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ON UNDERWATER DETONATIONS, I. A NEW METHOD FOR PREDICTING THE CJ DETONATION PRESSURE OF EXPLOSIVES

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ABSTRACT

The experimental detonation pressure of explosives has been found to correlate reasonably well with the theoretical specific impulse and density of these compositions. Two data sets were subjected to linear regression analysis, giving a number of possible correlations; however, the equation containing $I_{sp} \times \text{Density}^2$, a Kamlet-Jacobs like term, was found to show the best relationship for predicting, today's plastic bonded explosives. The complete equation is:

$$P_{\text{exptl}} = 44.4 (I_{sp} \times \text{Density}^2) - 21$$

INTRODUCTION

Explosives being developed for military use in recent years have consisted of polymeric binder matrices, filled with energetic ingredients. The multi-component, non-homogeneous compositions which have been and are being developed, especially those containing metal powders, have non-ideal detonation properties (an ideal explosive is one that can be described adequately by the steady-state theory)⁽¹⁾. The Kamlet-Jacobs (KJ)⁽²⁾ simplified computation method can predict the detonation properties of ideal explosives, but cannot always predict those of the less ideal ones, and it offers little possibility of being used to accurately predict the properties of metallized compositions. (Underwater explosives containing metal powders are of special interest to the Navy due to their potential target damage enhancement.)

The authors of this paper, propellant-oriented chemists, who in recent years became more involved in explosive development, have observed the

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remarkable similarity between the thermodynamic properties needed to calculate the performance characteristics of propellants and those of explosives. This similarity is especially evident between the Phi term (ν) in the Kamlet-Jacobs equation and the specific impulse (Isp) in the propellant calculations. Therefore, it appeared reasonable to examine the suitability of using specific impulse (Isp), which is easily obtained from the PEP(3)* computer code, to correlate the detonation properties of explosives. This paper reports the results of our study into the relationship between Isp and detonation pressure. Later papers will describe how Isp is related to detonation velocity and to cylinder energy. We hope to eventually use the Isp calculations for predicting the explosive performance of metallized compositions. (PEP computer calculations have been used for many years by propellant formulators to obtain rocket performance parameters of metallized propellants.)

*See appendix for an explanation of the PEP code and a sample printout.

DETONATION CALCULATIONS

The Kamlet-Jacob (KJ) equation accurately predicts the measured detonation pressure for a large number of explosive compounds. The KJ equation is given by:(2)

$$P_{CJ} = K \rho_0^2$$

where

$$K = 15.58$$

$$\phi = N(MW)^{1/2}(Q)^{1/2} = \text{phi}$$

ρ_0 = loading density of explosive, g/cc

P_{CJ} = Chapman-Jouguet Detonation Pressure in Kilobars

N = number of moles of gas from one gram of explosive

MW = average molecular weight of gases produced during explosion

Q = heat of detonation in cal/g, calculated using the H_2O/CO_2 arbitrary

First, we wanted to see if the I_{sp} could be directly substituted for the ϕ in the equation: $P_{(exptl)} = \phi \times \text{density}^2$.

Using the $P_{(exptl)}$, ϕ , and density data presented in Table 1 (this data is from the original paper by Kamlet and Dickinson published in 1968⁽⁴⁾ and is composed mostly of pressed and melt-cast ideal explosives), and the I_{sp} of the compositions calculated from the PEP code; the $\phi \times \text{density}^2$, and the $I_{sp} \times \text{density}^2$ of a number of explosives were plotted against their respective experimental detonation pressures (see Figures 1 and 2). A linear regression analysis of the data gave the results shown in Table 2.

A very good correlation was observed for both relationships, although the KJ equation gave a slightly better R^2 -correlation coefficient and standard error. The validity of using the Isp in place of the phi for determining detonation pressure was now clearly demonstrated.

Next, we wanted to find out if the exponent of 1 on the Isp and the exponent of 2 on the density gave the best fit to data. This time the linear regression analysis was conducted on the data in Table 1, using an equation of the form $\ln P(\text{exptl}) = N \ln (\text{Isp}) + M \ln (\text{Density}) + \text{intercept}$. The results presented below

$$N = 1.51 \pm 0.18 \quad M = 1.95 \pm 0.11$$

indicate that the exponents should be approximately 1.5 for Isp and 2.0 for density.

A similar linear regression analysis was then conducted on another data set. This data was obtained from the LLNL (Explosives Handbook⁽⁵⁾) and is shown in Table 3. Like Table 1, Table 3 is composed of some pressed and melt-cast explosives; but unlike Table 1, it also contains a number of plastic-bonded compositions (PBXs). (PBXs are representative of today's state-of-the-art military explosives).

These exponents were found to be quite different:

$$N = 0.93 \pm 0.21 \quad M = 2.25 \pm 0.11$$

The Table 3 data-set indicates that the exponent of the Isp is approximately 1.0 and the exponent of the density is approximately 2.25.

