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PREDICTING HIGH EXPLOSIVE DETONATION VELOCITIES FROM THEIR COMPOSITION AND STRUCTURE

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NAVAL WEAPONS STATION, YORKTOWN, VIRGINIA 23691

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20. ABSTRACT

A simple, empirical linear relationship between detonation velocity at theoretical maximum density and a factor, F, that is dependent solely upon chemical composition and structure is postulated for a gamut of ideal explosives. The explosives ranged from nitroaromatics, cyclic and linear nitramines, nitrate esters and nitro-nitrato aliphatics to zero hydrogen explosives, carbonless explosives and hydrogen rich explosives. Of the 64 explosives evaluated, 72% had calculated detonation velocity values within 3% of experimental and 95% within 7%. Only mixtures of TNM and NM and TNM itself varied grossly (>20%) from calculated velocities and the absolute error for all explosives is ± 2.8%.

Predicted C-J detonation pressures for 19 explosives had an absolute error of ± 10% and when TNM was excluded, an absolute error of ± 6.5%. With the exception of TNM and its mixtures, these results compare favorably with more complex predictive models.

F O R E W O R D

1. This is a report documenting the postulate that a simple, empirical linear relationship exists between detonation velocity and a factor, F, that is dependent solely upon the chemical composition and structure for a gamut of explosives.

Released by

W. McBride

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Under authority of
LEO A. HIBSON, JR.
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CONTENTS

PREDICTING HIGH EXPLOSIVE DETONATION VELOCITIES FROM THEIR COMPOSITION AND STRUCTURE

A simple, empirical linear relationship between detonation velocity and a factor, F, that is dependent solely upon chemical composition and structure is postulated for a gamut of explosives.

Since detonation velocity, D_0, is density dependent, the linear regression plot, Figure 1, of the factor, F, versus detonation velocity has been generated from detonation velocities either measured at or corrected to those obtainable at the theoretical maximum density (TMD) of the explosive tested. These D' values at their TMD's have been proximated from the relationship

$$D' = D_0 + (\rho_{TM} - \rho_0) \times 3.0$$

where D', ρ_{TM}, D_0, and ρ_0 are the detonation velocities and densities at their respective theoretical maximum and experimentally measured values expressed in millimeters per microsecond (mm/μsec) and grams per cubic centimeter (g/cc).

The relationship's principal feature is that F values are derived solely from molecular formulae and structures and require no prior knowledge of any measured, estimated or calculated physical, chemical or thermochemical properties.

The factor is expressed as

$$F = \frac{n(O) + n(N) - \frac{n(H)}{2n(O)} + \frac{n(A)}{4} - \frac{n(B)}{2} - \frac{n(C)}{2} - \frac{n(D)}{4} - \frac{n(E)}{4}}{\text{molecular wt}} \times 100$$

where, for one mole of the composition:

- $n(O)$ = number of oxygen atoms
- $n(N)$ = number of nitrogen atoms
- $n(H)$ = number of hydrogen atoms
- $n(A)$ = number of aromatic rings
- $n(B)$ = number of oxygen atoms in excess of those already available to form CO_2 and H_2O
- $n(C)$ = number of oxygen atoms doubly bonded directly to carbon as in a carbonyl $\overset{|}{\underset{|}{C}} = O$
- $n(D)$ = number of oxygen atoms singly bonded directly to carbon as in a $\overset{|}{\underset{|}{C}} - O - R$ linkage where R can equal -H, $-NH_4$, -C, etc.
- $n(E)$ = number of nitrato groups existing either in a nitrate ester configuration or as a nitric acid salt such as hydrazine mononitrate.

Carboxylate or ester type linkages, $O - \overset{|}{C} = O$, such as in TNETB, triethyltrinitrobutyrate, are simply treated as having one each (C) and (D) type oxygen species.

The rationale for the respective A - E adjustments is that they are simplistically related to heats of formation, i.e.,

- <u>A</u> accounts for the effect of an aromatic ring,
- <u>B</u> accounts for the fact that oxygen atoms in excess of those required to form CO_2 and H_2O are partially wasted as contributors to product heats of formation,
- <u>C</u> and <u>D</u> account for the fact that oxygen-carbon moieties contribute less energy to overall explosive performance during their bond breaking and reformation than do more easily disassociated oxygen atoms originally bonded exclusively to nitrogen atoms, and
- <u>E</u> accounts for the greater stability of the nitrate carbon-oxygen bonding in the case of the nitrate esters and by the imparted stability of salt configurations, e.g., in the cases of ammoniacal nitrates.

The linear regression plot, Figure 1, of the factor, F, versus detonation velocity, D', as expressed by the equation

$$F = 0.56\,D' + 0.17$$

or

$$\text{(1)} \qquad \text{Predicted } D' = \frac{(F - 0.17)}{0.56}$$

holds quite well for a broad spectrum of explosives that includes pure compounds, admixtures of explosives typified by cyclotols, and plastic bonded explosive compositions formulated with small portions of inert binder materials.

