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RUBY CODE CALCULATION OF DETONATION PROPERTIES I. C-H-N-O SYSTEMS

1 NOVEMBER 1963

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UNITED STATES NAVAL ORDNANCE LABORATORY, WHITE OAK, MARYLAND

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RUBY CODE CALCULATION OF DETONATION PROPERTIES I. C-H-N-O SYSTEMS

By
Donna Price and Harold Hurwitz

ABSTRACT: The RUBY code has been used to compute detonation properties for 23 solid high explosives (pure compounds), 5 liquids, and several mixtures at loading densities of TMD (the theoretical maximum density) and 0.95 TMD. It was found that the BKW equation of state parameters now in the code are adequate for many high explosives, but should be replaced by a recently available newer set of parameters to obtain good agreement between computed and experimental results for the larger variety (in oxygen balance) of high explosives.

It is shown that the detonation properties of the solid mixtures can be computed from those of the pure components. A comparison is made between the energy release exhibited by burning and by detonation; they are of the same order of magnitude, and the limit of the release in confined burning at high pressure is the detonation release.

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RUBY Code Calculation of Detonation Properties I.
C-H-N-O Systems

The work of this report was carried out under Task RUME 4E-000/212-1/F008-08-11, Problem 013, Explosive Hydrodynamic Calculations. The work should be of interest to scientists conducting research on explosives and detonation phenomena.

The report itself is a progress report on a continuing investigation of obtaining the most acceptable computed values of detonation properties of high explosives by use of the RUBY Code. As a result of the present work, changes in the computational scheme have been recommended. Subsequent reports will present results obtained after such improvements in the code.

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TABLES

RUBY CODE CALCULATION OF DETONATION PROPERTIES I. C-H-N-O SYSTEMS

Over twelve years ago, Christian and Snay[1] computed detonation parameters for some thirteen organic explosives and their mixtures at five different loading densities. At that time, digital computers were not generally available; the work was therefore carried out on desk computers and the calculations simplified by the use of arbitrary decomposition equations.

In recent years, with the aid of digital computers, a more refined method of obtaining values of the detonation parameters has been outlined by Cowan and Fickett[2]. As in the earlier work, the Kistiakowsky-Wilson equation of state was used for the detonation gas products. Although different co-volume factors were used in the two cases, the major difference is the computation of the composition of the detonation products in equilibrium at the C-J pressure and temperature, an operation made practical by the use of an electronic computer in the more recent work.

The documented advances in this field have extended the computational plan of Ref. (2). Two very similar codes[3,4] have been constructed for the computation of detonation parameters. Of these two, the RUBY code[3] was obtained by NOL from the Lawrence Radiation Laboratory; it has been slightly modified and improved for use at NOL with the IBM 7090 computer[5].

Mader[6] has carried out machine computations of detonation parameters for five pure organic explosives and a number of mixtures at a single loading density. However, no one has used the present codes and techniques to make a survey of different pure explosives and their mixtures which has the scope and value of the tabulations of Ref. (1). The present report covers some of the work in an effort designed to produce a reference manual of the best values that can be computed at the present time.

The entire program has been planned to study, in order,

(1) necessary modifications to the RUBY code for its most effective use in this work,

(2) a study of a representative group of organic (C-H-N-O) explosives and their mixtures at high loading density,

(3) a study of a selected group of organic explosives with varying loading densities,

(4) revision of the code if results of (3) indicate the necessity, and

(5) a study of more complex explosives such as metallized explosives, fluorine containing compounds, and composite propellants.

Work on item (1) and the beginning of that on item (2) are being reported separately[8]. The work reported here completes item 2 of the study. Its results for pure organic explosives and mixtures, applicable in the range of 90 - 100% voidless density, are expected to be immediately useful for two reasons: (1) most practical charges have loading densities within this range and (2) it is in this density range that theoretical and experimental results are most apt to agree.

While this report was being written, a second and more comprehensive report by Mader[7] was issued. Although it is not exactly the manual envisioned by the authors, its results will contribute greatly to the planned study and will considerably reduce the future work that needs to be done. Details of Ref. (7) will be discussed in the appropriate sections below.

HIGH EXPLOSIVES THAT ARE SINGLE COMPOUNDS

The explosives studied were selected to cover a wide range of oxidizing-reducing conditions; their formulae, molecular weight, oxygen balance and heats of formation are given in Table 1. Table 1A lists 22 solid organic explosives and Table 1B, four liquids. Both tables are arranged in order of increasing oxygen balance, and each table contains one inorganic high explosive.

The computed values of the detonation properties appear in Table 2. Each explosive has two sets of values shown as functions of its loading density ρ_o. The higher ρ_o is taken as the voidless or crystal density (TMD) for the material; the lower is 95% TMD. Intermediate values of the parameters can be obtained by linear interpolation, and values down to 90% TMD may be obtained by linear extrapolation although no parameter is exactly a linear function even within this narrow range[8]. Of course, the 95% TMD values for liquids in Table 2B are fictitious and hence bracketed. They are given to allow adjustments of the computed values to any future improved values of the liquid density at 25°C; moreover, they can be used with the thermal expansion coefficient (if it is known) to obtain a first approximation to the density effect caused by a change in temperature.

The detonation properties listed in Table 2 are pressure P, temperature T, density ρ, exponent K, and two internal energy differences. The subscript j refers to Chapman-Jouguet conditions o refers to the initial state at 298°K and 1 atm.

The change in internal energy across the detonation front, $E_j - E_o$ is, by the Hugoniot equation,

$$E_j - E_o = (1/2) P_j (V_o - V_j) \qquad (1)$$

with P_0 taken equal to zero ($P_0 \ll P_j$). Here E_j is the internal energy of the detonation products at P_j, T_j; and E_0 is that of the unreacted explosive at 298°K, 1 atm. V is specific volume. The chemical energy (detonation energy, heat of detonation), Δe, is the negative of the change in internal energy for the fictitious chemical reaction:

$$\text{Explosive } (T_0, P_0) \longrightarrow \text{C-J detonation products } (T_0, P_0).$$

Here

$$\Delta e = E_0(T_0, P_0) - E_1(T_0, P_0) \tag{2}$$

where the subscript 1 refers to the C-J products. In the code the detonation energy is computed as

$$\Delta e = -\Delta H(T_0, P_0) + nRT_0 = -\Delta E(T_0, P_0)$$

where n is the number of moles of gas formed in the actual reaction:

$$\text{Explosive } (T_0, P_0) \longrightarrow \text{C-J detonation products } (T_j, P_j).$$

Since

$$E_j = E_1(T_j, P_j)$$

it is clear that

$$E_j - E_0 = E_1(T_j, P_j) - E_1(T_0, P_0) - \Delta e \tag{3}$$

In other words, the change in internal energy across the detonation front is the amount of energy necessary to raise the temperature and pressure of the detonation products from T_0, P_0 to T_j, P_j minus the chemical energy Δe released in a fictitious reaction carried out at 298°K.

The remaining property of Table 2, K, is called an exponent because of the similarity of its definition to that for the adiabatic exponent of a gas. Cowan and Fickett[8] define the exponent K_j as

$$K_j = -\left(\frac{\partial \ln P}{\partial \ln V}\right)_S = \frac{\rho_0 D^2}{P_j} - 1 \tag{4}$$

where D is the detonation velocity. By combining the hydrodynamic equations derived from the laws of conservation of mass and momentum and neglecting P_0, it is evident that

$$P_j = \rho_0 D^2 \left(1 - \frac{\rho_0}{\rho_j}\right) \tag{5}$$

must also hold. Hence the exponent may be evaluated by

$$K_j = \left(1 - \frac{\rho_0}{\rho_j}\right)^{-1} - 1 = \rho_0/(\rho_j - \rho_0) \qquad (6)$$

This latter method is used in the RUBY code. The exponent K is discussed further in the appendix.