A linear regression analysis was then conducted on the relationships as determined from the ln-ln analyses of data from both Tables 1 and 3. Table 4 shows these results. Indeed, the term $\text{Isp}^{1.5} \times \text{density}^{2.0}$ did correlate as well as the $\text{Phi} \times \text{density}^2$ with the experimental detonation pressures given in Table 1. But it showed the poorest correlation for the LLNL data in

Table 3. On the other hand, the term $Isp^{1.0} \text{ density}^{2.25}$ gave the best correlation with the data in Table 3, but gave the least correlation for the data from Table 1. Because all these terms correlated reasonably well with the experimental detonation pressure ($R^2 > 0.95$), and since $Isp \times \text{density}^2$ was an acceptable compromise between the two sets of exponents, the exponents 1 and 2 were chosen. Also, because Table 1 contained mostly ideal explosive compositions, while Table 3 contained many less ideal compositions, e.g. PBX-explosives formed from energetic solids and binder ingredient; this equation was selected as more representative of today's state-of-the-art composite compositions. Thus, the equation for calculating the detonation pressure from the $Isp \times \text{density}^2$ function was derived from the data in Table 3.

$$P(\text{exptl}) = 44.4 Isp \times \text{density}^2 - 21$$

The validity of this relationship can be better demonstrated by plotting the various variables against the experimental detonation pressures given in Table 3. The four plots (Figures 3, 4, 5 and 6) show the Isp , density, $Isp \times \text{density}$, and the $Isp \times \text{density}^2$, respectively, as a function of the detonation pressure. Figure 3 demonstrates that the Isp alone showed some correlation. Figure 4 shows that the density alone gave a much better correlation but the data is quite scattered. In Figure 5, where the term $Isp \times \text{density}$ is used, we see a significant improvement in the correlation, although LX-17, which has a large density and a relatively small Isp , is still far from the line. Figure 6 shows the result of using $Isp \times \text{density}^2$. In this plot, all the compositions are reasonably close to the least squares line and exhibit a R^2 -correlation coefficient of 0.984.

The I_{sp} correlation works well, although the PEP computer code uses the assumption that the products are ideal gases, and the I_{sp} calculation is based on rocket motor pressure conditions (expansion from 1000 to 14.7 psi). Gases at the very high pressures of a Chapman-Jouguet (CJ) detonation are not considered ideal, but Fickett and Davis⁽⁶⁾ state: "Little is known about the properties of gases in the neighborhood of the CJ point of liquid and solid explosives."

CONCLUSION

A novel method has been found to predict the Chapman-Jouguet detonation pressure: using the theoretical rocket performance calculations from the PEP computer code. This method has been shown to agree with the earlier work of KJ for ideal explosives. The correlation obtained through the use of the PEP code have been extended to composite explosives, e.g. binders filled with solid explosive particulate material.

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GLOSSARY

Designation

BTF	Benzo-tris [1,2,5]-oxadiazole-1,4,7-trioxide
Comp B	RDX/TNT/WAX (63/36/1)
Cyclotol	RDX/TNT (75/25)
EDNA	Ethylene Dinitramine, (1,2-di-(nitramino)ethane)
FEFO	1,1'-[Methylene-bis-(Oxy)]-Bis-[2-fluoro-2,2-dinitroethane]
HMX	Octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine
LX-04	HMX/Viton A (85/15)
LX-10	HMX/Viton A (95/5)
LX-14	HMX/Estane (95.5/4.5)
LX-17	TATB/KEL-F 900 (92.5/7.5)
NG	1,2,3-Propanetriol trinitrate
NM	Nitromethane
Octol	HMX/TNT (75/25)
PBX-9010	RDX/KEL-F (90/10)
PBX-9011	HMX/Estane (90/10)
PBX 9404	HMX/NC/CEF (94/3/3)
Pentolite	PETN/TNT (50/50)
PETN	2,2-Bis[(Nitroxymethyl)-1,3-propanediol dinitrate (Pentaerythritol tetranitrate)]
RDX	Hexahydro-1,3,5-trinitro-1,3,5-triazine
TATB	2,4,6-Trinitro-1,3,5-benzenetriamine
TETRYL	N-Methyl-N,2,4,6-tetranitrobenzenamine
TNB	1,3,5-Trinitrobenzene
TNM	Tetranitromethane
TNT	2-Methyl-1,3,5-trinitrobenzene
CEF	Tris-b-chloroethylphosphate
Estane	Polyurethane solution system from B. F. Goodrich Co.
KEL-F	Chlorotrifluoroethylene/vinylidene fluoride copolymer (3/1) from 3M Company
Viton A	Vinylidene fluoride/hexafluoropropylene copolymer (60/40) from DuPont Chemical Co.

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APPENDIX: THE PEP CODE

The Propellant Evaluation Program (PEP) was developed by D.R. Cruise of Naval Weapons Center, China Lake. It assumes that the gases are ideal. The products are calculated using a free energy minimization technique. First, the enthalpy is calculated for the propellant at 1000 psi, then the propellant is burned and the gases expanded to 14.7 psi. The enthalpy is again calculated for the gases at this lower pressure. This difference in the two enthalpies is proportional to the work done by the expanding gases and is expressed as the specific impulse, ISP. The following information is needed to run the PEP:

1. heat of formation of each ingredient
2. atomic formula of each ingredient
3. composition of propellant or explosive

A sample calculation is given for the explosive LX-04, which is composed of 85% HMX and 15% Viton A.

LX04		H	C	N	O	F					
HMX		.088	.004	.088	.0080	.0080	85.000	61.	.0687		
VITON A		.004	.0050	.0000	.000	.0070	15.000	-1801.	.0650		
GRAM ATOM AMOUNTS FOR PROPELLANT WEIGHT OF 100.000										1.0000	
0 (H)	(C)	(N)	(O)	(F)							
2.576587	1.548873	2.295963	2.295963	.521159							
T(K)	T(F)	P(ATM)	P(Psi)	ENTHALPY	ENTROPY	CP/CV	GAS	RT/V			
2898.	4757.	68.02	1800.00	-21.87	245.98	1.2584	4.260	15.978			
1.33953	C0	1.14743	N2	.52993	H2O	.52104	HF				
.48452	H2	.28926	CO2	.81979	H	.80661	HO				
1.80E-03	NO	1.78E-04	O	1.17E-04	F	7.55E-05	O2				
4.33E-05	NH3	3.63E-05	CHO	3.36E-05	CNH						
T(K)	T(F)	P(ATM)	P(Psi)	ENTHALPY	ENTROPY	CP/CV	GAS	RT/V			
1285.	1710.	1.00	14.70	-91.31	245.98	1.3086	4.246	.236			
1.14797	N2	1.14265	CO	.68672	H2	.52116	HF				
.48620	CO2	.34891	H2O	.80803	NH3	.80802	CH4				
HYPOTHESIS	IMPULSE	GAMMA	THR. T	THR. P	CF	ISP*	OPT EX	EXH V	RHO-ISP		
B FROZEN	243.8	1.2807	2541.	37.36	1.575		7.63	7843.	459.3		
SHIFTING	445.8	1.2512	2577.	37.73	1.569		196.8	781.	7910.	463.3	
BOOST VELOCITIES FOR PROPELLANT DENSITY OF .06888 (S.G. OF 1.884)											