Data for experimental detonation velocities of 64 explosives reported in the literature are collated in Table I.* Chemical designations and compositions are given in Table II.

The correlation coefficient of the linear regression line calculates to be better than 95%. Explosives were chosen nonselectively to maximize the range of types and structures. Thus, of the 64 explosives, 55 were pure compounds and 9 were composites which ranged from nitroaromatics, nitroaliphatics, cyclic and linear nitramines, nitrate esters and nitro-nitrato aliphatics to zero hydrogen explosives, carbonless explosives and hydrogen rich explosives. Data sources are listed in Table II, references (1) through (8).

Most of the randomly selected data taken from Meyer, Table II, including that for EGDN, did not reference either a maximum theoretical density for the explosive or a description of the experimental measuring technique. In all those cases, the reported detonation velocity, D_0, was plotted in lieu of D'. Nonetheless, their calculated percent errors, with the exception of EDGN, were evenly distributed within ± 5%.

The accuracy for predicting D' values appears comparable to more complex treatments which require either additional thermochemical and bond formation data or, at minimum, some other experimentally measured property such as density. Thus, 72% of the explosives, regardless of type, had calculated D' values within 3% of experimental and 61 of 64 explosives (95%) calculated to within 7% of experimental values. Only ethyleneglycoldinitrate (EGDN), and a 1:0.25 mixture of nitromethane (NM)/tetranitromethane (TNM), and pure TNM itself exceeded experimentally reported values by 11%, 26% and 20%, respectively.

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*Molecular weights and atomic compositions for composited explosives were derived respectively from the sum of the weighted average molecular weights and the weighted average sums of each elemental mole fraction. When the explosive ingredient in PBX type composites exceeded 90%, its molecular weight was used as the proximate molecular weight of the mixture. Finally, elements other than C, H, N and O were factored out of the atomic compositions as in the cases of Kel-F or CEF. A sample calculation is given in the appendix.

The anomalous results for TNM and NM/TNM mixtures have yet to be explained. In a helpful critique, Dr. Charles Mader (ref (8), Table II) pointed out that for a series of NM/TNM mixtures - which by his calculations behave ideally - a maximum detonation velocity of 6.88 mm/μsec was obtained at the 1:0.25 NM/TNM ratio, i.e.,

Compound	Exptl D' (mm/μsec)	Calc'd D' (mm/μsec)	% error
NM	6.32	6.30	-
NM/TNM 1:0.25	6.88	8.68	+26
TNM	6.55	7.89	+20

However, Mader also noted (ref (9), Table II) that the F/D' relationship described here would probably not be applicable to systems having non-ideal behavior such as in the cases for many aluminum or ammonium nitrate-containing compositions.

Although Mader's calculations cannot be ignored, it seems possible that the liquid mixture 1:0.25 NM/TNM, even though balanced for CO_2 and H_2O production, does not behave ideally with a consequent measured D_0 lower than predicted as often is the case for many CO_2 - H_2O balanced AN compositions. For example, Dr. Ray McGuire (ref (10), Table II) has expressed his opinion that it is questionable whether or not TNM can be thought of as a reliably performing high explosive at all. Finally, Akst (ref (7), Table II) has pointed out that TNM also calculates to a higher value than experimental using Kamlet's equation.

For these reasons, the calculated D's for TNM and NM/TNM were not used in generating Eq. (1). Without them, the absolute error for the other 62 explosives is ± 2%, with them included it is ± 3%. Therefore, even with the unexplained TNM and NM/TNM results, it is believed that a realistic relationship between detonation velocity and structure/composition has been demonstrated for ideal explosives.

To maximize the usefulness of this relationship, it is hoped that it can be refined still further. For example, liquid explosives such as NG, EGDN, NIBTN and TNM all tended to have higher predicted than measured detonation velocities, suggesting, perhaps, some critical diameter or other shock sensitivity effect. Eventually it then may be possible to predict detonation pressures at theoretical maximum density, using compositional and structural relationships alone, by a procedure even simpler than those developed by Kamlet, et al., a decade ago (ref (6a-d), Table II). Thus, Figure 2 is a linear regression plot of experimental C-J pressures versus experimental detonation velocities of 11 explosives measured at, or within 2% of, their maximum theoretical densities.

This relationship

$$(2) \qquad P'_{C-J} = 93.3\ D' - 456$$

has a correlation coefficient of 0.99.