In Table 1 the explosives are arranged in order of increasing oxygen balance to demonstrate the range considered in oxidation-reduction compositions. The same order has been maintained in subsequent tables where it serves to show in Table 2 that oxygen balance alone is generally useless in predicting even the trends to be expected in detonation properties. Within the chemically related series of amino substituted trinitrobenzenes (TNB, TNA, DATB, and TATB), however, the number of substituted amino groups effects a corresponding trend in the oxygen balance; thus, within the series the oxygen balance seems to indicate the qualitative trends in the detonation properties, as would be expected. Even here no quantitative relationships appear. Table 2 also demonstrates the relative insensitivity of detonation energy to loading density and the relative sensitivity of C-J pressure to this factor. The changes were respectively about 1% and 10% for a 5% change in ρ_0. Other parameters exhibit sensitivities between these extremes.

In Table 3 are listed the composition of the detonation products found. For the equilibrium products considered, carbon has been taken as graphite rather than diamond or amorphous. Both the latter forms have been used by other workers—particularly in attempting to make computations agree with experimental results for TNT, e.g., Refs. (1) and (5). If subsequent more detailed study with the code indicates the necessity of a choice of different forms of carbon, such a modification will be made. Similarly, methane has been retained as a possible product because it is found after detonation in calorimeters and because its presence is indicated by the thermodynamic computations; some workers believe that methane formation is so slow that it should not be considered a possible detonation product.

In the earlier work[8] it was shown that only two minor components (NH_3 and CH_4) need be considered with the major products (C, $H_2O(g)$, CO_2, CO, and N_2) to obtain satisfactory values of the detonation properties of explosives up through PETN, i.e., up to an oxygen balance of -10% to CO_2. In materials of higher oxygen balance, equilibrium computations show that NH_3 and CH_4 disappear; minor components which then assume importance are oxygen and the oxides of nitrogen. These facts are reflected in the products shown in Table 3. In no case did atomic species or free radicals occur in significant amounts.

The increase in P_j caused by increasing ρ_o from 0.95 TMD to TMD is sufficient to show, in the data of Table 3, the effect of pressure on the soot reactions

$$2\ CO \rightleftarrows CO_2 + C$$

$$H_2 + CO \rightleftarrows H_2O(g) + C$$

When carbon is a product, the amount formed from the explosive at the higher density (hence, higher pressure) is always greater than that at the lower. In general, the amounts of $H_2O(g)$ and CO_2 are also greater although reversals sometimes occur because of the effect of the water-gas equilibrium. Additional examples of the pressure effect on the composition of the products will be given later.

COMPARISON OF COMPUTED VALUES WITH EXPERIMENTAL RESULTS

There is little point in comparing the computed values with all available detonation velocity, pressure, and temperature measurements. The hydrodynamic equations used result in ideal values of D and P_j, both of which can exhibit a diameter effect. (See Ref. (8) for a discussion of these parameters.) Experimental data should therefore be selected from studies made on large charges, made with the diameter as a variable, and made with the best available instrumentation. An earlier discussion[9] of a similar choice is still relevant; it led to the selection of data measured at Los Alamos Scientific Laboratory (LASL). The LASL data cited in Ref. (7) will be used for the present comparison.

Experimental values of D, P_j (where available), and T_j (where available) are given for nine pure explosives in Table 4. Except for TNT and NM, there is reasonable agreement in D (3%) and P (5%) with the computed values in explosives of oxygen balance up to the CO_2 level. For the higher oxygen content materials, HN and TNM, the agreement is very poor. The temperature measurements are too few and the agreements too poor to speculate on the inadequacy of the experimental method, the numerical treatment or both.

In Ref. (7) Mader tabulates four sets of BKW parameters:

a. those used in Ref. (6),

b. those obtained by fitting experimental values of D and P_j for RDX at 1.80 and 1.0 g/cc,

c. those obtained by fitting experimental values

of TNT, and

d. those obtained as in (b) but chosen to keep $(\partial P/\partial T)_V > 0$.

He made these computations with new co-volumes he had derived for H_2O and CO_2. He then gave sample computations using each of these four sets of parameters.

Table 4 lists the results only for set (a), that set now in the RUBY code. They differ only slightly* from the corresponding values in Ref. (6) computed with the old co-volumes and the same BKW parameters. Moreover, as would be expected, they differ only slightly from the values of this report.

Mader's results showed that use of the BKW parameters, set (d), very much improved the agreement with experimental values for NM, HN, and TNM; for the last material, and presumably for other oxygen rich explosives, the improvement was spectacular (a factor of 10 in per cent difference).

Neither Mader's calculations[7] nor those of Fickett[8] show the discontinuity observed experimentally[10] in the detonation velocity - loading density curve for TNT. No other low oxygen balance explosive has been studied as carefully as TNT, and the few data available for DATB[11] are inconclusive on the existence of such a discontinuity. TNT is known to exhibit increasing resistance to the initiation of high order detonation with increasing loading density; difficulty in initiating cast TNT and booster effects manifest in explosions of cast TNT are common experience. Although TNT does not exhibit the extreme "dead pressing" phenomena of NQ, its behavior is sufficiently similar to indicate obvious difficulty in establishing the steady state reaction. For these reasons, it is suggested that such a discontinuity is evidence of the beginning of non-ideal reaction, and that the present theory is applicable only to loading densities below that at which the discontinuity appears, i.e., below 1.53 g/cc for TNT.

In support of this suggestion, TNT (ρ_o = 1.64) results obtained with set (d) parameters gives D and P of 7.197 mm/μsec and 213 kbar, respectively; extrapolation of the low density portion of the D-ρ_o curve[10], gives D of 7.100 mm/μsec and P_J of 203 kbar (by adding a corresponding pressure increment from

* It is not clear whether the small differences arise from the new co-volumes or from considering a somewhat different set of products in the two cases.

Table 1 to the measured P_j). The K value for the extrapolated results is 3.07. These differences are now as small as those encountered in some higher oxygen materials. Moreover, the measured and computed velocities in the present work for DATB and TATB seem to be in reasonable agreement. Finally, liquid TNT (ρ = 1.447) shows better agreement with set (d) parameters than with set (c)[7].

If the suggested irregularity of reaction appears at high density in TNT alone, or at high density in all high carbon explosives, it seems possible that set (d) BKW parameters can be used for all explosives, but restricted to lower densities in those exhibiting atypical reaction of the TNT type.

Values of the exponent K listed under "Experimental" in Table 4 are bracketed because they are not measured but are computed from experimental values of D and P_j. Thus any experimental errors can be magnified in K.

In Table 5 a number of experimental values of D, for other explosives than those of Table 4, are compared with the computed values of Table 2. Although the measurements of Table 5 are considered less accurate than those of Table 4, the trend noted in Table 4 is confirmed. The higher oxygen content materials (TNETB on) surely require BKW parameters of set (d).

MIXTURES OF ORGANIC HIGH EXPLOSIVES

It has been known for some time that most mixtures of organic explosives exhibit effects that can be predicted by simple additivity of the effects of each pure component (e.g., Ref. (15)). There was, however, a question of the applicability of the additivity rule to a mixture consisting of an explosive with an oxygen balance negative to CO (e.g., TNT) mixed with another explosive of positive oxygen balance to CO (e.g., PETN). Pentolite 50/50 is such a mixture. On the basis of data available for pentolite six years ago, it was concluded[18] that rapid energy release phenomena such as detonation and fragmentation velocity would exhibit additivity whereas a long-time energy release in a calorimeter would not.