NOTE: Sample Calculation:
 (English to metric) $245.8 \frac{\text{lb sec}}{\text{lb mass}} \times \frac{9.807}{1000} = 2.410 \frac{\text{N sec}}{\text{g}}$

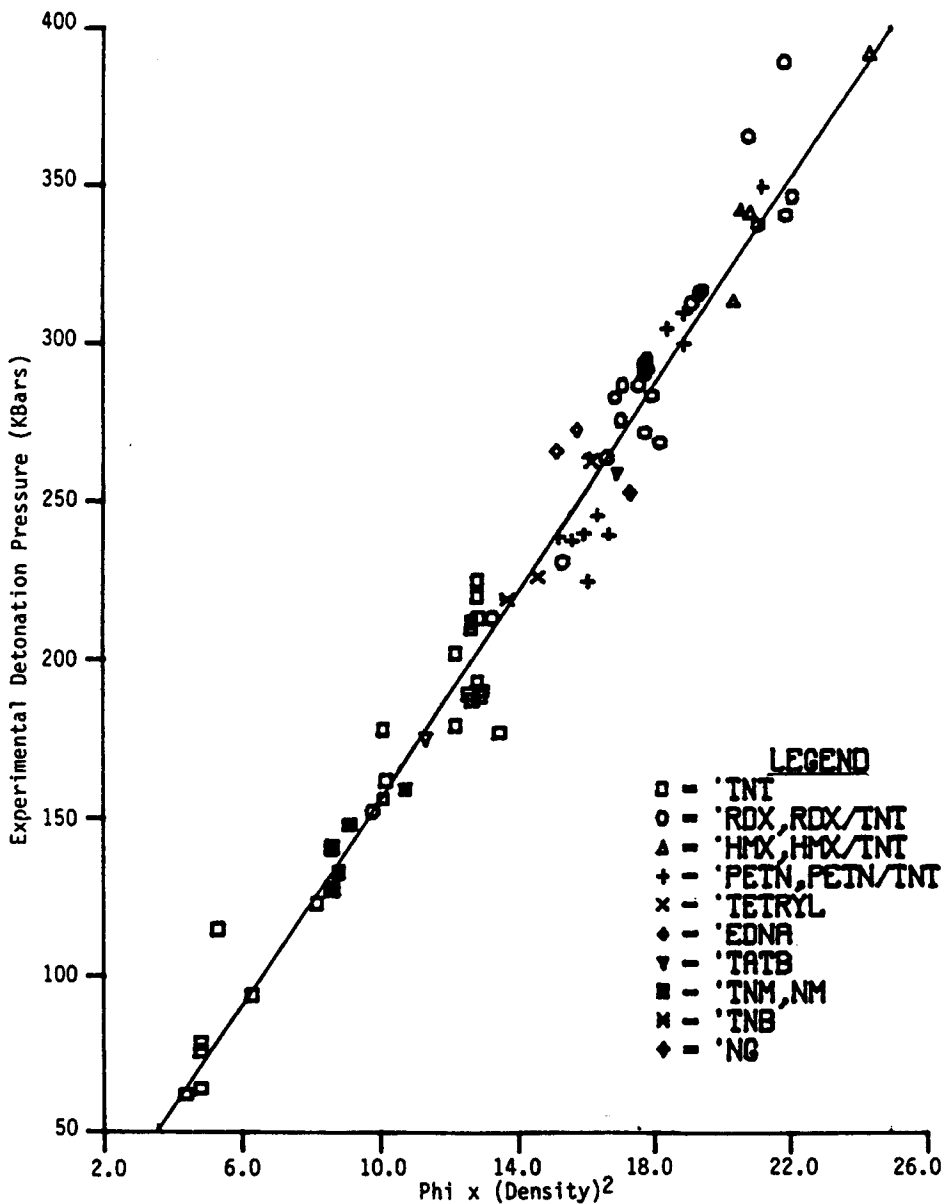


FIGURE 1.
Experimental Detonation Pressure Vs. $\Phi \times (\text{Density})^2$

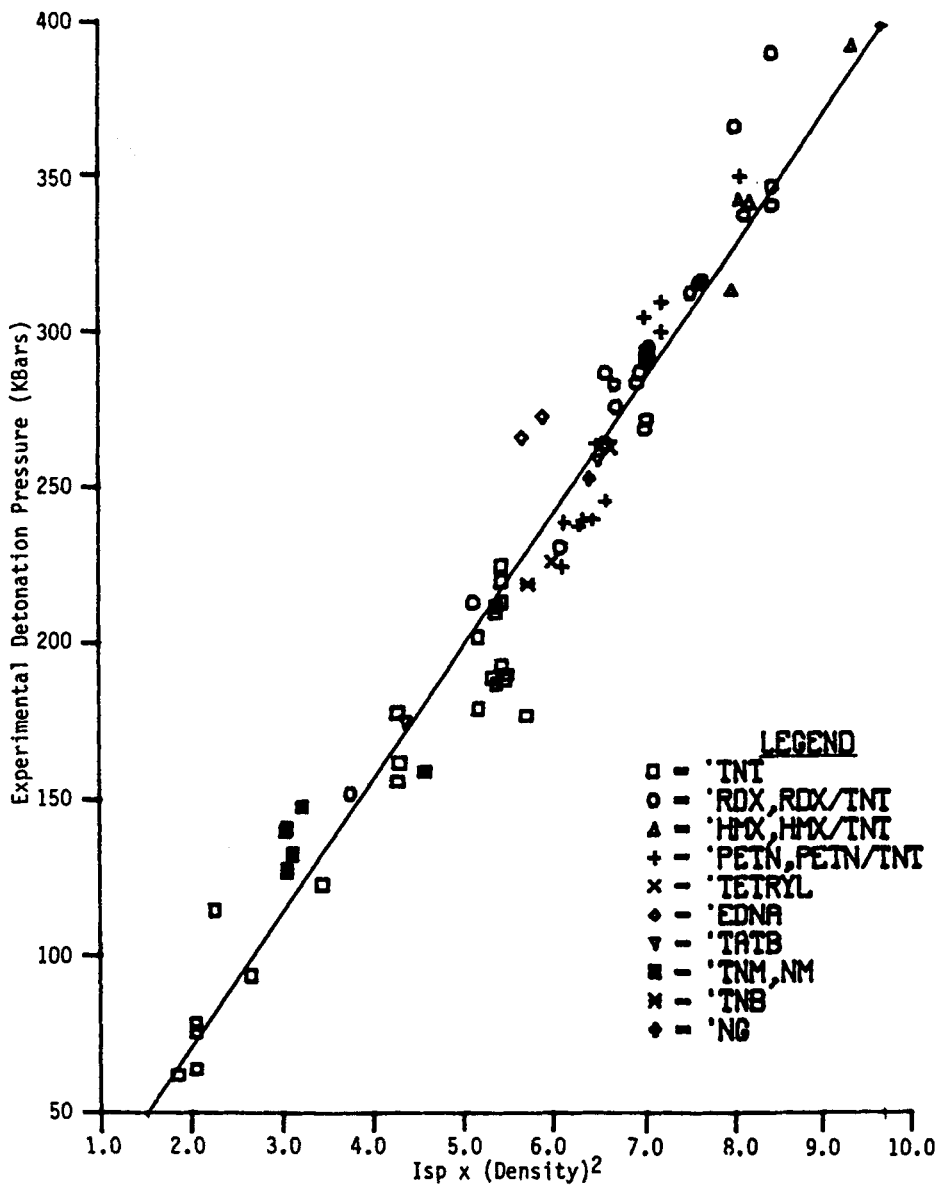


FIGURE 2.
Experimental Detonation Pressure Vs. $I_{sp} \times (\text{Density})^2$