Predicted P'_{C-J} values then were calculated from this equation using the predicted D' values of Eq. (1). A comparison of the experimental versus calculated C-J pressures for these 11 explosives is made in Table III along with 8 other explosives whose experimentally determined C-J pressures, P^0_{C-J}, were corrected to an arbitrary theoretical maximum, i.e.,

$$P'_{C-J} = P^0_{C-J} \times \left(\frac{\rho_{TMD}}{\rho_0}\right)^2$$

where super and subscripts indicate the experimentally determined value at that density.

The absolute error for all 19 values is $\pm$ 10.2% versus $\pm$ 4.4% for the same calculated data set reported by Kamlet (ref (6b), Table II). Omitting the as yet unexplained TNM data from the set gives absolute errors of $\pm$ 6.5% and $\pm$ 4.3%, respectively.

When Kamlet's observations (ref (6a-b), Table II) are recalled, namely: that no single C-J pressure measurement is universally accepted within 5% (i.e., as of the year 1968 prior to which all data cited was gathered); that experimental detonation pressures ranging from 177 to 220 kilobars have been reported for TNT at 1.63 to 1.64 g/cc density; and that NG and PETN data are either anomalous or suspect, the correlation between observed and calculated values by this method must be considered good in its present stage.

TABLE I. PREDICTED DETONATION VELOCITIES

No.	Xpl	TMD (g/cc)	Elemental composition C	H	N	O	Mol wt	Exptl D' (mm/μsec)	Factor F	Calc'd D' (mm/μsec)	% error
1	HNB	2+	6	-	6	12	348	9.50	5.24	9.05	-5
2	SORGUYL	2.01	4	2	8	10	322	9.15	5.09	8.79	-4
3	HMX	1.90	4	8	8	8	296	9.14	5.24	9.05	-1
4	BTNEU	1.86	5	6	8	13	386	9.00	5.25	9.07	+1
5	9404	1.87	4.20	8.26	7.73	8.09	296	8.89	5.17	8.93	+1
6	RDX	1.83	3	6	6	6	222	8.85	5.18	8.95	+1
7	BTNEN	1.96	4	4	8	14	388	8.85	5.12	8.84	0
8	HN	1.64	0	5	3	3	95	8.69	4.91	8.46	-3
9	BTF	1.90	6	-	6	6	252	8.61	4.86	8.38	-3
10	9011	1.80	5.12	9.41	7.55	7.73	296	8.59	4.96	8.55	0
11	OCTOL	1.83	4.94	7.14	6.53	7.44	278	8.54	4.87	8.39	-1
12	9010	1.82	3.35	5.86	5.86	5.86	222	8.49	5.05	8.71	+3
13	COMP C-4	1.59(?)	4.02	7.82	5.44	5.55	222	8.04	4.65	8.00	0
14	CYCLOTOL	1.77	3.96	5.73	5.24	5.98	223	8.33	4.86	8.38	+1
15	9205	1.72	4.04	6.94	5.50	5.55	222	8.32	4.72	8.13	-2
16	TNETB	1.78	6	6	6	14	386	8.30	4.93	8.50	+2
17	PETN	1.77	5	8	4	12	316	8.29	4.67	8.04	-3
18	MHN	1.73	6	8	6	18	452	8.26	4.71	8.11	-2
19	EDNA	1.71	2	6	4	4	150	8.23	4.83	8.32	+1
20	NQ	1.72	1	4	4	2	104	8.16	4.81	8.29	+2
21	DINGU	1.94	4	4	6	6	232	8.15	4.60	7.91	-3
22	DNPN	1.73	6	10	6	10	326	8.10	4.75	8.18	+1
23	COMP B-3	1.74	4.53	5.56	4.78	5.96	221	8.05	4.68	8.05	0
24	DINA	1.67	4	8	4	8	240	8.00	4.58	7.88	-2
25	TATB	1.94	6	6	6	6	258	7.94	4.55	7.82	-2
26	TETRYL	1.73	7	5	5	8	287	7.91	4.51	7.75	-2
27	NIBTN	1.64	4	6	4	11	286	7.86	4.89	8.45	+5
28	R-SALT	1.57(?)	3	6	6	3	174	7.80	4.60	7.91	+1
29	TPEON	1.58	15	24	8	26	732	7.71	4.24	7.27	-6
30	NG	1.60	3	5	3	9	227	7.70	4.72	8.13	+6
31	EDD	1.60	2	10	4	6	186	7.69	4.66	8.02	+4
32	DATB	1.84	6	5	5	6	243	7.67	4.46	7.66	0
33	HNAB	1.77	12	4	8	12	452	7.65	4.50	7.73	+1
34	PETRIN	1.54(?)	5	9	3	10	271	7.64	4.26	7.30	-4

TABLE I. PREDICTED DETONATION VELOCITIES (cont'd)