Since the earlier work, blast data for pentolite in N_2 have been obtained[18] and indicate straight additivity of the component effects in the relatively long blast phenomena. Subsequently, a calorimetric determination of the heat of detonation of pentolite was made[17]; for this even longer term energy release, additivity also held. It follows that mixtures, with solid components of an oxygen balance nearly up to the CO_2 level, follow the additivity principle. Consequently, it should be possible to predict the properties of the mixture from those computed for the pure components.

To investigate this possibility, RUBY was used to compute the detonation properties for two cyclotols and for pentolite 50/50; the results are given in Tables 6 and 7. Table 8 summarizes computed data for the components of the cyclotols, pentolite, and an RDX/TFNA mixture reported in Ref. (7). These data were used to predict mixture properties as follows:

$$D = \sum_i x_i D_i \tag{7}$$

where i is component index, x is weight fraction.

$$\rho_j = \left(\sum_i \frac{x_i}{\rho_{ji}} \right)^{-1} \quad \text{or} \quad V_j = \Sigma\, x_i V_{ji} \tag{8}$$

$$K_j = \rho_o/(\rho_j - \rho_o) \tag{9}$$

$$P_j = \rho_o D^2/(K_j + 1) \tag{10}$$

$$T_j = \sum_i x_i T_{ji} \tag{11}$$

Table 9 compares values obtained in the above manner with those computed by the code. It is evident that agreement is to 0.1% or better in ρ_j; 0.2% in D; 0.4% in K, 0.7% in P, and 1% in T. Although the energies have not been listed, they are strictly additive as are the products. In other words, for the explosives studied, there is no indication of interaction to produce products in the mixture differing from those produced by the individual components. It follows that the properties of the mixtures can be predicted to 1% or better from the computed values of the components.

Of course, the additivity treatment is inadequate when components interact as, for example, in the liquid mixtures of NM with TNM[7]. In this case, the detonation velocity of the mixture is greater than that of either component. No solid mixture exhibiting this behavior has been reported.

PROPERTIES OF EXPLOSIVES WHEN BURNED

Organic explosives are capable of a number of exothermal decompositions. All are of importance for safety considerations, and for consideration of the transient conditions involved in the build-up from burning to steady state detonation. For these reasons, the NOL code for propellant computations[18] has been used to compute properties and products to be expected from high explosive burning at constant pressure. In this case, the heat of reaction is the change in enthalpy for the fictitious reaction:

Explosive (T_o, P_o) $\longrightarrow$ deflagration products (T_o, P_o),

and is written

$$\Delta h = H_0(T_0,P_0) - H_1(T_0,P_0) = -\Delta H(T_0,P_0)$$

Table 10 lists comparison of computed energy release, temperature, and amount of gas products for a group of representative explosives (a) detonating at 0.95 TMD and (b) burning at 1 atm; this table also contains the major deflagration products. The trend in products formed vs oxygen balance is qualitatively the same as that for detonation products, e.g., less carbon and more CO_2 with increased oxygen balance. There are, however, large quantitative differences (See Table 3) attributable chiefly to the different equilibria at P_j and P_0.

The energy release in the burning (Δh) is of the same order of magnitude as that in detonation (Δe), but somewhat smaller; for atmospheric pressures, Δh ranges from $0.50\Delta e$ (low oxygen balance) to $0.65\Delta e$ (O.B. of zero to CO_2). Similarly, the flame temperature is of the same order of magnitude as T_j with a range of 0.75 to 1.00 T_j. The total product gas n ranges from 1.65 to 1.15 n_j.

It is seldom that explosives are burned at a pressure as low as 1 atm, possibly only when they are being destroyed by burning them in very thin layers. If they are used in propellants or are burned under confinement, the chamber pressure is perhaps 100 bar and the confined burning pressures can be 5 kbar and greater. Increasing the pressure at which the reaction occurs will increase Δh and decrease n. In the limit, burning at P_j will produce the same products found for detonation at P_j, because the equilibrium computations are independent of all kinetic considerations. The two codes do <u>not</u> produce the same results because the ideal gas law (adequate up to ca. 0.2 kbar) is used in the propellant code whereas the BKW equation (believed adequate down to ca. 0.2 kbar) is used in the RUBY code. Nevertheless, Table 11 shows the trends to be expected as the chamber pressure is increased for six representative high explosives. In the detonation pressure range, the results are inexact because of the inadequacy of the ideal gas law; for the same reason they show insensitivity to 10 - 15% changes in pressure within this range, and flame temperatures greater than T_j.

Table 12 contains the results obtained, for most of the explosives of Table 1, when the detonation pressure is used as the chamber pressure in computing the results of deflagration. The differences introduced by using the ideal gas law rather than the BKW equation of state can best be seen by comparing results of Table 12 with those of Tables 2 and 3.

It cannot be emphasized too strongly that the energy release of the burning explosive is of the same order of magnitude as that of the detonating explosive. The great difference between burning and detonation is the rate of energy release; this can differ by several orders of magnitude[19]. However, as the pressure, under which the burning takes place, increases, so too does the rate of energy release. Thus the high pressure burning approaches detonation as a limit in its rate of energy release.

CONCLUSIONS

1. Use of the RUBY code with its present set of parameters, BKW set (a), results in computed detonation properties in reasonable agreement with the measured properties of most of the explosives studied at high densities. Exceptions are NM, TNT, and explosives of high oxygen balance.

2. Replacement of BKW set (a) parameters with BKW set (d) parameters will bring all but one (TNT) of the above exceptions into line. The exceptional TNT behavior has been tentatively considered evidence of incomplete reaction.

3. Mixtures of organic solid high explosives behave additively. Computed detonation properties of the mixtures, good to 1% or better, can be obtained by an additive treatment of the computed properties of the pure components.

4. The energy release in burning of an explosive is of the same order of magnitude as that in detonation. The energy release in confined burning approaches the detonation energy as a limit at high pressures.

FUTURE WORK

The results already considered make it evident that the BKW parameters and co-volumes now in RUBY should be changed to the set (d) values of Ref. (7). After this has been done, scanning the D vs ρ_o curve of representative explosives will be carried out. The explosives, selected to cover a range in O.B. and also to be those for which D - ρ_o data are or should be available, are:

TNT (Compare with Ref. (10) data at $\rho_o \leq 1.53$)

DATB (Compare with Ref. (11) data and, if possible, additional points obtained at the higher densities to demonstrate presence or absence of a discontinuity.)

NQ (Compare with literature values and Ref. (20))

RDX (Compare with LASL data)

TNETB (Compare with Ref. (21))

HN (Compare with Ref. (22) and, if possible, extend diameter effect study of Ref. (23))

Of these, Mader[7] has reported scans of RDX with set (d) parameters as well as of HMX, PETN, Tetryl, and PA. He has reported only single results at high density with set (d) parameters for TNT and DATB; his reported scans for these explosives were carried out with set (c) parameters. Thus of the materials selected, computations must be made for NQ, TNETB, HN, and possibly TNT and DATE.

After acceptable agreement with experimental D vs ρ_o slopes is attained, the revised RUBY will be used to obtain tables similar to Tables 2 and 3, and selected adiabats from the C-J point down. At the same time, Sexton[17] is carrying out calorimetric determinations of heat of detonation for twelve explosives; these will be compared to both the numerical results and the experimental underwater and blast measurements.