Correlation Coeff. $R^2 = 0.049$

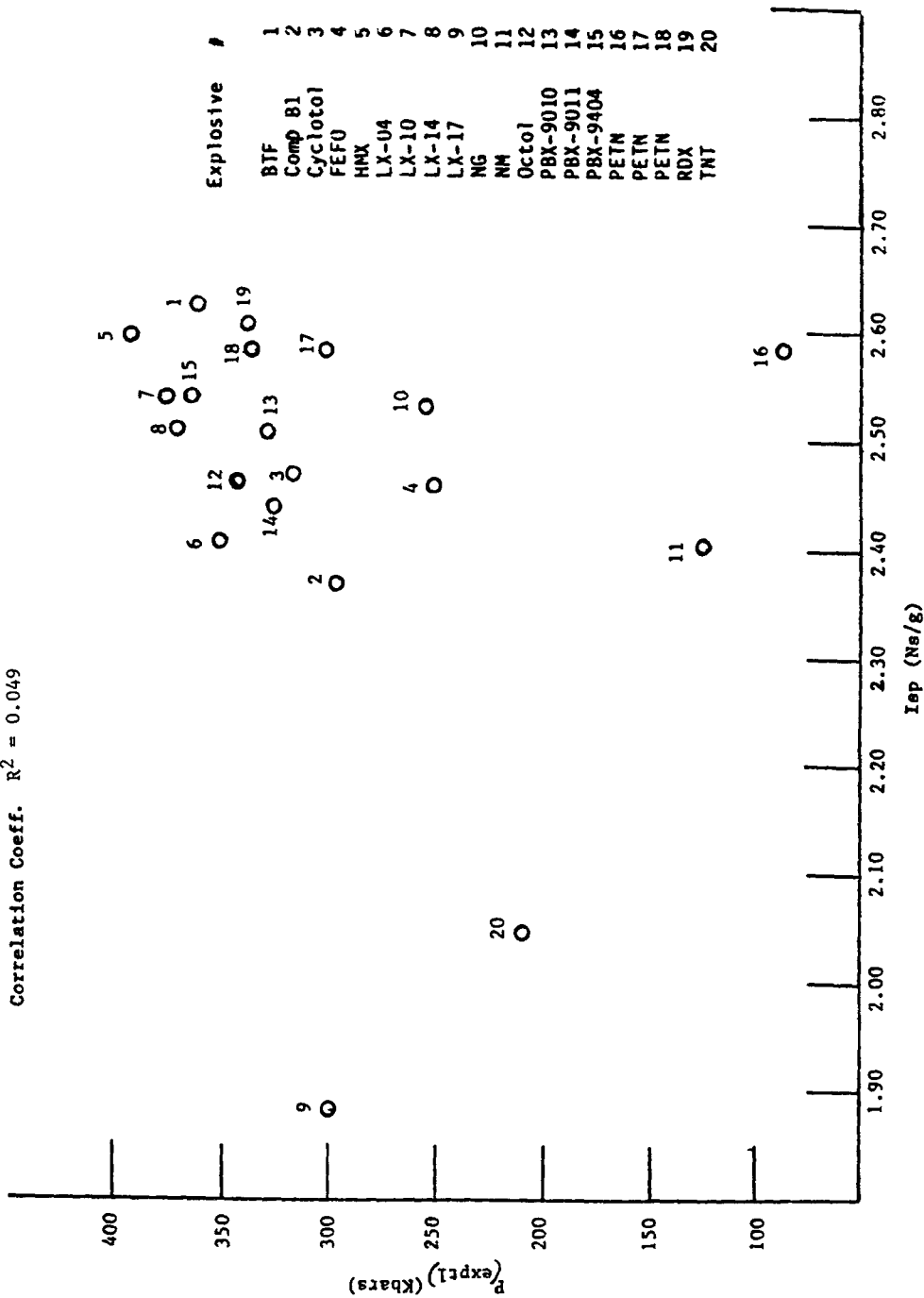


FIGURE 3.
Experimental Detonation Pressure Versus Isp

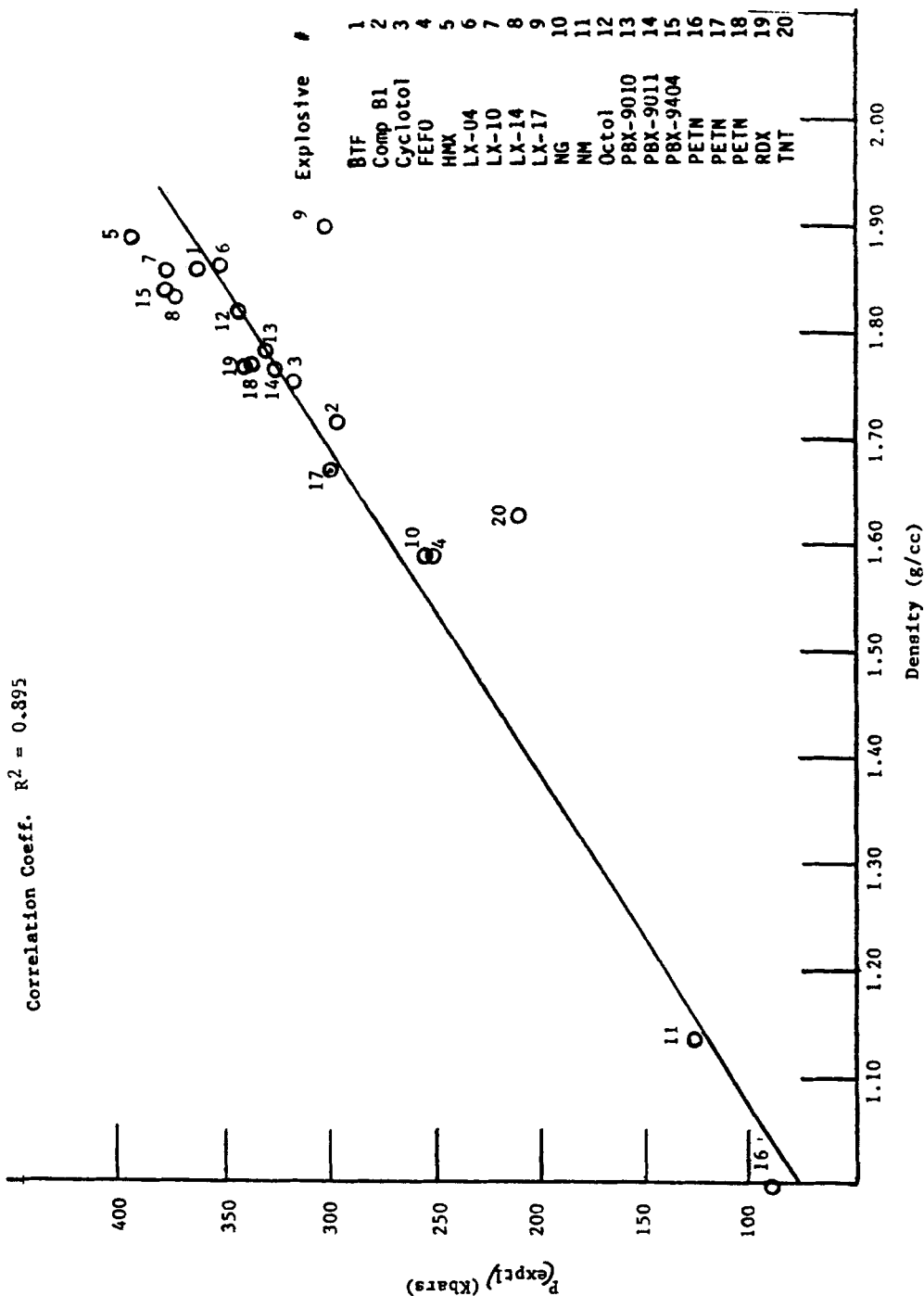


FIGURE 4.
Experimental Detonation Pressure Versus Density

Correlation Coeff. $R^2 = 0.927$

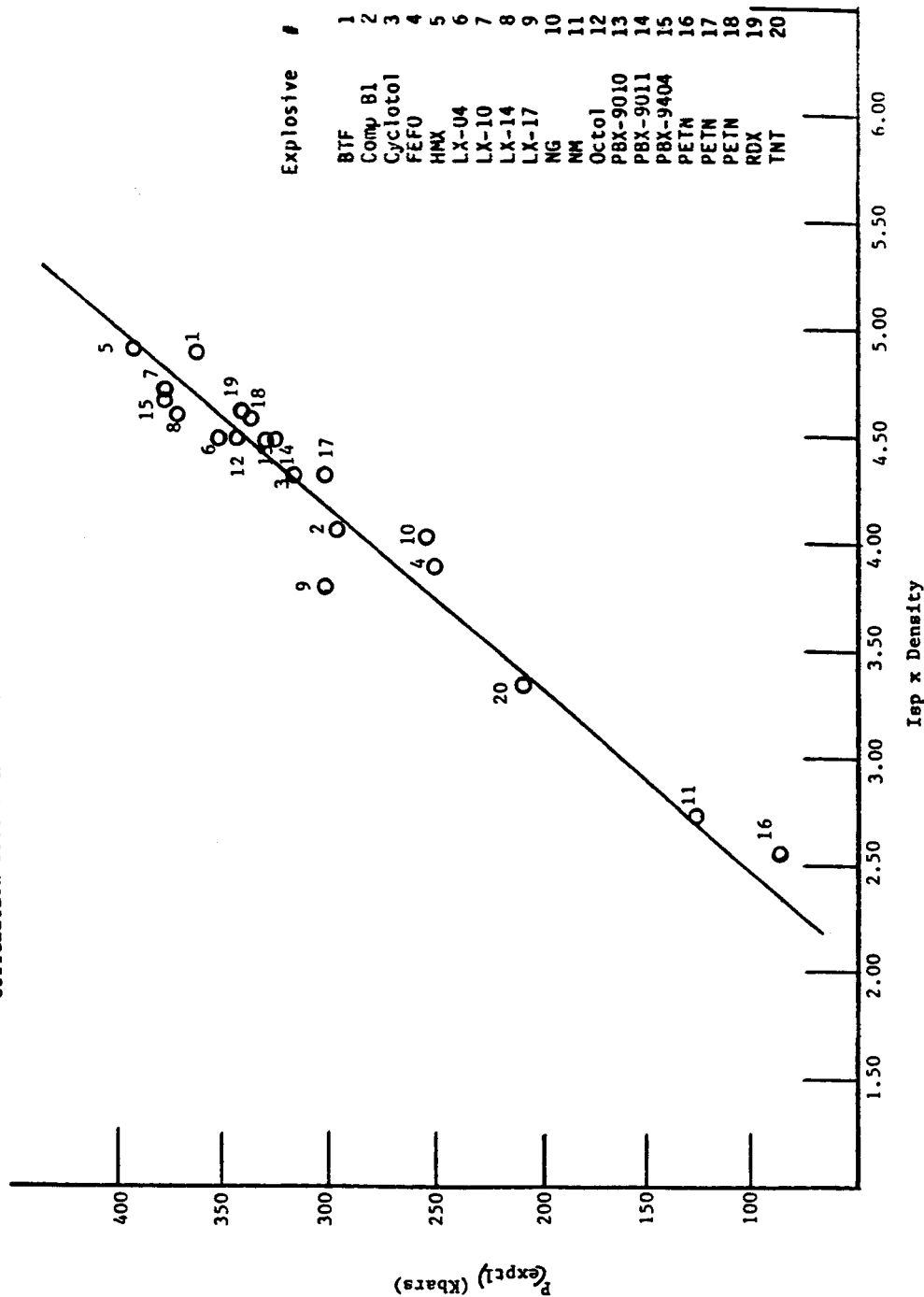


FIGURE 5.
Experimental Detonation Pressure Versus $Isp \times Density$

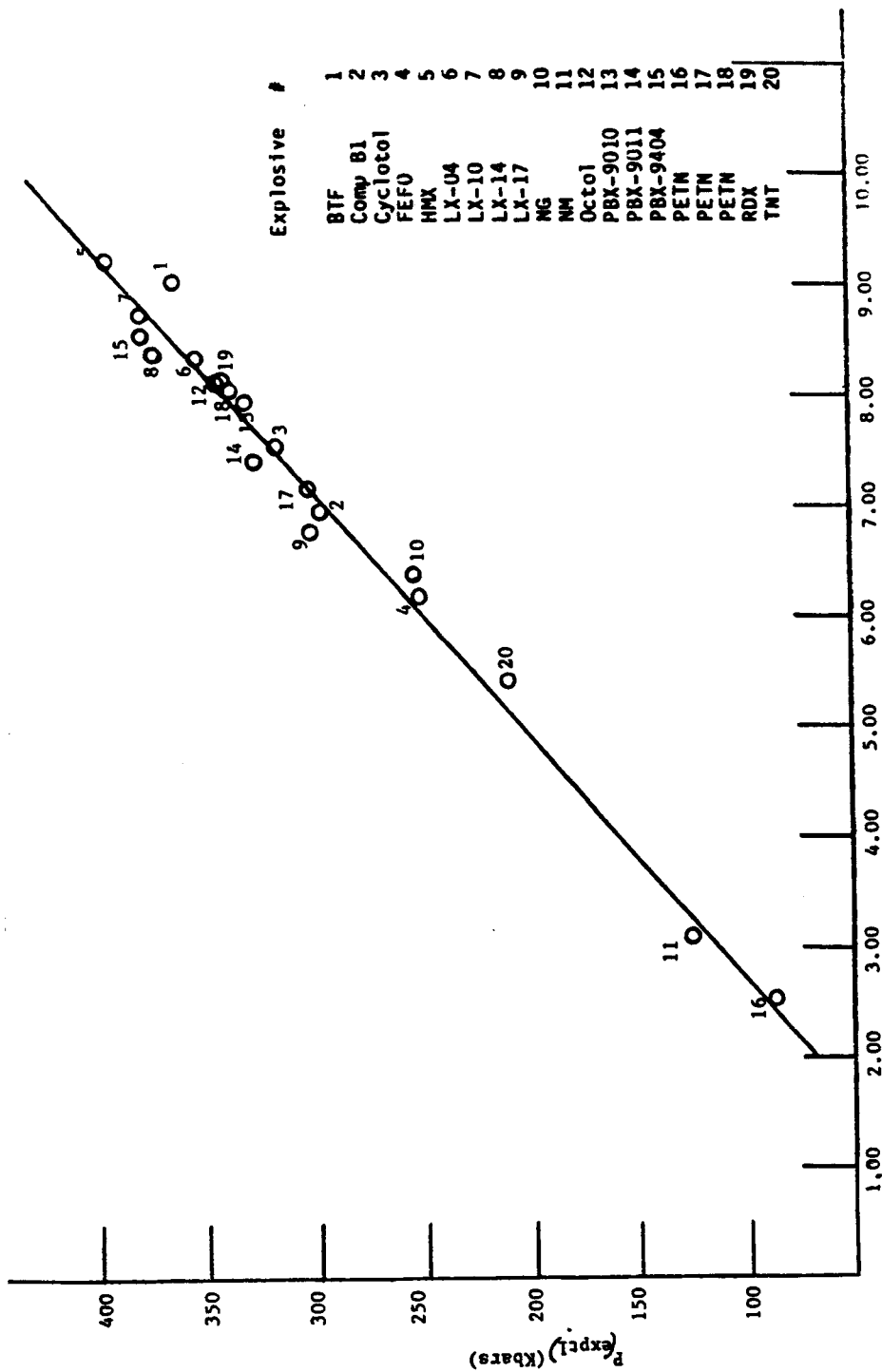


FIGURE 6.
Experimental Detonation Pressure Versus Isp x Density²

TABLE I
Comparison of Experimental and Calculated Detonation Pressures

Explosive	Isp* (Ns/y)	Isp x Density ²	P _(calc) (kbars)	P _(exptl) -P _(calc) (kbars)	Density** (g/cc)	P _{(exptl)**} (Kbars)	Phi**	phi x Density ²	P _(k_u) (kbars)	P _(exptl) -P _(k_u) (kbars)
TNT	2.048	1.848	63	- 2	0.95	62.2	4.838	4.366	64	- 2
		2.048	72	4	1.00	76.3		4.838	72	4
		2.048	72	6	1.00	78.5		4.838	72	7
		5.178	206	-27	1.59	179.0		12.231	193	-14
		2.048	72	- 8	1.00	64		4.838	72	- 8
		2.662	99	- 5	1.14	94		6.287	96	- 2
		3.461	133	-10	1.30	123		8.176	127	- 4
		4.306	169	- 7	1.45	162		10.172	159	3
		5.178	206	- 4	1.59	202		12.232	193	9
		5.508	229	-52	1.64	177	188.4	13.012	214	-37
		5.481	219	-31	1.63	188.4		12.949	205	-17
		5.508	221	-31	1.64	190		13.012	206	-16
		5.335	213	-24	1.614	189		12.603	199	-10
		5.375	215	- 5	1.62	210		12.697	201	9
		5.388	215	-28	1.622	187.2		12.728	201	-14
		5.375	215	- 3	1.62	212		12.697	201	11
		5.455	218	- 5	1.632	213		12.886	204	9
	5.441	218	2	1.630	220		12.854	204	16	
	5.441	218	7	1.63	225		12.854	204	21	
	5.441	218	-24	1.63	193		12.854	204	-11	
	4.276	168	10	1.445	178		10.102	158	20	
	4.276	168	-11	1.445	156		10.102	158	- 2	
	2.262	81	34	1.051	115		5.344	80	35	
RDX	2.611	8.152	334	4	1.767	338	6.784	21.182	340	- 2
		8.460	347	43	1.80	390		21.980	353	37
		8.042	329	37	1.755	366		20.895	336	30
		6.601	267	20	1.59	287		17.151	274	13
		5.118	204	9	1.40	213		13.297	211	2
		3.760	146	6	1.20	152		9.769	153	-1
		8.460	347	-6	1.80	341		21.980	353	-12
		6.937	282	2	1.63	283.7		18.024	288	-5
		8.460	347	8	1.80	347		21.980	356	-9
		7.023	285	-16	1.64	269		18.246	292	-23

TABLE 1 (Cont)

Explosive	Isp* (Ns/g)	Isp x Density ²	P(calc) (Kbars)	P(exptl)-P(calc) (Kbars)	Density** (g/cc)	P(exptl)** (Kbars)	Phi**	phi x Density ²	P(KJ) (Kbars)	P(exptl)-P(KJ) (Kbars)
HMX	2.601	9.390	387	6	1.90	393	6.772	24.447	394	-1
Tetryl	2.305	6.005	242	-15	1.614	226.4	5.615	14.627	233	-6
		6.661	270	-7	1.70	263		16.227	259	4
PETN	2.586	6.117	247	-22	1.538	224.7	6.805	16.097	257	-32
		6.358	257	-17	1.568	239.9		16.731	267	-27
		7.212	294	16	1.67	310		18.978	304	6
		7.212	294	6	1.67	300		18.978	304	-4
		8.102	332	18	1.77	350		21.319	343	7
		7.023	285	20	1.648	305		18.428	296	9
RDX/TNT										