No.	Xpl	TMD (g/cc)	Elemental composition C	H	N	O	Mol wt	Exptl D' (mm/μsec)	Factor F	Calc'd D' (mm/μsec)	% error
35	DNPTB	1.68	7	9	5	12	355	7.63	4.47	7.68	+1
36	TNPON	1.68(?)	8	6	4	10	318	7.60	4.23	7.25	-5
37	DPEHN	1.63	10	16	6	19	524	7.53	4.36	7.48	-1
38	PIC ACID	1.76	6	3	3	7	229	7.50	4.27	7.32	-2
39	DIPAM	1.79	12	6	8	12	454	7.49	4.46	7.66	+2
40	TNA	1.76	6	4	4	6	228	7.42	4.35	7.46	+1
41	XPL D	1.72	6	6	4	7	246	7.36	4.30	7.38	0
42	GTNB	1.63	10	12	6	16	472	7.34	4.26	7.30	-1
43	EGDN	1.48(?)	2	4	2	6	152	7.30	4.72	8.13	+11
44	TNB	1.64(?)	6	3	3	6	213	7.27	4.23	7.25	0
45	TACOT	1.85	12	4	8	8	388	7.25	4.19	7.18	-1
46	HNDP	1.64(?)	12	5	7	12	439	7.20	4.39	7.54	+5
47	HNDPO	1.70(?)	12	4	6	13	440	7.18	4.34	7.45	+4
48	HNS	1.74	14	6	6	12	450	7.12	4.06	6.95	-2
49	DNDMOA	1.52(?)	4	6	4	6	206	7.10	4.13	7.07	0
50	FIVONITE	1.59(?)	9	12	4	13	384	7.04	3.92	6.70	-5
51	DIAZ	1.63	6	2	4	5	210	7.00	4.19	7.18	+3
52	HNDS*	1.65(?)	12	4	6	13	456	7.00	4.19	7.18	+3
53	TNT	1.65	7	5	3	6	227	6.96	3.89	6.64	-5
54	NM/TNM**	...	1.00	2.40	1.60	3.20	88	6.88	5.03	8.68	+26
55	TNC	1.68(?)	7	5	3	7	243	6.85	3.97	6.79	-1
56.	DNPEN	1.60(?)	8	7	3	8	273	6.80	3.78	6.45	-5
57	ET PIC	1.60(?)	8	7	3	7	257	6.80	3.70	6.30	-7
58	TNAN	1.61(?)	7	5	3	7	243	6.80	3.96	6.77	0
59	DEGN	1.38	4	8	2	7	196	6.76	3.92	6.70	-1
60	TNM	1.65	1	0	4	8	196	6.55	4.59	7.89	+20
61	TMPTN	1.50(?)	6	11	3	9	269	6.44	3.95	6.75	+5
62	DNPF	1.60	10	12	4	12	380	6.38	3.68	6.27	-2
63	NM	1.16	1	3	1	2	61	6.32	3.69	6.30	0
64	TNN	...	10	5	3	6	263	6.00	3.45	5.86	-2

*Sulfur atom treated as an oxygen.
**1:025 mole ratio.

Note: (?) indicates that the reference value given is at the experimental condition and TMD data is not listed.

TABLE II. DATA SOURCES

No.	Explosive	Chemical designation	Ref() page
1	HNB	hexanitrobenzene	(5)
2	SORGUYL	tetranitroglycolcolurile	(3) 80
3	HMX	cyclotetramethylenetetranitramine	(1) 8.1
4	BTNEU	bis-trinitroethylurea	(4) 24
5	9404	HMX + NC + chlorethylphosphate	(1) 8.1
6	RDX	cyclotrimethylenetrinitramine	(1) 8.1
7	BTNEN	bis-trinitroethylnitramine	(4) 24
8	HN	hydrazinemononitrate	(4) 22
9	BTF	benzotrifuroxan	(1) 8.1
10	9011	HMX-Estane	(1) 8.1
11	OCTOL	HMX-TNT	(1) 8.1
12	9010	RDX-Kel-F	(1) 8.1
13	COMP C-4	RDX-polyisobutylene	(1) 8.1
14	CYCLOTOL	RDX-TNT	(1) 8.1
15	9205	RDX-polystyrene-ethylhexylphthalate	(1) 8.1
16	TNETB	triethyltrinitrobutyrate	(2) 373
17	PETN	pentaaerythritoltetranitrate	(1) 8.1
18	MHN	mannitol hexanitrate	(2) 197
19	EDNA	ethylenedinitramine	(2) 150
20	NQ	nitroguanidine	(1) 8.1
21	DINGU	dinitroglycolcolurile	(3) 79
22	DNPN	bis-dinitropropylnitramine	(4) 24
23	COMP B-3	RDX-TNT	(1) 8.1
24	DINA	dioxyethylnitraminedinitrate	(6a)
25	TATB	triaminotrinitrobenzene	(1) 8.1
26	TETRYL	trinitrophenylmethylnitramine	(1) 8.1
27	NIBTN	nitroisobutyltrinitrate	(2) 243
28	R-SALT	cyclotrimethylenetrinitrosamine	(4) 24
29	TPEON	tripentaaerythritoloctanitrate	(2) 381
30	NG	trinitroglycerine	(1) 8.1
31	EDD	ethylenediaminedinitrate	(7)
32	DATB	diaminotrinitrobenzene	(1) 8.1
33	HNAB	hexanitroazobenzene	(1) 8.1
34	PETRIN	trinitropentaaerythritol	(4) 17*
35	DNPTB	dinitropropyltrinitrobutyrate	(2) 113**
36	TNPON	trinitrophenoxyethylnitrate	(3) 307
37	DPEHN	dipentaaerythritolhexanitrate	(2) 119
38	PIC ACID	trinitrophenol	(2) 288
39	DIPAM	hexanitrodiphenylamine	(1) 8.1
40	TNA	trinitroaniline	(2) 282
41	XPL D	ammonium picrate	(2) 136
42	GTNB	ethyleneglycol di-trinitrobutyrate	(2) 133**
43	EGDN	ethyleneglycoldinitrate	(3) 193
44	TNB	trinitrobenzene	(4) 24
45	TACOT	tetranitrotetraazadibenzocyclooctatetrene	(1) 8.1

TABLE II. DATA SOURCES (cont'd)

No.	Explosive	Chemical designation	Ref() page
46	HNDP	hexanitrodephenylamine	(3) 144
47	HNDPO	hexanitrodiphenylamine oxide	(3) 146
48	HNS	hexanitrostilbene	(1) 8.1
49	DNDMOA	dinitrodimethyloxamide	(3) 82
50	FIVONITE	tetramethylolcyclopentanonetetranitrate	(3) 258
51	DIAZ	diazodinitrophenol	(2) 99
52	HNDS	hexanitrodiphenylsulfide	(3) 147
53	TNT	trinitrotoluene	(1) 8.1
54	NM/TNM	nitromethane/tetranitromethane (1:0.25)	(8)
55	TNC	trinitrocresol	(3) 305
56	DNPEN	dinitrophenoxyethylnitrate	(3) 85
57	ET PIC	ethyl picrate	(3) 104
58	TNAN	trinitroanisole	(3) 301
59	DEGN	diethyleneglycoldinitrate	(2) 103
60	TNM	tetranitromethane	(1) 8.1
61	TMPTN	trimethylolethylmethanetrinitrate	(3) 101
62	DNPF	dinitropropylfumarate	(2) 107
63	NM	nitromethane	(1) 8.1
64	TNN	trinitronaphthalene	(3) 306

*Calculated value.
**Error in formula and/or structure as listed.

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TABLE III. EXPERIMENTAL VERSUS CALCULATED C-J DETONATION PRESSURES

	Xpl	Exptl P^0_{C-J} (kbar)	Exptl P'_{C-J} (kbar)	Calc'd P'_{C-J} (kbar)	% error	Kamlet's[a] % error
	HMX	393	393	388	- 1.3	- 3.1
	OCTOL[b]	342	342	327	- 4.4	- 4.5
	PETN	340	340	294	-13.5	- 5.1
	CYCLOTOL[c]	316	323	326	+ 0.9	- 4.4
	COMP B-3	287	294	295	+ 0.3	- 4.3
I	TETRYL	263	272	267	- 1.8	- 3.9
	NG	253	253	303	+19.8	+ 6.7
	TNB	219	219	220	+ 0.5	- 2.3
	TNT	200[d]	205	164	-20.0	- 1.0
	TNM	159	159	280	+76.1	+ 5.6
	NM	133	138	132	- 4.3	+ 3.0
	9404	375	387	377	- 2.6	[e]
	RDX	338	357	379	+ 6.2	- 3.9
	9010	328	343	357	+ 4.1	[e]
II	PETN	300	337	294	-12.8	- 1.4
	EDNA	273	328	320	- 2.4	- 9.9
	TNETB	265	294	337	+14.6	+10.6
	TATB	259	285	274	- 3.9	+ 2.1
	DATB	251	268	259	- 3.4	+ 2.9
			Absolute error:		$\pm$10.2	$\pm$ 4.4
			Absolute error excluding TNM:		$\pm$ 6.5	$\pm$ 4.3

I: Measured at or within 2% of ρ'_{TMD} .

II. Measured at lower ρ_0 value and corrected to ρ'_{TMD}.

[a]At experimental density as reported in ref (6b), Table II.
[b]77:22.4 HMX:TNT.
[c]77:23 RDX:TNT.
[d]Average of seven values reported at 1.63 to 1.64 g/cc.
[e]Not available.