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Table 1A

Solid High Explosives Used in Computations

Material	Molecular Weight M.W.	Heat of Formation ΔHf Kcal/mole	Formula C	H	N	O	Name	Oxygen Balance* % to CO	to CO_2
R-Salt	174.13	66.8[a]	3	6	6	3	Cyclotrimethylenetrinitrosoamine	-28	
TNT	227.13	- 17.81	7	5	3	6	Trinitrotoluene	-25	
TATB	258.16	- 36.85[b]	6	6	6	6	Triaminotrinitrobenzene	-19	
DNPF	380.23	-222.0	10	12	4	12	Bis(2,2-dinitropropyl)fumarate	-17	
DATB	243.14	- 29.23[b]	6	5	5	6	Diaminotrinitrobenzene	-16	
NQ	104.07	- 21.9 [a]	1	4	4	2	Nitroguanidine	-15	
TNA	228.12	- 20.07[a]	6	4	4	6	Picramide	-14	
Expl.D	246.14	- 95.1 [a]	6	6	4	7	Ammonium picrate	-13	
TNB	213.11	- 11.40 [c]	6	3	3	6	Trinitrobenzene	-11	-56
EDNA	150.10	- 25.8 [d]	2	6	4	4	N,N' dinitroethylenediamine	-11	-32
Tetryl	287.15	4.67	7	5	5	8	Trinitrophenylmethylnitramine	- 8	
DNPN	326.19	- 65.0	6	10	6	10	Bis(2,2-dinitropropyl)nitramine	- 5	
PA	229.11	- 57.3	6	3	3	7	Picric Acid	- 3	
DINA	240.14	- 74.0 [e]	4	8	4	8	Diethylnitramine dinitrate	0	-27
RDX	222.13	14.71	3	6	6	6	Cyclotrimethylenetrinitramine	0	-22
HMX	296.17	17.93	4	8	8	8	Cyclotetramethylenetetranitramine	0	-22
Petrin	271.14	-149.0 [f]	5	9	3	10	Pentaerythritol trinitrate	3	-27
PETN	316.15	-125.0	5	8	4	12	Pentaerythritol tetranitrate	15	-10
TNETB	386.16	-118.62	6	6	6	14	Trinitroethyl trinitrobutyrate	21	- 4
BTNEU	386.16	- 72.7	5	6	8	13	Bis(trinitroethyl)urea	21	0
TC	133.15**	- 33.25 [b]				**		33	13
BTNEN	388.14	12.0	4	4	8	14	Bis(trinitroethyl)nitramine	33	16
HN	95.06	- 60.5	0	5	3	3	Hydrazine mononitrate	--	--

Table 1B

Liquid High Explosives Used in Computations

Material	Molecular Weight	Heat of Formation ΔHf Kcal/mole	Formula C	H	N	O	Name	Oxygen Balance* % to CO	to CO_2
EN	91.07	-45.51 [g]	2	5	1	3	Ethyl nitrate	-26	
NM	61.04	-27.04 [h]	1	3	1	2	Nitromethane	-13	
NG	227.09	-90.8 [i]	3	5	3	9	Nitroglycerine		3.5
TNM	196.04	13.0 [h]	1	0	4	8	Tetranitromethane		49
98% H_2O_2	33.422	-45.80 [j]	0	2	0	2	Hydrogen Peroxide	---	----
$H_2O_{1.9888}$									

* For $C_aH_bN_cO_d$, the oxygen balances are:

O.B. (CO_2), % = 1600(d-2a-0.5b)/M.W.
O.B. (CO), % = 1600(d-a-0.5b)/M.W.

** Classified Material. Atomic ratios C:H:N:O are:

1.636:1.454:2.182:5.091; "molecular weight" is for this unit.

Sources:
a. L. Médard and M. Thomas, Mem. poudres 31, 173-96 (1949).
b. W. S. McEwan, NOTS, private communication.
c. Burlot, Mem. poudres 29, 226 (1939).
d. L. Médard and M. Thomas, Mem. poudres 37, 129-38 (1955).
e. P. Tavernier and M. Lamouroux, Mem. poudres 37, 197-206 (1955).
f. NPP value computed from bond energies.
g. D. M. Fairbrother, H. A. Skinner, and F. W. Evans, Trans. Faraday Soc. 53, 779-83 (1957).
h. E. J. Prosen, U. S. Nat. Bur. Standards, private communication.
i. JANAF Thermochemical Data, addenda of June 1963, Confidential.
j. Circular 500, U. S. Nat. Bur. Standards (1952).
Other values from NavOrd 2986, addenda of Feb 1956, Confidential.

Table 2A

Computed Detonation Properties for Solid High Explosives

Material	Loading Density ρ_o g/cc	Detonation Velocity D mm/μsec	C-J Pressure P_j kbar	C-J Temperature T_j °K	C-J Density ρ_j g/cc	C-J Exponent K_j	Energies*, cal/g: Across Detonation Front $E_j - E_o$	Energies*, cal/g: Chemical Δe
R-Salt	1.60	8.019	263.9	2634	2.152	2.899	505.4	1383
	1.520	7.740	236.8	2728	2.054	2.846	484.0	1377
TNT	1.651	7.287	222.0	2736	2.211	2.949	407.1	1265
	1.5684	7.018	198.3	2803	2.110	2.895	387.9	1253
TATB	1.938	8.309	321.5	1913	2.551	3.161	476.4	1091
	1.8411	7.970	285.4	2039	2.435	3.098	451.9	1089
DNPF	1.60	7.327	214.7	2148	2.133	3.001	400.8	1079
	1.520	7.049	191.2	2230	2.035	2.949	380.7	1074
DATB	1.837	7.885	282.0	2265	2.439	3.051	452.8	1161
	1.7452	7.580	251.0	2374	2.328	2.995	430.2	1156
NQ	1.78	8.379	298.4	1385	2.338	3.188	478.4	922
	1.691	8.060	266.6	1493	2.233	3.121	457.2	922
TNA	1.77	7.588	257.3	2612	2.368	2.961	438.6	1240
	1.6815	7.309	229.8	2702	2.260	2.909	417.9	1230
Expl. D	1.72	7.551	244.0	2168	2.290	3.019	421.9	1092
	1.634	7.264	217.5	2264	2.185	2.963	401.5	1088
TNB	1.688	7.253	230.3	2988	2.279	2.855	423.0	1312
	1.6036	7.007	205.9	3048	2.171	2.824	401.4	1294
EDNA	1.75	8.702	330.9	2100	2.332	3.005	564.2	1315
	1.6625	8.384	296.0	2225	2.227	2.948	539.1	1312
Tetryl	1.73	7.678	264.7	2987	2.336	2.853	474.4	1395
	1.6435	7.419	237.2	3065	2.228	2.814	452.2	1379

