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Prediction of the Brisance of Energetic Materials

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Abstract: The brisance parameter can be used to show the shattering power of an energetic compound and the speed to reach its peak pressure. It determines the effectiveness with which an explosive can fragment a shell. Nowadays, the sand test or sand crushing test is the preferred method for brisance measurements but there is no reliable method for the prediction of the brisance parameter. In this paper, a method for the prediction of the brisance through sand test for pure and mixed energetic materials as well as aluminized explosives is reported. It is based on the molecular structure of the desired compound and once the conclusion is established any experimental data is redundant. The calculated brisance relative to 2,4,6-trinitrotoluene (= 100) shows good agreement with the measured values.

Keywords: Energetic compounds · Brisance parameter · Sand test · Molecular structure

1 Introduction

Upon detonation of an explosive, very high pressure is created in its shock wave. It will shatter rather than displace any object in its path [1, 2]. But subsequent expansion of gases performs volume work [1, 2]. Brisance can be defined as the ability of an explosive to wreck a solid object in direct contact or in vicinity of the detonation wave impact. It is essentially the shattering power of an explosive, which is distinguished from the total work capacity of explosives. The speed with which the explosive reaches its peak pressure is a measure of its brisance. Knowledge of the brisance is of practical importance since it determines the effectiveness of an explosive in military applications such as fragmenting shells, bomb casings, grenades and mines as well as in imparting high velocities to the resulting fragments.

Some efforts have been made to express the relationship between detonation velocity or detonation pressure and brisance [1, 2]. Several test methods have been used for the determination of the brisance of energetic materials [2]. Early test methods include lead block compression test, copper cylinder test, Quinan test and Hopkinson pressure bar method, which have been reviewed elsewhere [2].

The sand test or sand crushing test is a convenient method for measuring brisance of an explosive [2]. It consists of the determination of a standard amount of sand, which is crushed by a standard mass of explosive. As compared to various methods for determining the brisance of energetic compounds, experimental data of the sand test are available for different pure, mixture and aluminized explosives because it is a simple and convenient method.

Although nowadays the sand test is the preferred test for brisance measurements, there is no reliable method for its prediction. The purpose of this work is to introduce a reliable and simple method for predicting brisance as determined by the sand test for any pure and mixture of energetic materials with the general formula $C_aH_bN_cO_d$ as well as aluminized explosives. It is shown that this method is based on the molecular structure and that any further experimental data is redundant. Moreover, it can be easily used for some important classes of energetic compounds including nitroaromatics, acyclic and cyclic nitramines, nitrate esters and nitroaliphatics.

2 Materials and Methods

The brisance parameter can be directly related to detonation pressure or detonation velocity and indirectly to heat of detonation [1]. It was recently indicated that the detonation performance of energetic compounds can be correlated with their molecular structure [3–8]. The study of the reported sand crushing test of pure and mixture of energetic compounds with general formula $C_aH_bN_cO_d$ as well as aluminized explosives has shown that it is possible to obtain a simple correlation on the basis of elemental composition and molecular structure moieties. Different combinations of elemental composition were examined and optimized, the experimental data is given in Table 1. Several structural parameters of pure energetic compounds are also essential to improve the predicted results on the basis of the elemental

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Table 1. Comparison of the predicted $Bris_{relTNT}$[a)] of Equation (1) for pure energetic materials with experimental data related to TNT as standard with 100%.

No.	Compound	Formula	Exp.	Equation (1)	Dev
1	1,2,4-Butantriol trinitrate (BTTN)	$C_4H_7N_3O_9$	101 [2]	104	−3
2	Cyclotetramethylene tetranitramine (HMX)	$C_4H_8N_8O_8$	125–55 [2]	144	−19–11
3	Ammonium picrate (AP)	$C_6H_6N_4O_7$	84–87 [2]	100	−16–(−13)
4	Cyclotrimethylene trinitramine (RDX)	$C_3H_6N_6O_6$	140 [2]	134	6
5	Diazodinitrophenol (DDNP)	$C_6H_2N_4O_5$	97–104 [2]	100	−3–4
6	Dioxyethylnitramine dinitrate (DINA)	$C_4H_8N_4O_8$	71 [2]	69	2
7	Diethyleneglycol dinitrate (DEGDN)	$C_4H_8N_2O_7$	95 [2]	93	2
8	Dinitrobenzene (DNB)	$C_6H_4N_2O_4$	74–82 [2]	85	−11–(−3)
9	Dinitrodimethyloxamide (MNO)	$C_4H_6N_4O_6$	71 [2]	66	5
10	2,4-Dinitrophenol (DNPh)	$C_6H_4N_2O_5$	52 [2]	87	−35
11	Dipentaerythritol hexanitrate (DIPEHN)	$C_{10}H_{16}N_6O_{19}$	119 [2]	117	2
12	Erythritol tetranitrate	$C_4H_6N_4O_{12}$	132–143 [2]	137	−5–6
13	Ethylenediamine dinitrate (EDDN)	$C_2H_{10}N_4O_6$	96 [2]	102	−6
14	Ethylene dinitramine (EDNA)	$C_2H_6N_4O_4$	119 [2]	122	−3
15	Hexanitrodiphenylamine (Hexyl)	$C_{12}H_5N_7O_{12}$	117–120 [2]	113	4–7
16	Mannitol hexanitrate (MHN)	$C_6H_8N_6O_{18}$	137–143 [2]	135	2–8
17	Metriol trinitrate (MTN)	$C_5H_9N_3O_9$	99 [2]	99	0
18	Glyceryl trinitrate (NG)	$C_3H_5N_3O_9$	120 [2]	129	−9
19	Nitroguanidine (NQ)	$CH_4N_4O_2$	73 [10]	66	7
20	Nitroglycol (Ngu)	$C_2H_4N_2O_6$	129 [2]	120	9
21	Nitrourea	$CH_3N_3O_3$	60 [2]	65	−5
22	Pentaerythritol tetranitrate (PETN)	$C_5H_8N_4O_{12}$	129–141 [2]	132	−3–9
23	Pentryl	$C_8H_6N_6O_{11}$	129 [2]	134	−5
24	Trinitrophenol (Picric acid)	$C_6H_3N_3O_7$	103–110 [2]	99	4–11
25	1,3,5-Trinitrobenzene (TNB)	$C_6H_3N_3O_6$	110 [2]	96	14
26	2,3,4,6-Tetranitroaniline (TNA)	$C_6H_3N_5O_8$	102 [2]	111	−9
27	Tetranitrocarbazole (TNC)	$C_{12}H_5N_5O_8$	86–95 [2]	93	−7–2
28	Diglycerol tetranitrate	$C_6H_{10}N_4O_{13}$	108 [2]	110	−2
29	Tetranitromethane (TNM)	CN_4O_8	108 [2]	123	−15
30	Triethyleneglycol dinitrate (TEGDN)	$C_6H_{12}N_2O_8$	30 [11]	31	−1
31	Trinitrophenyl methylnitramine (Tetryl)	$C_7H_5N_5O_8$	113–123 [2]	125	−12–(−2)
32	Trimethylolpropane trinitrate	$C_6H_{11}N_3O_9$	108–115 [2]	94	14–21
33	Trinitroanisol (TNAns)	$C_7H_5N_3O_7$	100–110 [2]	94	6–16
34	2,4,6-Trinitrobenzoldehyde (TNBA)	$C_7H_3N_3O_7$	110 [2]	96	14
35	Trinitrobenzoic acid (TNBA)	$C_7H_3N_3O_8$	100 [2]	99	1
36	2,4,6-Trinitroresorcinol (Styphnic acid)	$C_6H_3N_3O_8$	94 [2]	101	−7
37	1,3,5-Triazido-2,4,6-trinitrobenzene (TATB)	$C_6H_6N_6O_6$	89 [11]	107	−18
38	2,4,6-Trinitrotoluene (TNT)	$C_7H_5N_3O_6$	100 [2]	91	9
39	2,4,6-Trinitroxylene (TNX)	$C_8H_7N_3O_6$	84 [2]	86	−2
40	Dinitroglycerinnitrolactate (GLTN)	$C_6H_9N_3O_{11}$	27 [10]	29	−2
41	Dinitroglycolurile (DNGU)	$C_4H_4N_6O_6$	88 [10]	78	10
42	Tetranitroglycolurile	$C_4H_2N_8O_{10}$	129 [10]	137	−8
43	Dinitrospirodihydantoin	$C_5H_2N_6O_8$	75 [11]	84	−9
44	Tripentaerythritol octanitrata (TEPON)	$C_{15}H_{24}N_8O_{26}$	129 [2]	121	8
45	Nitroaminoguanidine (NaGu)	$CH_5N_5O_2$	92 [12]	106	−14
46	2,3,4,6-Tetranitroaniline (TNA)	$C_6H_3N_5O_8$	102 [12]	111	−9
47	Dipicrylurea	$C_{13}H_6N_8O_{13}$	76 [13]	80	−4

a) $Bris_{relTNT}$: brisance as determined by sand test related to TNT as standard with 100%.

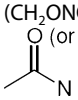
composition. It was found that a suitable correlation using a multiple linear regression method [9] has the following form:

$$Bris_{relTNT} = 85.5 + Bris_{core} - 35.96Bris^{-} + 19.69Bris^{+} \quad (1a)$$

$$Bris_{core} = 4.812c + 2.556(d - a - b/2) \quad (1b)$$

where $Bris_{relTNT}$ is the relative brisance with respect to TNT; $Bris_{core}$ is the core brisance, which is based on the number of nitrogen atoms and the distribution of oxygen atoms between carbon and hydrogen atoms; $Bris^{+}$ and $Bris^{-}$ are correcting positive and negative functions for those values obtained on the basis of $Bris_{core}$.

Table 2. Specification of $Bris^+$ or $Bris^-$ according to different compounds/fragments.

Energetic compound or molecular fragment	$Bris^+$ or $Bris^-$
$(CH_2ONO_2)_n$ or $C(CH_2ONO_2)_n$ or $(CH_2{-}NNO_2)_n$ or $(-HN-NO_2)_n$ where $n \leq 4$ and Aromatic-N(NO_2)– 	$Bris^+ = 1.0$ $Bris^- = 1.0$
Only $-ONO_2$ along with –COO–	$Bris^- = 2.0$
More than one –C–O–C–	$= 1.5 Bris^-$
Nitramine group	$= 1.0 Bris^-$

3 Results and Discussion

3.1 Prediction of $Bris^+$ and $Bris^-$ for Pure Energetic Materials

The values of $Bris^+$ and $Bris^-$ depend on the presence of some molecular moieties in the molecular structure of pure $C_aH_bN_cO_d$ energetic compounds, which can be specified according to the following situations (Table 2):

The correlation coefficient of Equation (1) is equal to 0.84 because the uncertainty in the determination of $Bris_{relTNT}$ is relatively high [9]. As indicated in Table 1, the calculated values of Equation (1) are compared with the measured values of $Bris_{relTNT}$ for different classes of pure energetic compounds. For some energetic compounds given in Table 1, there is a large difference between the predicted values and experimental data of $Bris_{relTNT}$.

3.2 Brisance for Mixture and Aluminized Explosives

For a mixture of different energetic components $Bris^+$ and $Bris^-$ are also equal to the specified $Bris^-$ values, if at least one of constituents follows the conditions of previous section. By knowledge of composition and empirical formula

Table 3. Comparison of the predicted values of $Bris_{relTNT}$ of Equation (1) for a mixture of energetic materials with the experimental data [2] related to TNT as standard with 100%.

No.	Compound	Formula	Exp.	Equation (1)	Dev
1	80/20 AN/TNT (Amatol)	$C_{0.617}H_{4.441}N_{2.264}O_{3.529}$	74	98	−24
2	60/40 AN/TNT (Amatol)	$C_{1.233}H_{3.881}N_{2.029}O_{3.307}$	90	96	−6
3	50/50 AN/TNT (Amatol)	$C_{1.542}H_{3.601}N_{1.911}O_{3.197}$	90	94	−4
4	40/60 AN/TNT (Amatol)	$C_{1.85}H_{3.322}N_{1.793}O_{3.086}$	94	93	1
5	75/25 RDX/TNT (Cyclotol)	$C_{1.784}H_{2.578}N_{2.357}O_{2.688}$	130	116	14
6	70/30 RDX/TNT (Cyclotol)	$C_{1.871}H_{2.553}N_{2.288}O_{2.685}$	128	115	13
7	65/35 RDX/TNT (Cyclotol)	$C_{1.958}H_{2.528}N_{2.219}O_{2.682}$	126	115	11
8	60/40 RDX/TNT (Cyclotol)	$C_{2.04}H_{2.50}N_{2.15}O_{2.68}$	125	114	11
9	30/70 RDX/TNT (Cyclotol)	$C_{2.564}H_{2.353}N_{1.736}O_{2.661}$	112	111	1
10	60/40 EDNA/TNT (Ednatol)	$C_{2.033}H_{3.281}N_{2.129}O_{2.657}$	112–117	113	−1–4
11	55/45 EDNA/TNT(Ednatol)	$C_{2.\ 121}H_{3.191}N_{2.061}O_{2.656}$	103	112	−9
12	60/40 TNT/HNDPhA[a)] (Novi,60)	$C_{2.944}H_{1.777}N_{1.431}O_{2.679}$	105	89	16
13	50/50 PETN/TNT (Pentolite)	$C_{2.333}H_{2.367}N_{1.294}O_{3.22}$	123	111	12
14	40/60 PETN/TNT (Pentolite)	$C_{2.483}H_{2.334}N_{1.299}O_{3.105}$	118	110	8
15	30/70 PETN/TNT (Pentolite)	$C_{2.633}H_{2.301}N_{1.305}O_{2.989}$	113	109	4
16	60/470 PETN/TNT (Pentolite)	$C_{2.183}H_{2.4}N_{1.288}O_{3.336}$	127	111	16
17	70/30 PETN/TNT (Pentolite)	$C_{2.033}H_{2.433}N_{1.283}O_{3.451}$	131	112	19
18	25/75 PETN/TNT (Pentolite)	$C_{2.708}H_{2.285}N_{1.308}O_{2.932}$	111	109	2
19	10/90 PETN/TNT (Pentolite)	$C_{2.934}H_{2.236}N_{1.316}O_{2.759}$	105	108	−3
20	48/52 TNT/AP (Picratol)	$C_{2.748}H_{2.3268}N_{1.48}O_{2.748}$	94	90	4
21	95/5 Nitromethane/Ethylenediamine (PLX)	$C_{1.611}H_{4.941}N_{1.665}O_{3.276}$	105	91	14
22	30/50/20 RDX/Tetryl/TNT (PTX-1)	$C_{2.244}H_{2.142}N_{1.946}O_{2.733}$	119–122	113	6–9
23	42/27/31 RDX/PETN/TNT (PTX-2)	$C_{1.951}H_{2.501}N_{1.887}O_{2.98}$	125–127	114	11–13
24	30/70 TNT/Tetryl (Tetrytol)	$C_{2.632}H_{1.88}N_{1.616}O_{2.744}$	120	112	8
25	25/75 TNT/Tetryl (Tetrytol)	$C_{2.6}H_{1.857}N_{1.637}O_{2.751}$	120	111	9
26	35/65 TNT/Tetryl (Tetrytol)	$C_{2.665}H_{1.903}N_{1.595}O_{2.737}$	118	111	7
27	60/40 TNT/Tetryl (Tetrytol)	$C_{2.826}H_{2.018}N_{1.49}O_{2.701}$	113	109	4
28	70/30/PA/HNDPhA (Trridite)	$C_{2.654}H_{1.259}N_{1.395}O_{2.96}$	89	91	−2
29	60/40/PA/HNDPhA (Trridite)	$C_{2.665}H_{1.242}N_{1.424}O_{2.927}$	84	91	−7
30	90/10/PA/HNDPhA (Trridite)	$C_{2.631}H_{1.293}N_{1.338}O_{3.024}$	100	91	9
31	60/40/TNAns/HNDPhA (Type98 Expl)	$C_{2.822}H_{1.69}N_{1.379}O_{2.822}$	98	90	8

a) HNDPhA = hexanitrodiphenylamine.

Table 4. Comparison of the predicted values of $Bris_{relTNT,Al}$[a)] of Equation (2) for aluminized explosives with the experimental data [2] related to TNT as standard with 100 %.

No.	Compound	Formula	Exp.	Equation (2)	Dev
1	67/22/11 TNT/AN/Al (Ammonal)	$C_{2.066}H_{2.576}N_{1.435}O_{2.596}Al_{0.408}$	100	92	8
2	40/21/21/18 TNT/AN/RDX/Al (DBX)	$C_{1.517}H_{2.499}N_{1.621}O_{2.412}Al_{0.667}$	121	113	8
3	60/24/16/TNT/HNDPhA/Al (Hexamite)	$C_{2.506}H_{1.595}N_{1.176}O_{2.242}Al_{0.593}$	116	133	−17
4	40/40/20 TNT/AN/Al (Minol-2)	$C_{1.233}H_{2.881}N_{1.529}O_{2.557}Al_{0.741}$	95	114	−19
5	45/37/38/RDX/TNT/Al (Torpex)	$C_{1.749}H_{2.031}N_{1.705}O_{2.194}Al_{0.667}$	122	122	0
6	42/40/18/RDX/TNT/Al (Torpex-2)	$C_{1.749}H_{2.031}N_{1.705}O_{2.194}Al_{0.667}$	122	122	0
7	29/49/22 TNT/HMX/Al (HTA-3)	$C_{1.801}H_{2.016}N_{1.664}O_{2.192}Al_{0.667}$	132 to 160	124	8 to 36
8	80/20 TNT/Al (Tritonal)	$C_{1.081}H_{2.162}N_{2.162}O_{2.162}Al_{0.741}$	108 to 114	109	−15 to −9
9	90/10 TNT/Al (Tritonal)	$C_{2.775}H_{1.982}N_{1.189}O_{2.379}Al_{0.371}$	111 to 114	114	2 to 5

a) $Bris_{relTNT,Al}$: brisance as determined by sand test for aluminized explosives related to TNT as standard with 100 %.

Table 5. Standardized coefficient values and some statistical parameters of Equation (1).

Variable	Coefficient[a)]	Standard error[b)]	P-value[c)]	Lower bound[d)] (95 %)	Upper bound[e)] (95 %)
Intercept	85.52	4.588014	6.31E-22	76.26	94.78
C	4.81	0.955659	9.48E-06	2.88	6.74
d-a-b/2	2.56	0.588584	8.71E-05	1.37	3.74
$Bris^-$	−35.96	3.373453	1.61E-13	−42.76	−29.15
$Bris^+$	19.69	5.02468	0.0003	9.55	29.83

a) Coefficient = The fit parameters; b) Standard error = SEP, given in text; c) P-value = The probability of rejecting a true null hypothesis; d) