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EQUATION OF STATE OF HIGH EXPLOSIVE AND CALCULATION OF DETONATI N WAVES

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ABSTRACT

This report summarizes the derivation of the equation of state of H. E. (Composition 'B' at density $\rho_0 = 1.67$) used in the most recent implosion calculations, and includes condensed tables of the important variables. The results of calculations on various types of detonation wave made with this equation of state are reported, and compared with earlier calculations based on γ - law equations.

In a fundamental report on detonation waves [1), G. I. Taylor has given the theory of plane and expanding waves and the results for detonation waves in TNT, using an equation of state for the explosive gases found by Jones. In this report we give a brief account of the derivation of the equation of state used here in various numerical calculations and of the results of calculations on detonation waves.

1. Equation of State

The first numerical calculations made on detonation waves used a $\gamma = 3$ equation of state for the explosive, and neglected changes of entropy. Experiments had indicated that this form was a fair approximation for pressures of the order of the detonation pressure, though it was certainly in error at lower pressures; furthermore this form was well adapted to certain analytic and semi-analytic calculations.

Subsequently, however, a desire for greater accuracy in implosion calculations led to the use of a somewhat more accurate equation of state. In his report [2), Jones has calculated the normal (Chapman-Jouguet) adiabatic for certain explosives, T.N.T. at loading densities of 1.0 and 1.5 gm/cm^3, and Composition 'B' at a loading density of 1.5; these were obtained by calculating the composition and thermodynamic properties of the mixture of explosive gases.

For the purpose of calculating the convergent detonation wave in an implosion the equation of state of Composition 'B' was required for a loading density of 1.67 gm/cm^3 and for a range of entropies about normal conditions. To obviate the necessity of making a fresh calculation, analagous to those of Jones, for these cases, the following perturbation method was used.

1) G.I. Taylor, Detonation Waves, A C 639; BM19.
2) RC-371, BM-647, and earlier reports RC-212, RC-306.

The equation of state calculated by Jones is a certain adiabatic $p(v_1 S_1)$ where the subscript $_1$ refers to conditions at the head of an ordinary detonation wave in Composition B at a loading density $\rho_o = 1.5$ gm/cm^3. At the detonation front the internal energy E may be derived from the shock conditions

$$E(v_1, S_1) = 1/2\ p_1(v_o - v_1) \qquad (1)$$

and therefore along the adiabatic

$$E(v_1\ S_1) = (1/2)\ p_1\ (v_o - v_1) - \int_{v_1}^{v} p dv \qquad (2)$$

For entropies S slightly different from S_1 we have

$$E(v, S) = E(v, S_1) + T(S - S_1) \qquad (3)$$

$$p(v, S) = p(v, S_1) - \left(\frac{\partial T}{\partial v}\right)_{S_1} (S - S_1) \qquad (4)$$

Since Jones has given T along his adiabatic, so that $(\partial T/\partial v)_{S_1}$ is also known, the problem is solved when the entropy change $(S - S_1)$ corresponding to the new conditions is determined.

For the Chapman-Jouguet adiabatic the changes in v and S are determined by perturbation of the equation of conservation of energy and of the Chapman-Jouguet condition, combined with equations (3) and (4). However, these conditions involve first and second derivatives of pressure and temperature at the detonation front; these derivatives are somewhat erratic so that the direct application of these conditions does not lead to a satisfactory result. The values finally chosen were obtained by compromising with additional conditions derived from the experimentally determined detonation velocity (7,800 m/sec) and variation of detonation velocity with loading density (3,800 m/sec/gm/cm^3). These values corresponded to a γ - value equal to 3.9, so that the detonation pressure was 0.2073 megabars. The new Chapman-Jouguet adiabatic was then calculated from formula (4); the primary points determined are listed in Table 1 (cf, Table 3 of Jones' paper). The remaining calculations, for higher detonation pressures, were then straightforward.

The equation (4) is of the form

$$p = f_1(v) + \Delta S\, f_2(v) \qquad (5)$$

A condensed table [3] of smoothed values of $f_1(v)$ and $f_2(v)$ is given in Table 2, together with the equation of the Hugoniot curve $p = \psi(v)$ that satisfies the shock conditions.

