)}{(n+1)\Gamma(1+y)f_3 f_5}\right\}\right]. \tag{22}$$

Function f_5 in (21) and (22) is given as

$$f_5=\frac{(1-z_0)n\overline{f}_4}{(n+1)}\left[1+\frac{(z-1)(1+\overline{y})}{n\overline{f}_4(1-z_0)}\right]. \tag{23}$$

Solving (16) and (20) for $\mathrm{d}z/\mathrm{d}R$, $\mathrm{d}y/\mathrm{d}R$ we get

$$\mathrm{d}y/\mathrm{d}R=-H_3G_1/[H_1G_1+H_2G_2], \tag{24}$$

$$\mathrm{d}z/\mathrm{d}R=-H_3G_2/[H_1G_1+H_2G_2]. \tag{25}$$

Equations (24) and (25) are two differential equations which give the variation of y and z in terms of the radius of convergence R. T is obtained from (6). Once z and y are known, other parameters can be obtained from the jump conditions (9)–(11).

4. Discussion of results and conclusions

Equations (24) and (25) are integrated by the Runge-Kutta method of fourth order, using a computer DEC-20. Variations of detonation parameters are calculated for four basic explosives and one mixture *i.e.* PETN, RDX, TETRYL, TNT and composition-B (RDX:TNT; 60:40). To calculate y, c_v and values of Γ for the detonation products of the explosives are required. We have calculated c_v using input data given by Mayer (1981). Value of c_v and Γ are given in table 1. To evaluate Γ we have taken $(\partial \ln D/\partial \ln \rho_0) = 0{\cdot}81$ as given by Zeldovich and Kompaneets (1960).

Figure 3 gives a plot of the variation of y and T with (R/R_0), where R_0 is the total radius of the charge. It is seen that y first decreases and then increases, *i.e.* initially the rate of increase of elastic pressure is greater as compared to the thermal pressure but later on in few cases (*e.g.* TNT) the thermal pressure becomes greater. Variation of y *i.e.* ratio of thermal pressure to elastic pressure for five explosives are given in table 2 and the total pressure is given in table 3. From figure 4, it is seen that during convergence, the thermal pressure increases at a higher rate compared to the elastic pressure. The

Table 1. Values of the characteristic detonation parameters of high explosives.

Explosive	ρ_0 (g/cc)	D (m/s)	n	Γ	c_v (cal/g-degree)	$\bar{y}$	$\bar{C} \times 10^{10}$
RDX	1·64	8475	3·02	0·5603	0·3654	0·2126	2·77
Tetryl	1·64	7556	2·97	0·4950	0·3755	0·2364	2·29
PETN	1·65	7854	3·04	0·5862	0·3331	0·2381	2·32
Comp-B	1·69	7862	2·75	0·1985	0·3746	0·0784	2·80
TNT	1·64	6950	3·16	0·7396	0·3913	0·3756	1·66

Table 2. Variation of y vs R/R_0 for various explosives.

Distance R/R_0	TNT	PETN	Tetryl	Comp-B	RDX
1·0	0·3757	0·2381	0·2362	0·0784	0·2126
0·9	0·3653	0·2314	0·2295	0·0759	0·2067
0·8	0·3558	0·2251	0·2228	0·0735	0·2012
0·7	0·3470	0·2198	0·2169	0·0713	0·1967
0·6	0·3413	0·2167	0·2121	0·0695	0·1938
0·5	0·3402	0·2166	0·2100	0·0686	0·1943
0·4	0·3478	0·2229	0·2130	0·0693	0·2005
0·3	0·3740	0·2419	0·2264	0·0737	0·2186
0·2	0·4487	0·2949	0·2665	0·0870	0·2684
0·1	0·7419	0·4879	0·4163	0·1322	0·4479
0·09	0·8181	0·5356	0·4516	0·1422	0·4921
0·08	0·9223	0·5974	0·4972	0·1547	0·5477
0·07	1·0377	0·6803	0·5570	0·1700	0·6227

Table 3. Variation of pressure p (kbar) vs R/R_0 for various explosives.