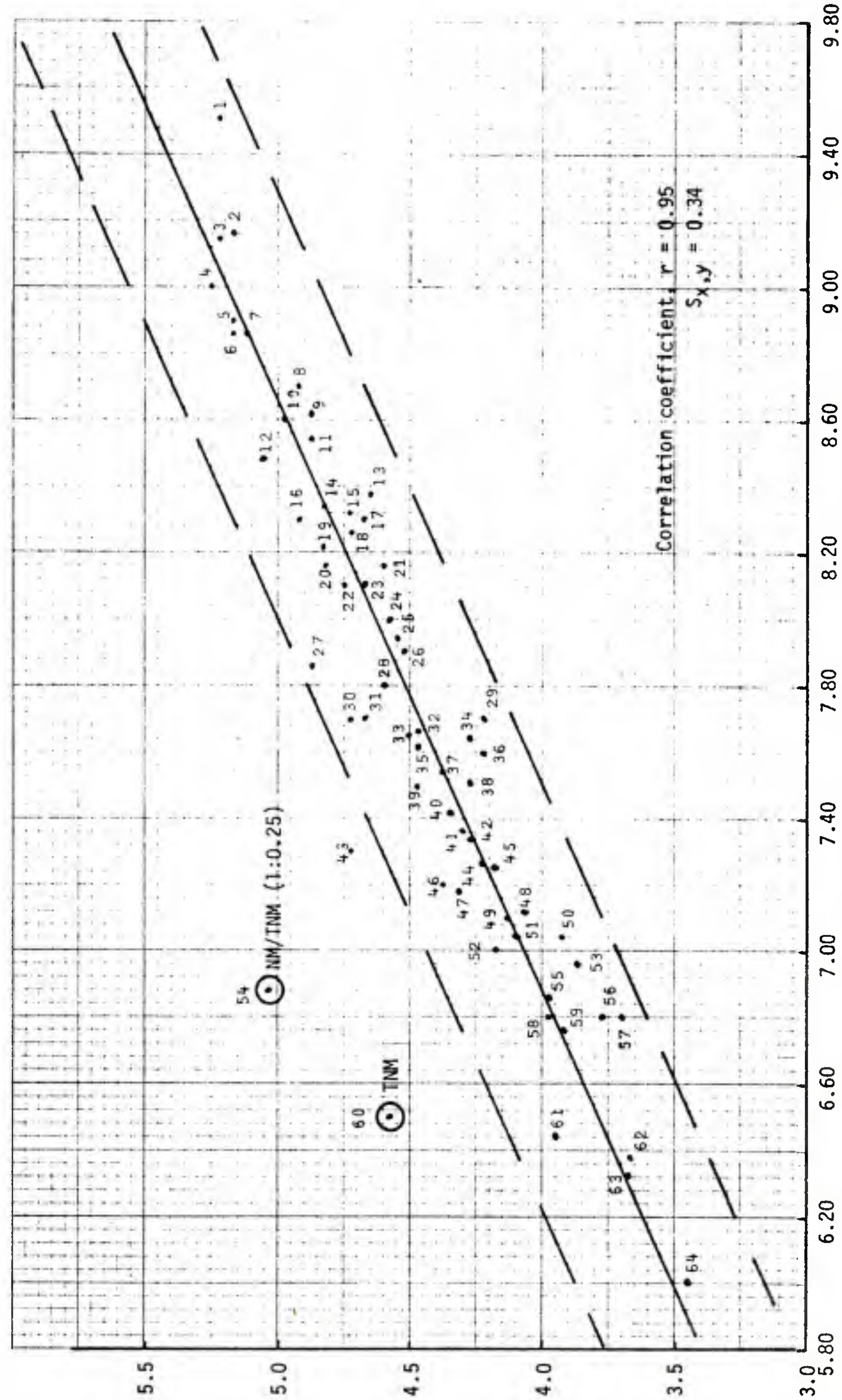

FIGURE 1. LINEAR REGRESSION PLOT OF FACTOR F VS DETONATION VELOCITY D'

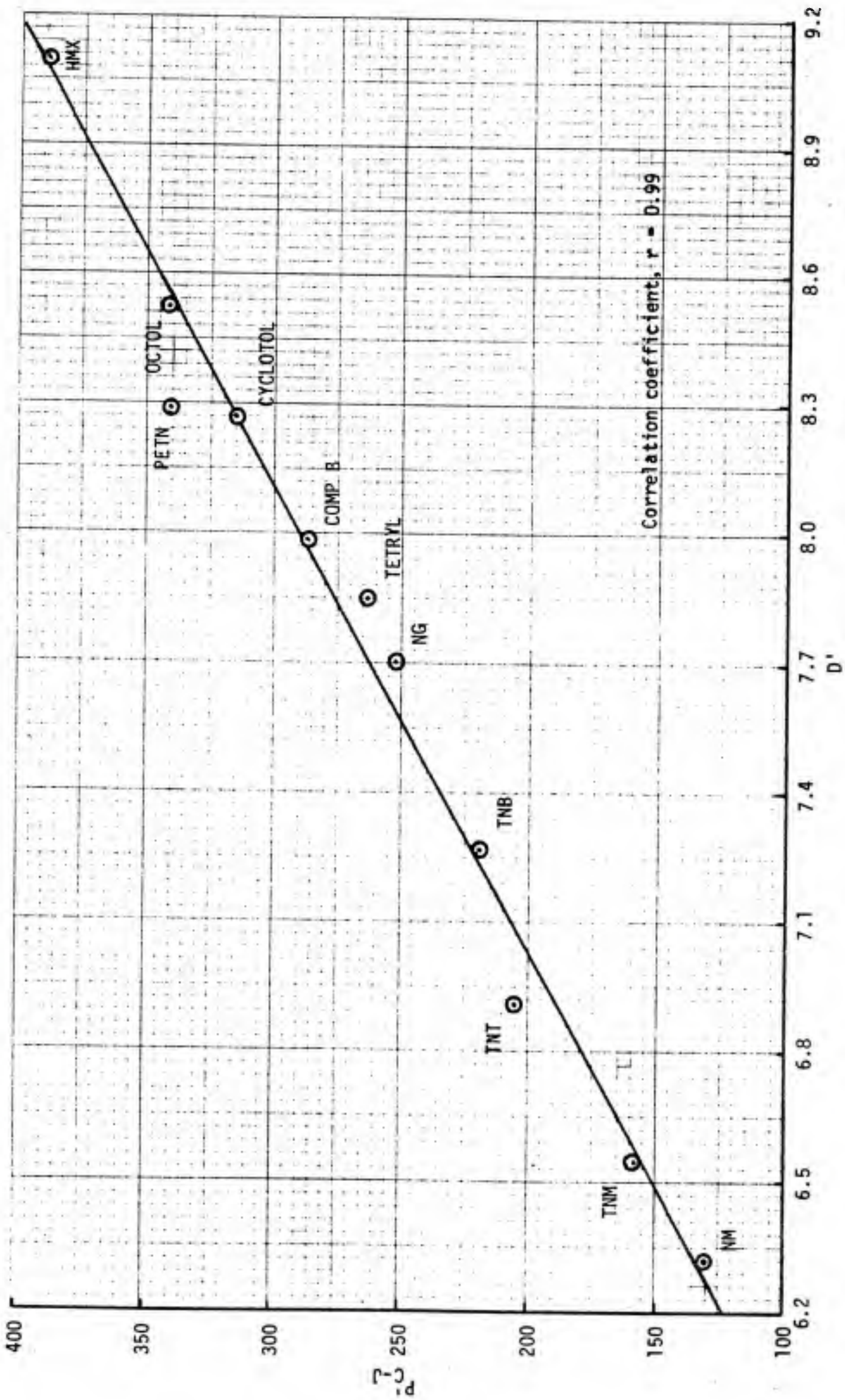

FIGURE 2. LINEAR REGRESSION PLOT OF P'_{C-J} EXPERIMENTAL VS D' EXPERIMENTAL

APPENDIX

The calculation of the factor, F, requires that for each explosive, pure or composited, the elemental composition in one mole must be used. This is due to the fact that the $\frac{\cancel{m}\cdot n(H)}{\cancel{m}\cdot 2n(O)}$ ratio is fixed since the molar quantity, m, cancels. That is, the value of this ratio would change when divided by m multiples or fractions of the molar weights, i.e.,

$\dfrac{\frac{n(H)}{2n(O)}}{m\cdot(MW)}$, whereas the values for the other components of the equation,

i.e., $\dfrac{\cancel{m}\cdot n(O)}{\cancel{m}\cdot(MW)}$, $\dfrac{\cancel{m}\cdot n(N)}{\cancel{m}\cdot(MW)}$, $\dfrac{\cancel{m}\cdot n\frac{(A)}{4}}{\cancel{m}\cdot(MW)}$, etc., obviously would not vary.

Example:

For 100 grams (g) of Cyclotol:

		C	H	N	O
$\frac{75\ g}{222.1}$ RDX =	0.34 mole for $C_3H_6N_6O_6$	1.01	2.03	2.03	2.03
$\frac{25\ g}{227.1}$ TNT =	0.11 mole for $C_7H_5N_3O_6$	0.77	0.55	0.33	0.66
	0.45 mole =	1.78	2.58	2.36	2.69
	1 mole =	3.96	5.73	5.24	5.98

and the equivalent MW = 222.2 .

For TNT A = 1 and for the mix its correction is $\frac{1}{4} \times \frac{.11}{.45} = 0.06$

$$F = \frac{5.98 + 5.24 - \frac{5.73}{2 \times 5.98} + .06}{222.2} \times 100 = 4.86$$

Predicted D' = (4.86 - .17) ÷ 0.56 = 8.38 mm/μsec

D' = observed = 8.33 mm/μsec or a 0.6% error.

ADDENDUM

Since the completion of this paper, our attention has been called to one by I. N. Aizenshtadt, translated from Fizika Goreniyva, Vol. 12, No. 5 pp 754-8, Sep-Oct 1976 and copy written by Plenum Publishing Corp., 227 W. 17th St., New York, N.Y. 10011. The author calculates detonation velocities for condensed explosives from one of three empirical equations that are dependent upon ΔH_f and which differ upon whether or not:

$$d > 2a + \frac{b}{2} \quad \text{then} \quad D_{1.60} = \left(\frac{1500a + 920b + 728c + 352d + 7.3\Delta H_f}{MW}\right)^{1/2}$$

$$d = 2a + \frac{b}{2} \quad \text{then} \quad D_{1.60} = \left(\frac{729.6a + 730b + 728c + 710d + 7.3\Delta H_f}{MW}\right)^{1/2}$$

$$d < 2a + \frac{b}{2} \quad \text{then} \quad D_{1.60} = \left(\frac{-39.6a + 540b + 728c + 1120d + 7.3\Delta H_f}{MW}\right)^{1/2}$$

where a, b, c, and d are again the respective numbers of carbon hydrogen, nitrogen and oxygen atoms in a CHNO type explosive molecule.

Table A compares the detonation velocities calculated by the three methods listed, extrapolated to their TMD values. The explosives were selected randomly except that the list deliberately includes the worst cases calculated in this paper, i.e., TNM and EGDN.

It can be seen that Aizenshtadt's procedure is considerably less accurate in absolute terms than either the method presented here or that of Kamlet-Jacobs.

TABLE A

COMPARISON OF
ROTHSTEIN-PETERSEN (R-P); AIZENSHTADT (Aiz); KAMLET-JACOBS (K-J)
SHORT METHODS FOR CALCULATING DETONATION VELOCITY AT TMD

Xpl	Exptl D' (mm/μsec)	R-P calc'd D' (mm/μsec)	% error	Aiz calc'd $D_{1.60}$ (mm/μsec)	Aiz calc'd D' (mm/μsec)	% error	K-J calc'd D' (mm/μsec)	% error
TNT	6.96	6.64	- 5	7.03	7.23	+ 4	6.99	0
TETRYL	7.91	7.75	- 2	7.25	7.77	- 2	7.79	- 2
RDX	8.85	8.95	+ 1	8.03	8.95	+ 1	8.89	0
HMX	9.14	9.05	- 1	8.03	9.23	+ 1	9.12	0
PETN	8.29	8.04	- 3	7.86	8.54	+ 3	8.70	+ 5
TNB	7.27	7.25	0	6.91	6.91	- 5	7.16	- 2
PIC ACID	7.50	7.32	- 2	6.94	7.58	+ 1	7.51	0
TNA	7.42	7.46	+ 1	7.08	7.72	+ 4	7.48	+ 1
NG	7.70	8.13	+ 6	7.80	7.80	+ 1	8.32	+ 8
NM	6.32	6.30	0	8.45	6.91	+ 9	6.48	+ 2
EGDN	7.30	8.13	+11	...	...	...	...	...
DATB	7.67	7.66	0	7.19	8.15	+ 6	7.63	0
BTNEU	9.00	9.07	+ 1	7.64	8.68	- 4	8.99	0
XPL D	7.36	7.38	0	7.28	8.40	- 7	7.29	- 1
TNM	6.55	7.89	+20	6.11	6.27	- 4	6.67	+ 2
R-SALT	7.80	7.91	+ 1	8.07	7.97	+ 2	7.61	- 3
TATB	7.94	7.82	- 2	7.32	8.34	+ 5	7.98	+ 1
DNPF	6.38	6.27	- 2	7.40	7.40	+16	6.89	+ 8
NQ	8.16	8.29	+ 2	8.27	8.63	+ 6	7.69	- 6
EDNA	8.23	8.32	+ 1	8.31	8.64	+ 5	8.28	0
DNPN	8.10	8.18	+ 1	7.88	8.27	+ 2	8.22	+ 2
DINA	8.00	7.88	- 2	8.37	8.62	+ 8	8.21	+ 3
PETRIN	7.64	7.30	- 4	8.68	8.50	+11	7.61	0
TNETB	8.30	8.50	+ 2	7.71	8.34	0	8.59	+ 4
BTNEN	8.85	8.84	0	7.27	8.71	- 2	9.05	+ 2
HN	8.69	8.46	- 3	8.82	8.98	+ 3	8.50	- 2
	Absolute error:		± 2.8			± 4.5		± 2.2
	Absolute error excluding TNM:		± 2.1			± 4.5		± 2.2

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