For the calculation of plane and expanding detonation waves we also need the following quantities,

$$c = v\sqrt{-\partial p/\partial v} \qquad (6)$$

$$\sigma = \int_{v_1}^{v} \sqrt{-\partial p/\partial v}\; dv \qquad (7)$$

$$f = (p/c^2)\; dc^2/dp \qquad (8)$$

The values of these quantities, calculated for the Chapman-Jouguet adiabatic, are given in Table 3.

The low-pressure end of the adiabatic was represented by the empirical formula

$$p = (v/v_o)^{-1.2}\left\{ .0072456 + \frac{0.0153190}{(v/v_o)} + \frac{0.113443}{(v/v_o)^3} \right\} \text{megabars} \qquad (9)$$

This holds for $(v/v_o) > 2.5$; $v_o = 0.5988$ cm^3/g^m.

2. Plane Detonation Waves

If x denotes the distance travelled by the wave and t the time since initiation, the pressure and velocity distribution in the wave are determined by the equations [4]

$$\left.\begin{aligned} u + c &= x/t \\ u - \sigma &= \text{constant} \end{aligned}\right\} \qquad (10)$$

3) Complete tables are available, prepared by the IBM group.
4) See Taylor's report or LA-1[illegible].

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These solutions are given in Table 4 for the above equation of state and for $\gamma = 3$ $(p = (16/27)\ \rho_0 C^3/D$ with same values of ρ_0, D). The Pressure distribution is also shown in Fig. 1, together with that calculated by Taylor for T.N.T. of density 1.51.

3. Expanding Detonation Waves

The pressure and velocity distribution behind an expanding wave have been calculated as a preliminary to the numerical integration of the air-blast coming from a spherical charge of H.E. The equations determining the solution[4] may be written in the form.

$$\frac{d\psi}{dz} = \frac{\psi\xi}{(1-\xi)^2\psi^2 - \xi^2}\left\{2\xi - f(1-\xi)\psi^2\right\} \qquad (11)$$

$$\frac{d\xi}{dz} = \frac{3\xi^2 - (1-\xi)^2\psi^2}{(1-\xi)^2\psi^2 - \xi^2}\cdot\xi \qquad (12)$$

Here z is the similarity variable

$$z = \log_e (x/Dt) \qquad (13)$$

and

$$\xi = ue^{-z}\ ; \quad \psi = u/c \qquad (14)$$

f is the quantity defined by equation (8), and is a known function of $\phi = \xi e^{z}/\psi$.
The boundary conditions at $z = o$ are

$$\xi = 1/\gamma + 1 \quad ; \psi = 1/\gamma \qquad (15)$$

The first step in the solution was the preparation of a smooth table of values of f as a function of ϕ ; this is reproduced in Table 5. The numerical integration was carried out with ξ as independent variable starting from $z = o$; subsequently, when ξ became small, z was used as independent variable. It was found that ξ and ψ became zero at $z = -0.74$ approximately so that within the sphere $x/Dt = 0.478$ the explosive is at rest at a pressure of .0603 mb. The pressure and velocity distributions for this solution are

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given in Table 6, and for the $\gamma = 3$ equation of state in Table 7. The pressure distributions in the two cases are illustrated in figure (2), together with that calculated by Taylor for T.N.T. of density 1.51.

For the subsequent IBM calculations it was desirable to have the hydrodynamic variables listed as functions of X/Dt, where X is a Lagrangean radial coordinate. It follows from the similarity hypothesis that

$$\frac{X}{Dt} = \left(\frac{1 - \xi}{v/v_o}\right)^{1/3} \frac{x}{Dt} \tag{16}$$

and this quantity is included in Table 5.

For starting the IBM calculation it was useful also to have an expansion of the solution near $z = o$ of the form

$$x/Dt = 1 - a_2\theta^2 - a_3\theta^3 - a_4\theta^4 \tag{17}$$

where

$$\theta^2 = 1 - X/Dt \tag{18}$$

The general formulae for the coefficients a_i are

$$\left.\begin{aligned} a_2 &= \gamma/(\gamma + 1) \\ a_3 &= \frac{4}{3} \cdot \frac{\gamma}{\gamma+1} \Big/ \sqrt{(\gamma+1)\ (f + 2)} \\ a_4 &= \frac{\gamma\ (5 - \gamma)}{3(\gamma+1)^2\ (f+2)} - \frac{\gamma}{(\gamma+1)^2}\left(1 - \frac{p'p'''}{3(p'')^2}\right) \end{aligned}\right\} \tag{19}$$

where γ, f have their values at the detonation front. For the modified Jones' equation of state these have the values

$$\left.\begin{aligned} a_2 &= 0.79592 \\ a_3 &= 0.13283 \\ a_4 &= -0.05 \end{aligned}\right\} \tag{20}$$

The last coefficient is uncertain on account of the p''' term.

4. <u>Convergent Detonation Waves</u>

The first calculations of convergent detonation waves were made with

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the isentropic $\gamma = 3$ equation of state; these were reported in LA-143. Subsequently, another calculation was made elsewhere, also using a $\gamma = 3$ equation of state but admitting changes of entropy according to a perfect-gas law for the Hugoniot curve; this did not differ much from the former, and a comparison of the two solutions was made in a report by J. Calkin, LA-262.

Later a new calculation of the convergent wave was made using the modified Jones' equation of state and formed the basis for all recent implosion calculations (from IBM problem N onwards). The preparatory analytic calculations were reported by J. Keller in LA-424, which also included comparisons of the effect of convergence for different γ - law equations of state.

Complete numerical details of the calculation are available in IBM problem N. We include in this report Figs. 3 and 4 to illustrate this solution; the former represents the variation of detonation pressure with radius of convergence, and the latter the pressure distribution at a time $t = a/2D$ (where a is the initial radius). Comparative curves for γ -laws have been taken from LA-424 and included in these figures.

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TABLE 1

V	P	
Cm^3/gm	$dynes/cm^2$	
.5110	1.6363	$x\ 10^{11}$
.5384	1.5050	
.6084	1.0963	
.6823	8.124	$x\ 10^{10}$
.7568	6.017	
.8335	4.449	
.9154	3.253	
1.012	2.302	
1.138	1.543	
1.331	9.41	$x\ 10^{9}$
1.491	6.986	
1.725	4.790	
2.063	3.233	
2.567	2.094	
3.346	1.323	
4.595	8.168	$x\ 10^{8}$
6.682	4.760	
10.34	2.638	
17.12	1.407	
30.62	6.783	$x\ 10^{7}$
59.96	2.922	
131.4	1.141	
334.1	3.723	$x\ 10^{6}$
1050.4	9.460	$x\ 10^{5}$

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TABLE 2

megabars

V/V_o	$f_1(v)$		$f_2(v)$	$\psi(v)$
.500	.9624		2.114	
.550	.7232		1.738	
.600	.5579		1.507	
.650	.4371		1.260	.4612
.700	.3486		1.048	.3586
.750	.2677		.852	.2702
(CJ) .796	.2073		.693	.2073
.800	.2034		.680	
.850	.1685		.544	
.900	.1442		.440	
.950	.1288		.381	
1.00	.1140		.348	
1.50	.03466		.239	
2.00	.01296		.112	
2.50	.006871		.051	
5.0	1.626	$\times 10^{-3}$		
10.0	5.610	$\times 10^{-4}$		
20.0	2.204			
50.0	6.908	$\times 10^{-5}$		
100.0	2.946			
200.0	1.269			
500.0	4.199	$\times 10^{-6}$		
1000.0	1.824			
∞	0			

$V_o = 0.5988$ cm^3/gm

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TABLE 5

V/V$_o$	C/D	σ/D	f
(CJ) .796	.7959	0	10.13
.800	.7749	.00402	10.81
.820	.6883	.02199	7.66
.840	.6365	.03791	5.58
.860	.5996	.05244	4.58
.880	.5720	.06589	3.63
.900	.5529	.07851	2.39
.920	.5409	.09053	1.70
.940	.5326	.10206	1.19
.960	.5272	.11322	.75
.980	.5240	.12405	.45
1.00	.5219	.13462	.34
1.10	.5095	.18381	.66
1.20	.4913	.22741	1.04
1.30	.4674	.26582	1.44
1.40	.4405	.29949	1.77
1.50	.4132	.32894	1.94
1.60	.3879	.35477	1.88
1.70	.3636	.37758	2.47
1.80	.3365	.39760	2.84
1.90	.3122	.41512	2.49
2.00	.2892	.43053	3.26
2.5	.2077	.4845	
3.0	.1723	.5189	
3.5	.1502	.5437	
4.0	.1354	.5627	
4.5	.12490	.5780	
5.0	.11717	.5908	
10.0	.08825	.6604	
20.0	.07512	.7165	
50.0	.06495	.7803	
100.0	.05949	.8234	
200.0	.05498	.8630	
500.0	.04988	.9110	
1000.0	.04645	.9444	
∞	0	1.4137	

D = 0.78 cm/μsec

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TABLE 4

Plane Detonation Wave (fixed wall)

x/Dt	Jones' Equation of State: u/D	Jones' Equation of State: $P/\rho_0 D^2$	$\gamma = 3$: u/D	$\gamma = 3$: $P/\rho_0 D^2$
1.0000	.2041	.2041	.2500	.2500
.9760	.2001	.2002	.2380	.2382
.8624	.1821	.1840	.1812	.1873
.8037	.1672	.1713	.1519	.1642
.7513	.1517	.1608	.1257	.1452
.7102	.1382	.1517	.1051	.1313
.6785	.1256	.1438	.0893	.1206
.6346	.1020	.1299	.0673	.1082
.6040	.0800	.1178	.0520	.09967
.5298	.0203	.08797	.0149	.08090
.5010	0	.07768	.0005	.07430
.5000			0	.07407
0	0	.07768	0	.07407

TABLE 5

C/D	f
(CJ) .796	11.026
.780	10.927
.760	10.703
.740	10.258
.720	9.457
.700	8.327
.680	7.255
.660	6.488
.640	5.828
.620	5.168
.600	4.572
.580	3.862
.560	2.986
.540	1.724
.520	0.481
.500	0.851
.480	1.264
.460	1.525
.440	1.750
.420	1.950
.400	2.130
.380	2.300
.360	2.460
.340	2.620
.320	2.780
.300	2.940

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TABLE 6

x/Dt	X/Dt	u/D	$P/\rho_o D^2$
1.00000	1.00000	.2041	.2041
.99756	.99697	.1936	.1936
.98821	.98544	.1819	.1820
.96902	.96206	.1687	.1691
.93714	.92416	.1533	.1553
.89314	.87248	.1376	.1410
.84641	.81909	.1220	.1284
.80564	.77460	.1080	.1194
.77101	.73549	.0957	.10940
.74077	.70158	.0845	.10110
.67032	.62856	.0578	.08619
.60653	.56473	.0343	.07440
.54881	.50839	.0158	.06537
.49659	.45893	.0031	.05979
.47688	.44126	0	.05932
0	0	0	.05932

TABLE 7

Expanding Wave ($\gamma = 3$)

x/Dt	u/D	$P/\rho_o D^2$
1.00000	.2500	.2500
.99920	.2400	.2400
.99968	.2300	.2300
.99639	.2200	.2200
.99197	.2100	.2102
.98599	.2000	.2004
.96929	.1800	.1812
.94564	.1600	.1626
.91456	.1400	.1449
.87577	.1200	.1282
.82920	.1000	.1127
.77500	.0800	.09843
.71329	.0600	.08555
.64383	.0400	.07408
.56457	.0200	.06407
.4536	0	.05531
0	0	.05531

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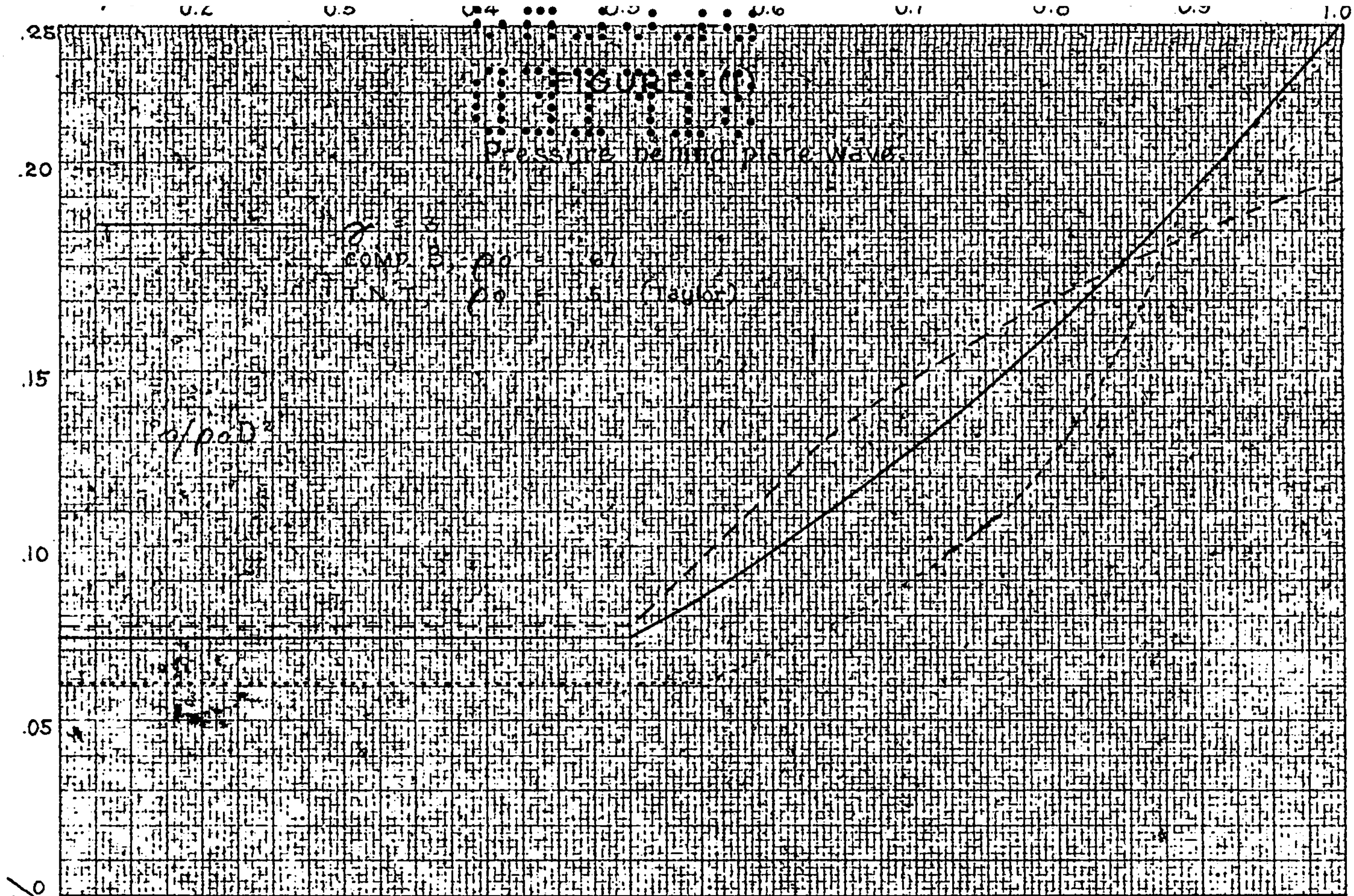


FIGURE (1)
Pressure behind plane wave
γ = 3
COMP B, ρo = 1.67
T.N.T., ρo = 1.51 (Taylor)
p/ρoD²
.25
.20
.15
.10
.05
0
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

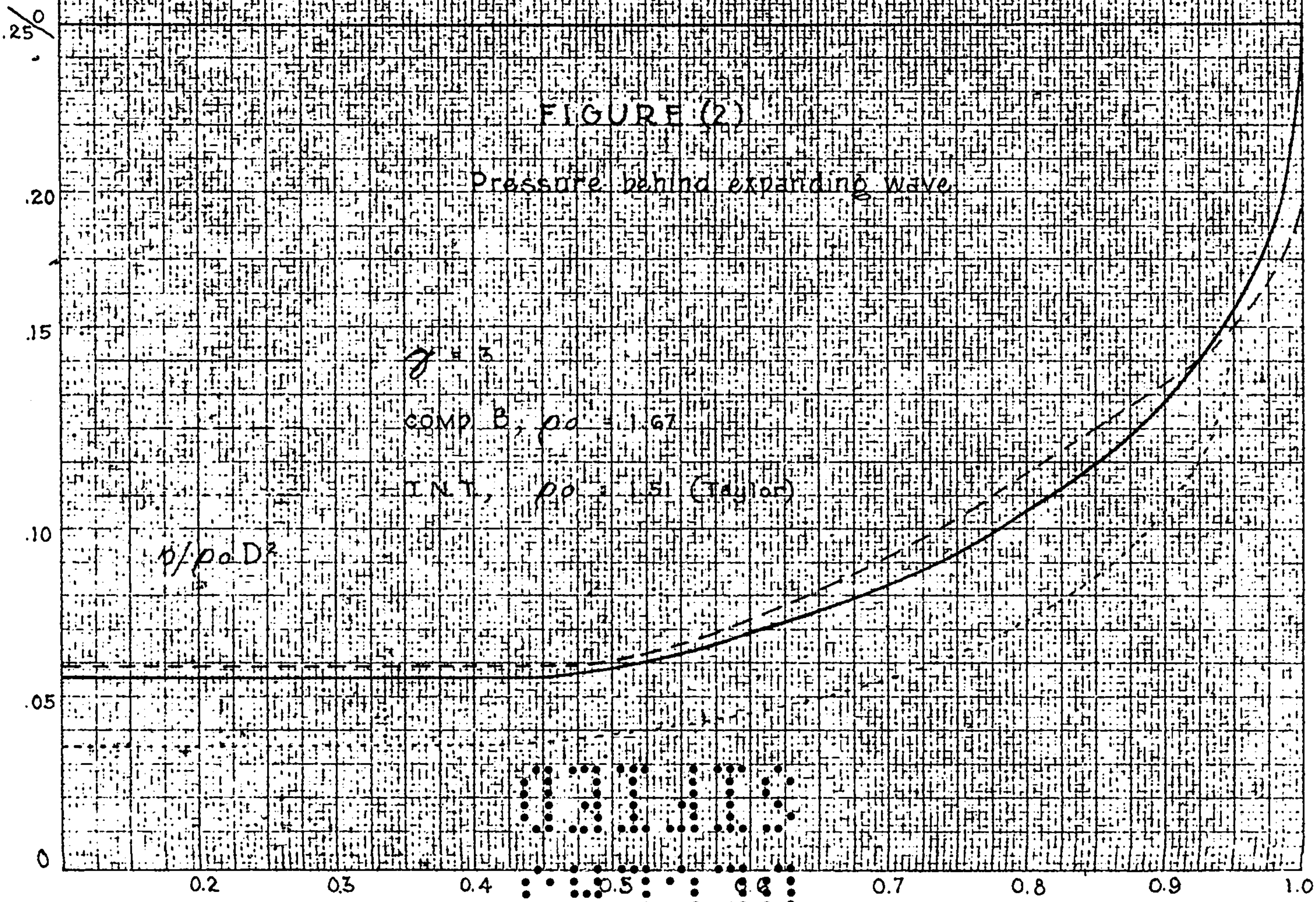


FIGURE (2)
Pressure behind expanding wave
γ = 3
COMP B, ρo = 1.67
T.N.T., ρo = 1.51 (Taylor)
p/ρoD²
.25
.20
.15
.10
.05
0
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

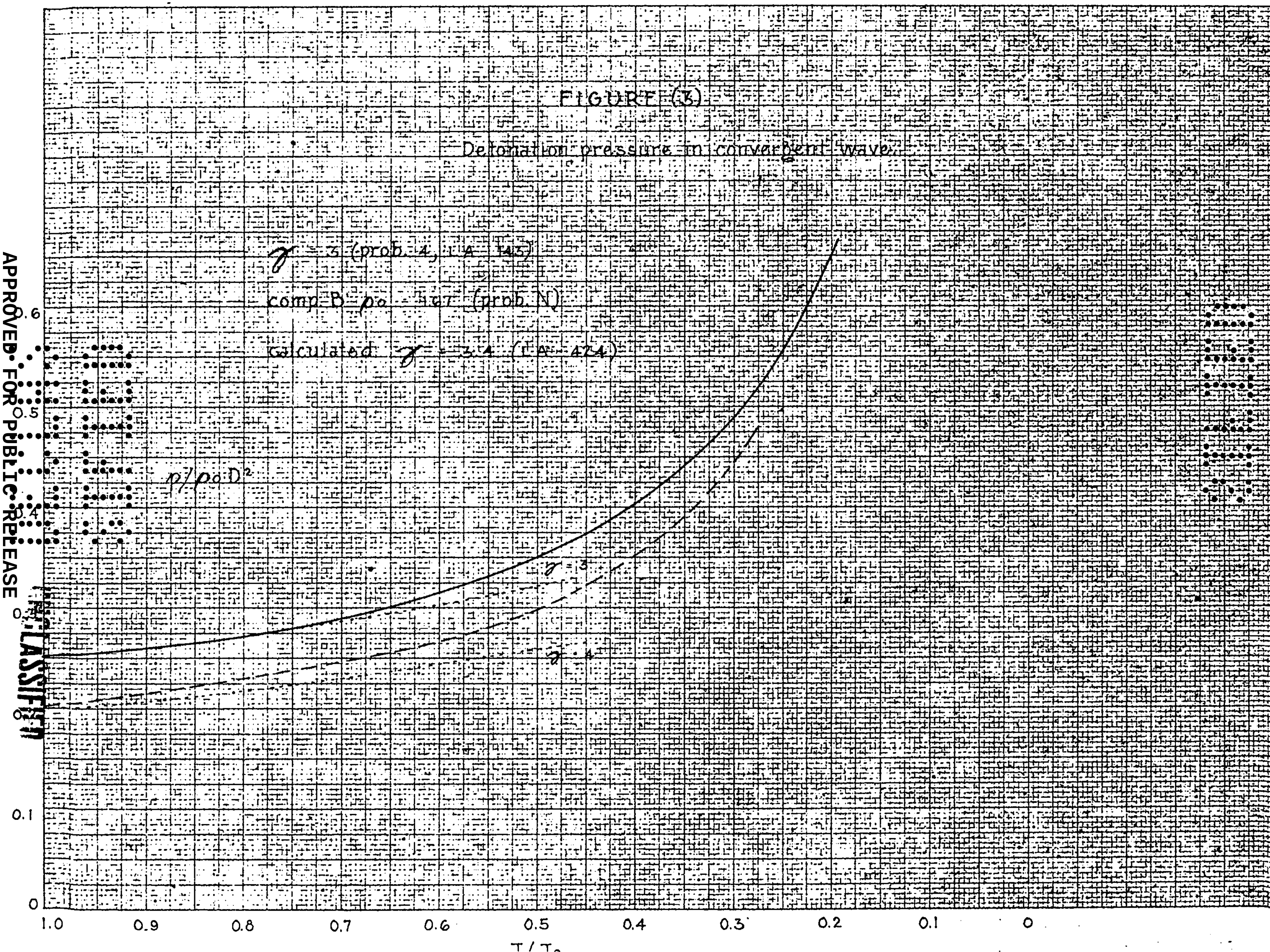
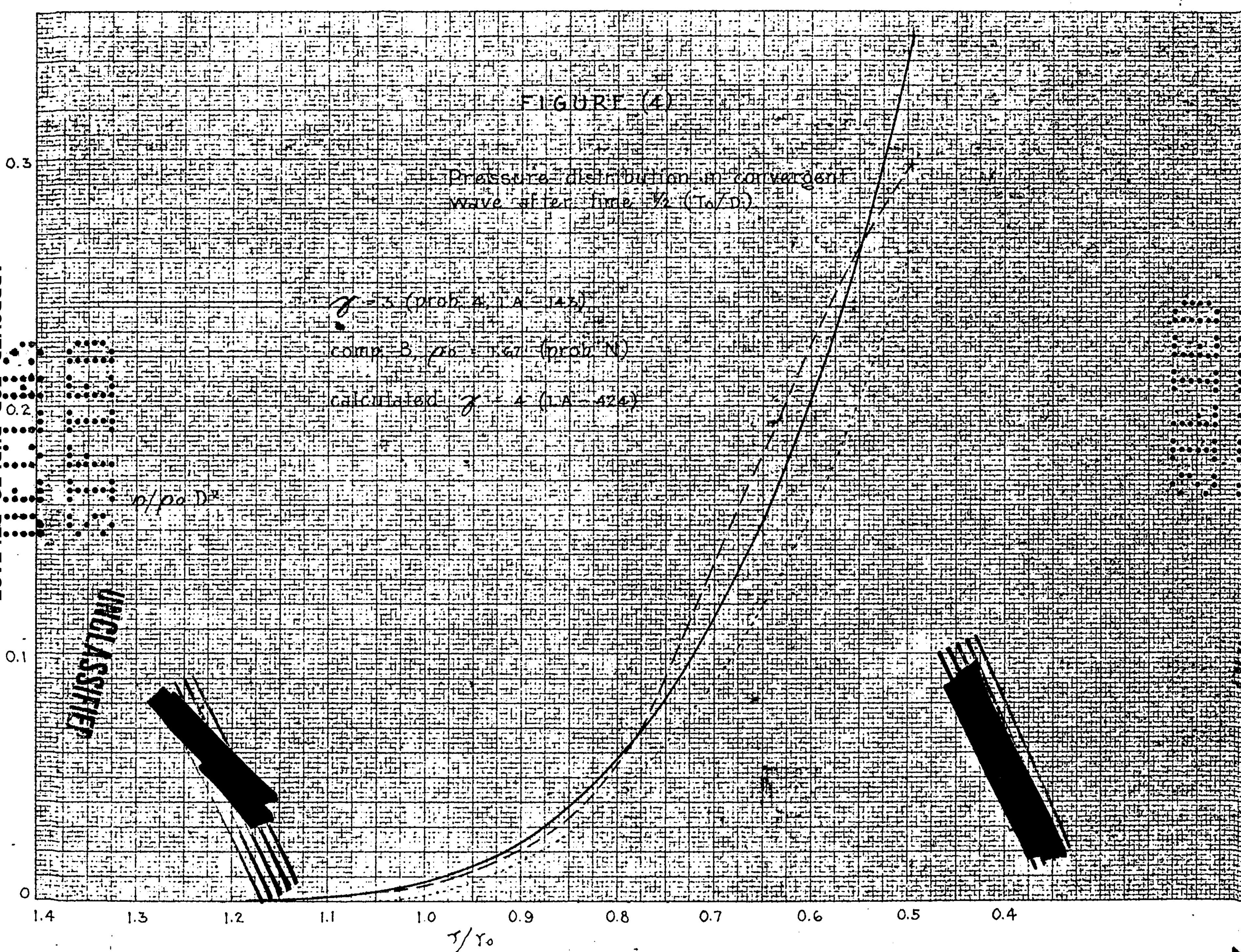


FIGURE (3)
Detonation pressure in convergent wave
comp B
(prob. N)
calculated
$p/\rho_0 D^2$
0.6
0.5
0.4
0.1
0
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0



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