Distance R/R_0	TNT	PETN	Tetryl	Comp-B	RDX
1·0	210·646	290·576	253·873	287·203	312·943
0·9	227·498	292·316	274·183	310·176	337·978
0·8	248·562	320·736	299·570	338·896	370·837
0·7	278·053	358·629	332·574	376·232	413·084
0·6	315·969	405·995	378·271	427·929	475·673
0·5	368·691	476·368	441·739	499·729	550·779
0·4	452·889	584·633	543·288	608·865	675·956
0·3	598·230	768·684	710·845	801·289	888·757
0·2	912·097	1171·970	1068·810	1200·500	1364·430
0·1	2089·610	2620·020	2325·480	2492·900	3029·280
0·09	2411·900	3004·360	2640·280	2803·070	3473·660
0·08	2864·780	3518·620	3059·170	3202·280	4052·260
0·07	3380·870	4235·880	3630·380	3719·240	4866·260

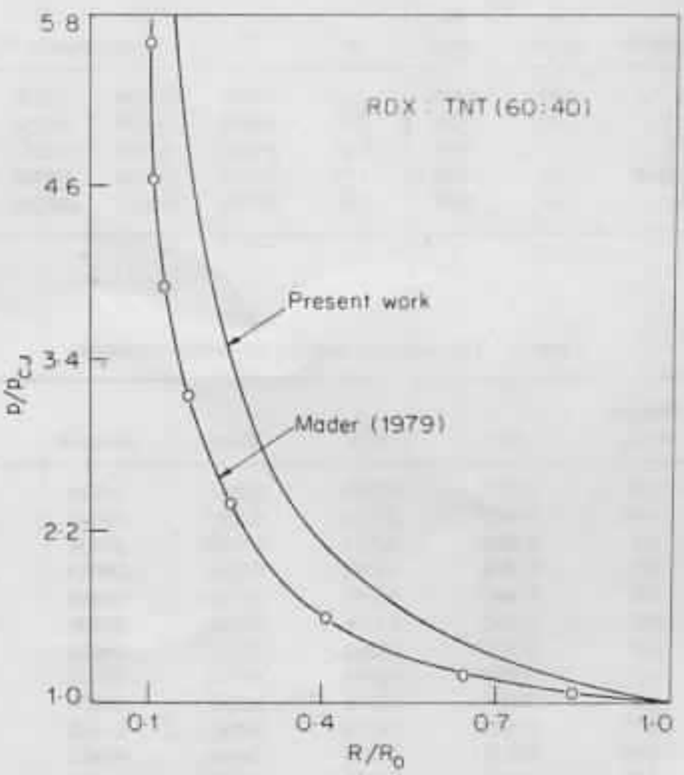

Figure 1. Variation of p/p_{CJ} vs R/R_0 due to convergence of detonation in a typical explosive (composition-B).

pressure when the polytropic equation of state is used (paper I), is initially lower but becomes higher than the total pressure of the present paper, as the detonation wave moves towards the centre of convergence. A typical case of composition-B is shown in figure 2.

Figures 1 and 2 give the variation of p/p_{CJ} and U/D vs (R/R_0) as the detonation wave converges from its initial radius R_0 to the centre of convergence. Results are compared with that of Mader (1979). The pressure and detonation velocity obtained by present method is slightly greater as compared to that of Mader (1979). This is because we have used a different equation of state. Mader has used the BKW equation of state with Arrhenius rate law. It is to be noted that BKW equation of state is calibrated for CJ values of detonation parameters and its accuracy at higher pressures is under question. Moreover it has been shown (Singh 1981) that the BKW equation of state gives much lower pressures as compared to that given by polytropic equation of state. This lower trend of Mader's values may be due to BKW equation of state only. We have not come across any experimental data, by which the law of convergence in explosives may be verified.

The Zeldovich equation of state is more realistic as it reduces to other forms of equations of state in special cases. The equation reduces to

$$pv = RT$$

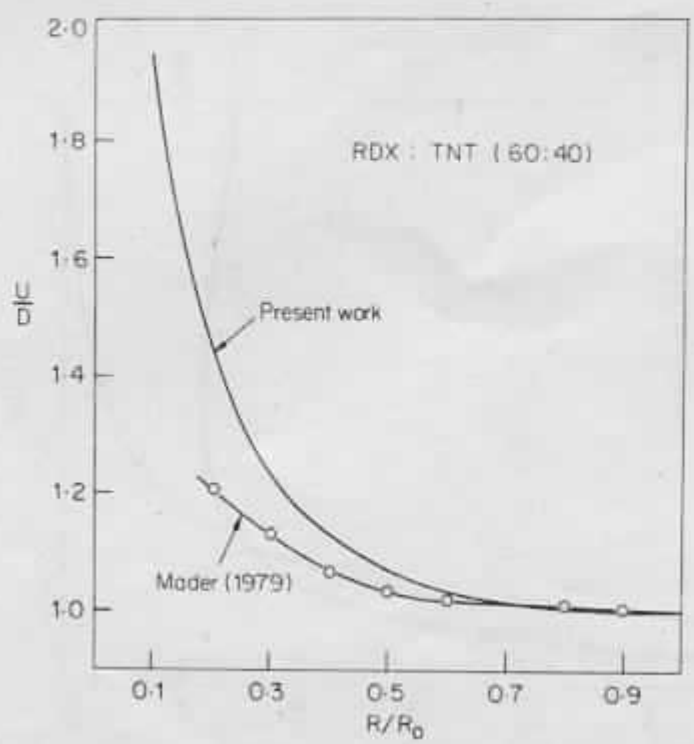

Figure 2. Variation of U/D vs R/R_0 due to convergence in composition-B.

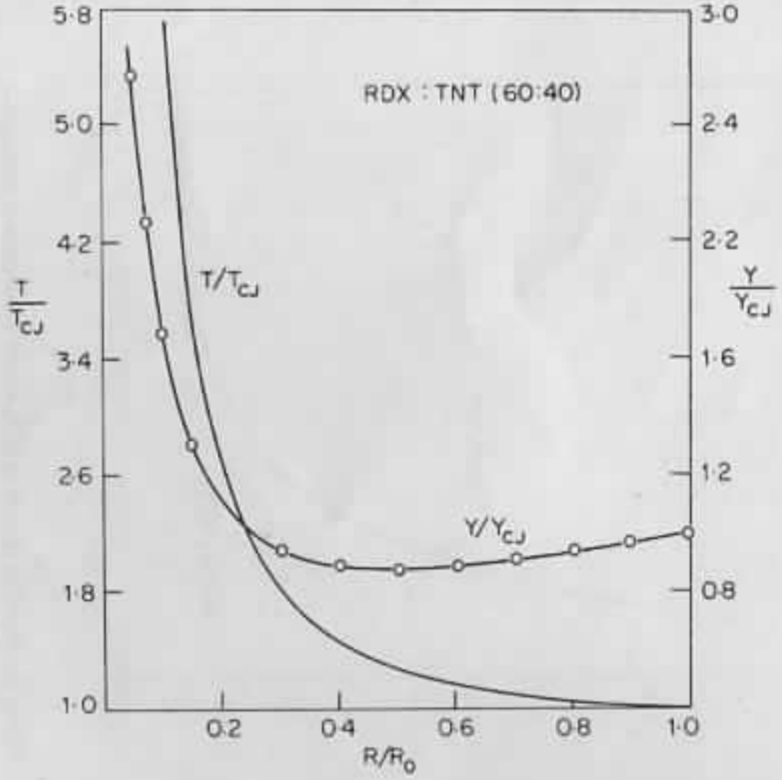

Figure 3. Variation of pressure ratio y and temperature T vs R/R_0 due to convergence in composition-B.

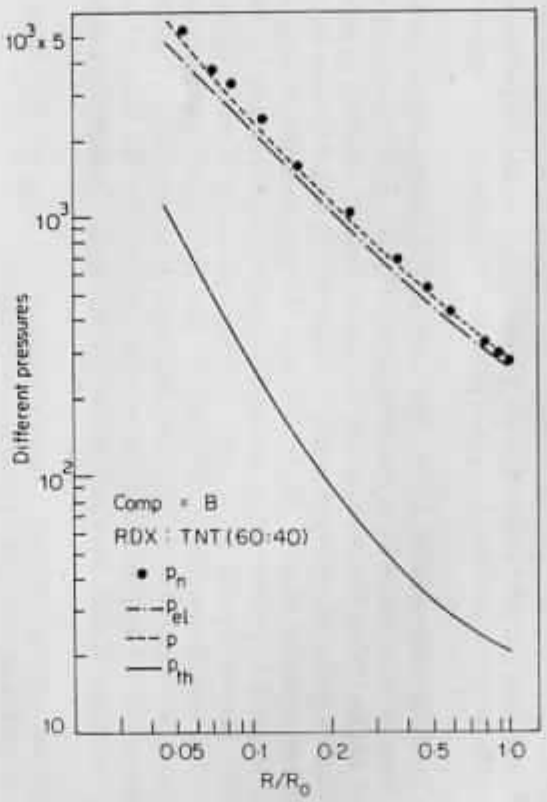

Figure 4. Variation of different pressures due to convergence in composition-B.

for $y \to \infty$ and $p = \tilde{C}\rho^{n}$ for $y = 0$. This means, it represents both gaseous and solid behaviour of detonation products. The only approximation in the present paper is regarding heat of detonation, which is assumed to be constant during the process of convergence.

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