Table 2A Continued

Material	Loading Density ρ_o g/cc	Detonation Velocity D mm/μsec	C-J Pressure P_j kbar	C-J Temperature T_j °K	C-J Density ρ_j g/cc	C-J Exponent K_j	Energies*, cal/g Across Detonation Front	Energies*, cal/g Chemical Δe
DNPN	1.73	8.268	302.6	2571	2.325	2.909	534.8	1411
	1.6435	7.978	271.3	2679	2.219	2.856	511.5	1402
PA	1.76	7.370	245.5	2747	2.368	2.895	427.9	1245
	1.672	7.113	220.0	2829	2.260	2.844	409.1	1232
DINA	1.70	8.311	302.5	2577	2.290	2.881	547.8	1441
	1.615	8.025	271.6	2684	2.186	2.830	524.6	1432
RDX	1.802	8.567	340.7	2668	2.427	2.882	582.0	1486
	1.7119	8.278	306.3	2793	2.317	2.830	558.2	1477
HMX	1.903	8.895	382.0	2506	2.550	2.941	608.7	1488
	1.8078	8.581	342.5	2649	2.434	2.886	582.6	1481
Petrin	1.54	7.638	236.2	2641	2.089	2.804	481.7	1352
	1.463	7.389	212.8	2719	1.994	2.754	463.0	1340
PETN	1.78	8.337	324.0	2812	2.412	2.818	569.7	1521
	1.691	8.065	291.9	2925	2.302	2.768	547.6	1508
TNETB	1.78	7.961	300.0	3005	2.425	2.760	535.7	1462
	1.691	7.714	270.6	3127	2.313	2.718	514.2	1452
BTNEU	1.86	8.242	333.0	2935	2.525	2.795	563.7	1489
	1.767	7.970	299.6	3087	2.410	2.746	540.9	1485
TC	1.84	7.583	281.0	2620	2.506	2.764	484.9	1226
	1.748	7.343	253.0	2758	2.389	2.725	464.3	1226
BTNEN	1.96	7.971	330.2	2651	2.667	2.772	533.7	1296
	1.862	7.720	297.2	2807	2.543	2.734	510.9	1297
HN	1.68	8.460	290.0	1218	2.214	3.146	497.5	908
	1.596	8.157	260.3	1318	2.114	3.079	477.9	908

* 1 mgbar - cc = 23.9 kcal = 10^6 abs. joules.

Table 2B

Computed Detonation Properties for Liquid High Explosives

Material	Loading Density ρ_o g/cc	Detonation Velocity D mm/μsec	C-J Pressure P_j kbar	C-J Temperature T_j °K	C-J Density ρ_j g/cc	C-J Exponent K_j	Energies, cal/g: Across Detonation Front	Energies, cal/g: Chemical Δe
EN	1.17	6.849	147.4	2607	1.600	2.723	404.5	1315
	(1.1115	6.632	132.9	2645	1.526	2.680	388.2	1302)
NM	1.13	6.739	141.4	2732	1.560	2.630	411.8	1310
	(1.0735	6.544	127.6	2764	1.486	2.603	394.0	1294)
NG	1.591	7.590	249.1	3176	2.185	2.680	508.4	1488
	(1.51145	7.356	224.7	3295	2.084	2.639	488.2	1485)
TMM	(1.52	5.445	119.5	1698	2.069	2.770	249.3	558)
	(1.444	5.288	108.2	1772	1.973	2.730	240.2	558)
98%H_2O_2 $H_2O_{1.9+}$	1.4419	6.436	137.4	701	1.873	3.347	262.0	385.2

Table 3A

Composition of Detonation Products for Solid H. E.

Material	Loading Density ρ g/cc	Gas Products n Moles/1000 g. HE	Partial Volumes cc/g HE gas $V_1(g)$	Partial Volumes cc/g HE carbon $V_1(c)$	C-J Products, moles/1000 g H.E. Graphite	CH_4	CO	CO_2	H_2O	H_2	NH_3	O_2	NO	N_2O	NO_2
R-Salt	1.60	34.48	0.4062	0.0585	15.27	0.5203	0.4916	0.9484	14.84	16.78	0.8985				
	1.520	34.58	0.4288	0.0580	14.80	0.6554	0.7492	1.025	14.43	16.73	0.9922				
TNT	1.651	26.02	0.3650	0.0872	21.98	0.1208	1.507	7.207	10.50	6.514	0.1798				
	1.5684	26.32	0.3872	0.0877	21.62	0.1478	2.109	6.944	10.42	6.507	0.1942				
TATB	1.938	29.07	0.3286	0.0634	17.33	0.0117	0.0591	5.838	11.51	11.59	0.0610				
	1.8411	29.10	0.3459	0.0648	17.26	0.0208	0.1305	5.830	11.45	11.58	0.0859				
DNPF	1.60	29.09	0.3975	0.0713	17.99	0.0790	0.3742	7.866	15.45	5.198	0.1233				
	1.520	29.20	0.4191	0.0722	17.80	0.0981	0.6124	7.790	15.37	5.188	0.1440				
DATB	1.837	27.88	0.3452	0.0648	17.19	0.0320	0.2942	7.160	10.06	10.23	0.1037				
	1.7452	27.99	0.3638	0.0657	17.03	0.0460	0.5192	7.078	10.00	10.22	0.1254				
NQ	1.78	38.39	0.3928	0.0348	9.429	0.0258	*	0.1532	18.91	19.13	0.1704				
	1.691	38.38	0.4127	0.0352	9.328	0.0477	*	0.2308	18.75	19.09	0.2461				
TNA	1.77	26.72	0.3573	0.0650	16.88	0.0547	0.9038	8.464	8.469	8.704	0.1257				
	1.6815	26.96	0.3772	0.0654	16.60	0.0690	1.381	8.250	8.421	8.698	0.1387				
Expl.D	1.72	28.56	0.3750	0.0617	15.94	0.0402	0.3009	8.095	11.95	8.072	0.1062				
	1.634	28.67	0.3951	0.0625	15.78	0.0568	0.5196	8.017	11.89	8.062	0.1263				
TNB	1.688	25.80	0.3749	0.0639	16.18	0.0704	2.382	9.527	6.719	6.979	0.1194				
	1.6036	26.22	0.3970	0.0635	15.72	0.0810	3.239	9.112	6.691	6.977	0.1236				
EDNA	1.75	36.66	0.3934	0.0353	9.682	0.0549	0.1259	3.462	19.60	13.23	0.1850				
	1.6625	36.70	0.4137	0.0354	9.492	0.0939	0.2425	3.496	19.42	13.20	0.2558				
Tetryl	1.73	27.93	0.3760	0.0520	13.51	0.0900	1.965	8.808	8.278	8.624	0.1652				
	1.6435	28.32	0.3975	0.0514	13.08	0.1067	2.750	8.440	8.230	8.618	0.1755				
DNPH	1.73	32.49	0.3929	0.0373	10.00	0.1074	0.7011	7.584	14.79	9.088	0.2172				
	1.6435	32.68	0.4136	0.0370	9.693	0.1445	1.117	7.440	14.66	9.071	0.2527				
PA	1.76	25.74	0.3703	0.0520	13.37	0.0434	1.321	11.45	6.328	6.503	0.0879				
	1.672	26.05	0.3906	0.0519	13.04	0.0510	1.951	11.15	6.307	6.501	0.0921				
DINA	1.70	33.63	0.4086	0.0281	7.540	0.1231	0.7446	8.249	16.07	8.215	0.2263				
	1.615	33.84	0.4300	0.0275	7.212	0.1644	1.181	8.099	15.93	8.197	0.2621				

Table 3A (Continued)

Material	Loading Density ρ g/cc	Gas Products n Moles/1000 g. HE	Partial Volumes cc/g HE gas $V_j(g)$	Partial Volumes cc/g HE carbon $V_j(c)$	C-J Products, moles/1000 g H.E. Graphite	CH_4	CO	CO_2	H_2O	H_2	NH_3	O_2	NO	N_2O	NO_2
RDX	1.802	34.06	0.3900	0.0220	6.047	0.0897	0.7085	6.660	12.98	13.39	0.2294				
	1.7119	34.27	0.4103	0.0214	5.732	0.1232	1.141	6.510	12.85	13.37	0.2726				
HMX	1.903	33.91	0.3697	0.0225	6.315	0.0584	0.3743	6.758	13.12	13.42	0.1785				
	1.8078	34.04	0.3887	0.0221	6.078	0.0861	0.6701	6.672	13.00	13.39	0.2240				
Petrin	1.54	32.92	0.4509	0.0278	7.090	0.1726	1.406	9.772	15.93	5.426	0.2132				
	1.463	33.23	0.4748	0.0267	6.683	0.2137	2.026	9.518	15.82	5.416	0.2329				
PETN	1.78	32.14	0.4064	0.0083	2.241	0.1156	1.107	12.35	12.15	6.234	0.1836				
	1.691	32.45	0.4274	0.0070	1.866	0.1410	1.730	12.08	12.07	6.226	0.1997				
TNETB	1.78	30.65	0.4118	0.0006	0.1675	0.0662	1.799	13.51	7.445	7.705	0.1274				
	1.691	30.89	0.4323	0	0	0.0381	2.280	13.22	7.535	7.716	0.1047				
BTNEU	1.86	31.11	0.3960	0	0	*	0.0984	12.85	7.764	10.32	*	0.0205	0.0253	0.0173	0.0097
	1.767	31.13	0.4148	0	0	*	0.1518	12.80	7.764	10.31	*	0.0349	0.0425	0.0187	0.0129
TC	1.84	29.50	0.3991	0	0	-	*	12.29	5.463	7.516	*	2.968	0.1673	0.0942	0.9991**
	1.748	29.60	0.4186	0	0	-	0.0044	12.29	5.463	7.587	*	3.123	0.2288	0.0820	0.8209**
BTNEN	1.96	30.06	0.3749	0	0	*	*	10.30	5.153	9.271	*	3.428	0.1939	0.1642	1.546
	1.862	30.21	0.3932	0	0	*	0.0042	10.30	5.153	9.389	*	3.674	0.2767	0.1425	1.271
HN	1.68	44.60	0.4517	0	-	-	-	-	26.30	15.67	*	2.413	*	0.0038	0.2151
	1.596	44.61	0.4730	0	-	-	-	-	26.30	15.68	*	2.431	*	0.0043	0.1955

* Negligible; ≤ 0.003

** H, H_2, O, OH, negligible

Table 3B

Composition of Detonation Products for Liquid H. E.

Material	Loading Density ρ_o g/cc	Gas Products n Moles/1000 g. HE	Partial Volumes cc/g HE gas $V_j(g)$	Partial Volumes cc/g HE carbon $V_j(c)$	C-J Products, moles/1000 g H.E. Graphite	CH_4	CO	CO_2	H_2O	N_2	NH_3	O_2	NO	N_2O	NO_2
EM	1.17	36.62	0.5588	0.0663	15.53	1.0625	2.179	3.192	24.38	5.175	0.6313				
	(1.1115	36.90	0.5910	0.0643	14.77	1.281	2.755	3.155	23.88	5.153	0.6746)				
MM	1.13	38.35	0.6057	0.0354	8.215	0.9539	3.322	3.891	21.66	7.856	0.6704				
	(1.0735	38.71	0.6403	0.0327	7.441	1.141	4.058	3.743	21.22	7.834	0.7146)				
NG [a]	1.591	31.85	0.4577	0	0	*	0.0536	13.16	11.01	6.382	*	0.8400	0.1971	0.0396	0.1695
	(1.51145	31.88	0.4798	0	0	*	0.0872	13.12	11.01	6.380	*	0.8648	0.2379	0.0346	0.1437)
TMM [b]	(1.52	30.28	0.4834	0	0	-	*	5.101	-	9.847	-	14.63	0.0475	0.0078	0.6472)
	(1.444	30.31	0.5068	0	0	-	*	5.101	-	9.871	-	14.69	0.0661	0.0078	0.5794)
H_2O_2 [c] (98%)	1.4419	44.33	0.5340	0	-	-	-	-	29.92	-	-	14.41	-	-	-
H_2O_{Loss}															

*Negligible; $\leq$ 0.003

[a] H, He, N, O, OH, negligible

[b] H, O negligible

[c] OH negligible

Table 4

Comparison of Computed and Measured Values of C-J Properties

Material	Detonation Properties	Experimental Ref. 7	Theoretical This Report	Theoretical Ref. 7[a]	% Difference $100(D_t-D_e)/D_e$, etc.[c]
TNT	D	6.950[b]	7.251	7.248	4.3[b]
ρ_o = 1.64	P	190	219	219	15.3
	T	-	2745	2765	-
	K	(3.16)	2.94	2.94	7.0
DATB	D	7.520	7.722	7.681[d]	2.7
ρ_o = 1.788	P	259	265	271[d]	2.3
	T	-	2323	2363[d]	-
	K	(2.90)	3.02	2.90[d]	4.1
Tetryl	D	7.560	7.588	7.587	0.4
ρ_o = 1.70	P	-	255	261	-
	T	-	3014	2903	-
	K	-	2.84	2.81	-
RDX	D	8.754	8.561	8.527	-2.2
ρ_o = 1.80	P	347	340	343	-2.0
	T	-	2671	2688	-
	K	(2.98)	2.88	2.82	-3.4
PETN	D	7.980	8.001	8.008	0.3
ρ_o = 1.67	P	300	284	286	-5.3
	T	3400	2957	2992	-13.0
	K	(2.55)	2.76	2.75	8.2
HN	D	8.691	8.265	8.366	-4.9
ρ_o = 1.626	P	-	271	280	-
	T	-	1282	1393	-
	K	-	3.10	3.06	-

Table 4 (Continued)

Material	Detonation Properties	Experimental Ref. 7	Theoretical This Report	Theoretical Ref. 7[a]	% Difference $100(D_t-D_e)/D_e$, etc.[c]
NM ρ_o=1.128	D	6.290	6.732	6.838	7.2
	P	141	141	146	0
	T	3380	2733	2915	-19.2
	K	(2.17)	2.63	2.61	21.2
NG ρ_o=1.59	D	7.580	7.587	7.636	0.1
	P	-	249	251	-
	T	3470	3177	3265	-8.5
	K	-	2.68	2.70	-
TNM ρ_o=1.64	D	6.360	5.693	5.741	-10.5
	P	159	137	141	-13.8
	T	2800	1581	1621	-43.5
	K	(3.17)	2.83	2.84	-10.7

a. Values given for equation of state parameters from Ref. 6. These are essentially those used in RUBY code for the present computations.

b. 7.100 by extrapolation of linear portion of D-ρ_o curve of Ref. 10; this gives a difference of 2.1% from theoretical.

c. Theoretical values of column 4; experimental values of column 3.

d. C. L. Mader, private communication. These values are computed with ΔH_f = -29.23 kcal/mole. Values of Ref. 7 were computed for ΔH_f = -6 kcal/mole, and the set of values shown in column 4 of Table III' is misplaced from another table. The correct values are 7772, 279.4, 2548, and 2.87 respectively.

Table 5

Comparison of Computed and Measured Detonation Velocities

Material	ρ_o	D, mm/μsec.		Difference $(D_t-D_e)/D_e$ %	Reference
		Experimental	Theoretical		
R-Salt	1.57	7.800	7.914	1.5	12
TATB	1.802	7.658	7.833	2.3	13
NQ	1.55	7.650	7.555	-1.2	12
TNA	1.72	7.300	7.430	1.8	12
Expl. D	1.55	6.850	6.984	2.0	12
TNB	1.640	7.269	7.113	-2.1	13
EDNA	1.6625	8.237	8.384	1.8	12
DNPN	1.73	8.100	8.268	2.1	14
PA	1.71	7.350	7.224	-1.7	12
TNETB	1.70	8.200	7.739	-5.6	14
BTNEU	1.86	9.000	8.242	-8.4	14
BTNEN	1.96	8.850	7.971	-9.9	14

Table 6

Computed Detonation Properties for Mixtures of Solid Organic Explosives

Material	Loading Density ρ_e g/cc	Detonation Velocity D mm/μsec	C-J Pressure P_j kbar	C-J Temperature T_j °K	C-J Density ρ_j g/cc	C-J Exponent K_j	Energies*, cal/g: Across Detonation Front $E_j - E_o$	Energies*, cal/g: Chemical Δe
RDX/TNT	1.745	8.117	294.9	2717	2.347	2.899	518.0	1407
64/36	1.65775	7.834	264.3	2819	2.239	2.850	494.8	1396
RDX/TNT	1.765	8.280	310.9	2703	2.375	2.892	541.0	1435
77/23	1.67675	7.995	278.9	2813	2.266	2.843	517.1	1425
Pentolite	1.713	7.827	270.3	2792	2.307	2.883	485.5	1392
50/50	1.62735	7.557	243.2	2882	2.204	2.821	467.4	1379

Table 7

Composition of Detonation Products of Mixtures

Material	Loading Density ρ_o g/cc	Gas Products n Moles/1000 g. HE	Partial Volumes cc/g HE		C-J Products, moles/1000 g H.E.						
			gas $V_j(g)$	carbon $V_j(c)$	Graphite	CH_4	CO	CO_2	H_2O	N_2	NH_3
RDX/TNT 64/36	1.745	31.16	0.3819	0.0442	11.78	0.1038	0.9806	6.877	12.06	10.91	0.2233
	1.65775	31.40	0.4026	0.0439	11.44	0.1354	1.487	6.678	11.95	10.89	0.2544
RDX/TNT 77/23	1.765	32.20	0.3849	0.0360	9.707	0.0991	0.8800	6.801	12.39	11.80	0.2271
	1.67675	32.44	0.4057	0.0356	9.375	0.1317	1.361	6.620	12.27	11.79	0.2627
Pentolite 50/50	1.713	29.11	0.3873	0.0462	12.09	0.1165	1.358	9.751	11.33	6.375	0.1804
	1.62735	29.42	0.4079	0.0457	11.71	0.1417	1.992	9.471	11.25	6.368	0.1951

Table 8

Summary of Computed Values for Mixture Components

	ρ_o	D	P_j	T_j	ρ_j	$\bar{K}_j$
TNT	1.651	7.287	222.0	2736	2.211	2.949
	1.5684	7.018	198.3	2803	2.110	2.895
RDX	1.802	8.567	340.7	2668	2.427	2.882
	1.7119	8.278	306.3	2793	2.317	2.830
RDX*	1.80	8.754	346.7	2588	2.404	2.979
PETN	1.78	8.337	324.0	2812	2.412	2.818
	1.691	8.065	291.9	2929	2.302	2.768
TFNA*	1.692	7.569	242.2	2205	2.256	3.002

*Computed values from Ref. (7); BKW parameters of set d used.
TFNA is 1, 1, 1-Trifluoro-3, 5, 5-trinitro-3-azahexane, $C_5H_7N_4O_6F_3$.

Table 9

Comparison of Computed Values for Mixtures with Those Predicted from Computed Values for Components

Material	C-J Properties	Computed for Mixture	Calculated from Computed Results for Components	% Difference	Material	Computed for Mixture	Calculated from Components	% Difference
	D	8.117	8.106	-0.1		7.834	7.824	-0.1
RDX/TNT	P	294.9	293.2	-0.6	RDX/TNT	264.3	263.1	-0.4
64/36	ρ	2.347	2.345	-0.1	64/36	2.239	2.238	-0.05
ρ_o=1.745	T	2717	2693	-0.9	ρ_o=1.65775	2819	2797	-0.8
	K	2.899	2.910	0.4		2.850	2.857	0.2
RDX/TNT	D	8.280	8.273	-0.1	RDX/TNT	7.995	7.988	-0.1
77/23	P	310.9	309.8	-0.4	77/23	278.9	278.2	-0.2
ρ_o=1.765	ρ	2.375	2.374	-0.05	ρ_o=1.67675	2.266	2.266	0
	T	2703	2684	-0.7		2813	2795	-0.6
	K	2.892	2.900	0.3		2.843	2.846	0.1
	D	7.827	7.812	-0.2		7.557	7.542	-0.2
Pentolite	P	270.3	269.2	-0.4	Pentolite	243.2	241.5	-0.7
50/50	ρ	2.307	2.307	0	50/50	2.204	2.202	-0.1
ρ_o=1.713	T	2792	2774	-0.6	ρ_o=1.62735	2882	2866	-0.6
	K	2.883	2.883	0		2.822	2.833	0.4
	D	8.278	8.279	0.01				
RDX/TFNA*	P	302.2	302.0	-0.03				
59.902/	ρ	2.343	2.342	-0.05				
40.098	T	2446	2434	-0.5				
ρ_o=1.754	K	2.977	2.981	0.1				

*Data from Ref. (7), BKW parameters set d. Mixture composition is here displayed as weight per cent; in Ref. (7) it is shown as 65/35 mole per cent.

Table 10

Comparison of Burning at One Atmosphere and Detonation

Material	Energy, cal/g Δe 95% TMD	Energy, cal/g Δh 1 atm.	Temperature, °K T_j* 95% TMD	Temperature, °K T_f Flame	Gas Products moles/kgram n_j*	Gas Products moles/kgram n	**Major Products of Burning, moles/kg CO	CO_2	H_2O	H_2	N_2	H	OH	O_2	O	NO
TNT	1253	618	2803	1991	26.39	44.01	26.41	0.0008	0.0016	6.604	10.99					
DATB	1156	531	2374	1815	27.99	45.23	24.67	0.0019	0.0030	10.28	10.27					
NQ	922	613	1493	1844	38.38	48.05	8.112	1.496	8.112	19.22	11.10	0.0118				
Tetryl	1379	834	3065	2470	28.32	46.78	23.23	0.8892	2.531	8.615	10.99	0.4962	0.0238	-	0.0007	0.0013
DINA	1432	997	2684	2787	33.84	42.84	12.30	4.361	11.12	8.285	4.613	1.093	0.7639	0.1093	0.1109	0.0876
RDX	1477	1003	2793	2923	34.27	42.47	10.36	3.148	8.302	13.41	3.860	1.579	1.108	0.2389	0.2725	0.1976
PETN	1508	971	2929	2896	32.45	38.12	8.593	7.222	9.716	6.173	1.646	0.8948	1.685	1.330	0.5521	0.3056
TNETB	1452	895	3127	2903	30.89	35.09	7.509	8.029	5.942	7.555	0.7980	0.6077	1.467	2.086	0.6796	0.4270
TC	1226	824	2758	2829	29.60	32.95	3.697	8.594	4.399	7.884	0.2749	0.2710	1.306	5.123	0.7816	0.6199

*Values from Tables 2 and 3.
**Carbon is a major product only for TNT; there 4.4 moles/kg appear.

Table 11

Effect of Chamber Pressure on Computed Values

Material	Chamber Pressure kbar	Heat of Reaction Δh cal/g	Flame Temperature °K	Main Products, moles/kg							
				Total Gas, n	CO	CO_2	H_2O	N_2	H_2	C	CH_4
TNT	10^{-3}	618	1991	44.01	26.41	0.0008	0.0016	6.604	10.99	4.404	0
	170	955	2775	33.77	14.12	3.69	4.92	6.603	2.78	11.36	1.65
	222	973	2813	33.10	13.30	3.97	5.10	6.603	2.49	11.81	1.67
Tetryl	10^{-3}	834	2470	46.78	23.23	0.8892	2.531	8.615	10.99	0	0
	214	1021	3128	37.22	17.74	3.22	3.68	8.71	2.71	2.26	1.16
	252	1034	3157	36.86	17.19	3.43	3.81	8.71	2.55	2.58	1.17
RDX	10^{-3}	1003	2923	42.47	10.36	3.15	8.30	13.41	3.86	0	0
	302	1250	3517	40.07	9.48	3.79	9.93	13.50	3.10	0	0
	346	1252	3523	39.59	9.34	3.85	9.91	13.50	2.99	0	0
PETN	10^{-3}	971	2896	38.12	8.59	7.22	9.72	6.17	1.65	0	0
	260	1389	3875	34.89	5.66	10.15	11.81	6.30	0.78	0	0
	302	1390	3877	34.70	5.64	10.17	11.81	6.30	0.78	0	0
NM	131	1071	2690	45.21	10.58	3.83	14.52	8.19	6.11	0	1.97
	151	1079	2705	44.94	10.35	3.98	14.56	8.19	5.80	0	2.11
NG	226	1392	3977	32.44	0.71	12.50	10.71	6.24	0.07	0	0
	256	1395	3983	32.42	0.68	12.53	10.72	6.24	0.07	0	0

Table 12

Computed Results for Burning at Detonation Pressure

Material	Chamber* Pressure kbar	Flame Temperature °K	Heat of Reaction Δh, cal/g	Main Products, moles/kg							
				C	CH_4	CO	CO_2	H_2O	N_2	H_2	Total Gas n
R-Salt	246	2962	1113	1.97	4.04	9.83	1.39	4.61	17.23	4.54	41.65
TNT	170	2775	955	11.36	1.65	14.12	3.69	4.92	6.60	2.78	33.77
TATB	268	2562	857	8.01	1.90	9.20	4.14	5.77	11.62	2.05	34.68
DNPF	159	2347	815	6.94	2.45	10.65	6.27	8.38	5.26	2.51	35.51
DATB	231	2679	886	7.60	1.53	11.46	4.08	5.05	10.28	2.16	34.57
NQ	275	2242	782	0	3.20	3.75	2.66	10.15	19.2	2.68	41.65
TNA	205	2828	922	6.98	1.16	14.24	3.92	4.22	8.77	2.22	34.53
Expl. D	190	2479	823	6.06	1.77	11.13	5.42	6.46	8.13	2.19	35.10
TNB	179	3001	958	6.14	0.79	17.57	3.65	3.28	7.04	2.18	34.52
EDNA	273	2845	1074	0	1.87	8.18	3.27	11.93	13.32	4.32	42.90
Tetryl	252	3157	1034	2.58	1.17	17.19	3.43	3.81	8.71	2.55	36.86
DNPN	248	3061	1097	0	1.21	12.89	4.30	9.17	9.20	3.74	40.51
PA	190	2859	882	3.43	0.64	17.18	4.93	3.50	6.55	1.76	34.57
DINA	245	3181	1167	0	0.48	11.15	5.02	12.11	8.33	3.57	40.69
RDX	302	3517	1250	0	0.23	9.48	3.79	9.93	13.50	3.10	40.07
HMX	339	3510	1247	0	0.28	9.38	3.84	9.92	13.50	3.02	39.98
Petrin	205	3003	1086	0	0.42	11.70	6.32	12.54	5.53	3.21	39.73
PETN	260	3875	1389	0	0	5.66	10.15	11.81	6.30	0.78	34.89
TNETB	246	4117	1376	0	0	2.96	12.58	7.44	7.63	0.20	31.43
BTNEU	285	4090	1361	0	0	1.29	11.66	7.52	10.07	0.10	31.86
TC	237	3744	1167	0	0	0.21	12.08	5.30	7.56	0.01	30.24
EN	115	2453	1004	0	5.00	12.66	4.30	11.68	5.49	5.77	44.91
NM	151	2705	1079	0	2.11	10.36	3.93	14.56	8.19	5.80	44.94
NG	226	3977	1392	0	0	0.71	12.50	10.71	6.24	0.07	32.44

*P_j value for solids at 0.95 TMD, liquids at NTP. Computations carried out on code designed by H. G. Snay.

APPENDIX

COMMENTS ON THE EXPONENT K

Since the sound speed c is defined by

$$c^2 = - V^2 (\partial P/\partial V)_S , \tag{A1}$$

the definition of K may be written

$$K = - \frac{V}{P} \left(\frac{\partial P}{\partial V}\right)_S = \frac{c^2}{P V} . \tag{A2}$$

A frequently used approximation for the internal energy of a compressed gas is

$$E = \frac{PV}{k-1} . \tag{A3}$$

It is possible to show that k=K under certain conditions. Rearranging Eqn. (A3) gives

$$P = \frac{(k-1)E}{V} . \tag{A4}$$

Considering the gas pressure as a function of E and V,

$$dP = \left(\frac{\partial P}{\partial E}\right)_V dE + \left(\frac{\partial P}{\partial V}\right)_E dV$$

$$\left(\frac{\partial P}{\partial V}\right)_S = \left(\frac{\partial P}{\partial E}\right)_V \left(\frac{\partial E}{\partial V}\right)_S + \left(\frac{\partial P}{\partial V}\right)_E \tag{A5}$$

Since

$$dE = TdS - PdV$$

$$\left(\frac{\partial E}{\partial V}\right)_S = - P . \tag{A6}$$

Using Eqn. (A6) and evaluating the remaining partials from Eqn. (A4) gives:

$$\frac{c^2}{V^2} = - \left(\frac{\partial P}{\partial V}\right)_S = P \frac{k-1}{V} + \frac{(k-1)E}{V^2}$$

$$= P \frac{k-1}{V} + \frac{P}{V}$$

$$= \frac{kP}{V}$$

or

$$\frac{c^2}{PV} = k . \tag{A7}$$

Since Eqns. (A2) and (A7) are identical, it follows that for explosives having all gas products

$$K = k \ .$$

K defined by Eqn. (A2) and k defined by Eqn. (A3) are the same.

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Detonation	DETO	Density	DENS	Release	RELE
High explosives	HIGX	Composition	CMPO	Burning	BURN
Carbon	CARB	Loading	LOAI	High pressure	HIGP
Hydrogen	HYDG	Explosives	EXPL	Experiment	EXPE
Nitrogen	NITG	Solid	SOLI	Organic	ORGA
Oxygen	OXYG	Liquid	LIQU		
Systems	SYST	Compounds	CMPU		
Computer	COMP	Mixtures	MIXT		
Code	CODE	Equation-of-state	EQUS		
Velocity	VELC	Parameters	PARA		

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Task RUME 4E-000/212-1/F008-08-11.

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The Ruby code was used to compute detonation properties (velocity, pressure, temperature, density and product composition) for about 30 explosives at two loading densities. The results indicated the need of improved values of equation of state parameters in the code.

1. Detonation - Calculations
2. Explosives, High - Detonation
3. Codes - Ruby
I. Title
II. Price, Donna
III. Hurwitz, Harold, jt. author
IV. Project

Abstract card is unclassified.

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