50/50	2.301	6.090	246	-14	1.627	231.1	5.806	15.369	245	-14
60/40	2.373	6.603	267	-3	1.668	264.1	5.992	16.671	266	-2
		6.698	272	11	1.680	283		16.912	270	13
		6.980	284	3	1.715	287		17.624	282	5
64/36	2.401	7.078	288	7	1.717	295	6.063	17.874	286	9
		7.053	287	6	1.714	293		17.812	285	8
		7.053	287	-15	1.714	272		17.812	285	-13
		7.045	286	4	1.713	290.4		17.791	285	5
65/35	2.408	7.081	288	4	1.715	292	6.086	17.900	286	9
75/25	2.472	6.714	272	4	1.648	276	6.292	17.088	273	3
77/23	2.485	7.550	308	5	1.743	313	6.319	19.197	308	5
		7.628	311	5	1.752	316		19.396	311	5
78/22	2.491	7.672	313	4	1.755	317	6.331	19.500	313	4
HMX/TNT										
75/25	2.463	8.007	328	-14	1.803	314	6.288	20.441	328	-14
76.77/23.3	2.474	8.096	331	12	1.809	343	6.310	20.649	332	11
77.67/22.4	2.479	8.220	337	5	1.821	342	6.321	20.961	337	5
EUNA	2.421	5.683	228	38	1.532	266	6.473	15.192	242	24
		5.908	238	35	1.562	273		15.793	252	21

TABLE 1 (Cont)

Explosive	Isp* (Ns/g)	Isp Density ²	P(calc) (Kbars)	P(exptl)-P(calc) (Kbars)	Density** (g/cc)	P(exptl)** (Kbars)	Phi**	phi x Density ²	P(kJ) (Kbars)	P(exptl)-P(kJ) (Kbars)
PETN/TNT										
50/50	2.332	6.504	263	1	1.670	264	5.796	16.164	258	6
		6.598	267	-21	1.682	246		16.398	262	-16
45/55	2.294	6.451	261	-20	1.677	240	5.680	15.974	255	-15
40/60	2.253	6.305	255	-16	1.673	238	5.586	15.635	249	-11
35/65	2.210	6.150	248	-9	1.668	239	5.492	15.280	243	-4
NM										
	2.405	3.060	116	25	1.128	141	6.767	8.610	134	7
		3.060	116	11	1.128	127		8.610	134	-7
		3.060	116	12	1.128	128		8.610	134	-6
		3.043	115	25	1.125	140		8.564	133	7
		3.125	118	15	1.14	133		8.794	137	-4
		3.230	123	25	1.159	148		9.090	142	6
TATB										
	1.913	6.527	264	-5	1.847	259	4.976	16.975	271	-12
		4.363	171	4	1.51	175		11.346	179	-4
TNB										
	2.132	5.734	230	-11	1.64	219	5.105	13.730	218	1
TNM										
	1.701	4.574	180	-21	1.64	159	4.007	12.302	169	-10
NG										
	2.535	6.425	260	-7	1.592	253	6.837	16.284	277	-24
STD error of estimate =										18

*Calculations from PEP code

**Data from KJ Paper (ref. 4)

TABLE 2
Linear Regression Analysis of Data

<u>x variable</u>	<u>Y variable</u>	<u>Intercept</u>	<u>Slope</u>	<u>R²**</u>	<u>Std Error (Kbars)</u>
phi x density ²	P(exptl)	-8 ± 10*	16.42 ± 0.68	0.969	14
Isp x Density ²	P(exptl)	-15 ± 14*	42.8 ± 2.2	0.951	18

* Least-square value of the coefficient ± its standard error
 ** R² = correlation coefficient squared

TABLE 3
Explosive Parameters

Explosive	#	Isp* (Ns/g)	Density** (g/cc)	P(exptl)** (Kbars)	Isp x Density	Isp x Density ²	P(calc) (Kbars)	P(exptl) - P(calc) (Kbars)
RIF	1	2.632	1.859	360	4.893	9.096	383	-23
Comp B1	2	2.372	1.717	295	4.073	6.993	289	6
Cyclotol	3	2.472	1.752	316	4.331	7.588	316	0
FEFO	4	2.461	1.59	250	3.913	6.222	255	-5
HMX	5	2.601	1.89	390	4.916	9.291	392	-2
LX-04	6	2.411	1.865	350	4.497	8.386	351	-1
LX-10	7	2.544	1.860	375	4.732	8.801	370	5
LX-14	8	2.514	1.833	370	4.608	8.447	354	16
LX-17	9	1.884	1.900	300	3.580	6.801	281	19
NG	10	2.535	1.59	253	4.031	6.409	264	-11
NM	11	2.405	1.135	125	2.730	3.098	117	8
Octol	12	2.463	1.821	342	4.485	8.167	342	0
PBX-9010	13	2.510	1.783	328	4.475	7.980	333	-5
PBX-9011	14	2.391	1.765	324	4.485	7.449	310	-14
PBX-9404	15	2.544	1.840	375	4.681	8.613	361	-14
PETN	16	2.586	0.99	87	2.560	2.535	92	-5
PETN	17	2.586	1.67	300	4.319	7.212	299	-1
PETN	18	2.586	1.77	335	4.577	8.102	339	-4
RDX	19	2.611	1.767	338	4.614	8.152	341	-3
TNT	20	2.048	1.630	210	3.338	5.441	221	-11

*PEP code calculation

**LLNL Explosive Handbook Data (ref. 5)

TABLE 4
Results of Regression Analysis

	<u>Intercept*</u>	<u>Slope*</u>	<u>R²</u>	<u>STD Error</u>
Isp x Density ²	-15 ± 14	42.8 ± 2.2	0.951	18
Isp ^{3/2} x Density ²	4 ± 10	25.8 ± 1.1	0.966	15
Isp x Density ^{2.25}	3 ± 13	35.1 ± 1.9	0.947	18
Phi x Density ²	-8 ± 10	16.42 ± 0.68	0.969	14
a. Isp x Density ²	-21 ± 21	44.4 ± 2.8	0.984	10
Isp ^{3/2} x Density ²	1 ± 34	26.4 ± 2.9	0.954	18
Isp x Density ^{2.25}	2 ± 18	36.0 ± 2.1	0.986	10

Table 1 data

Table 3 data

*95% Confidence level

Note a: This expression was selected from the data set that was more representative of today's state-of-the-art composite PBX explosives.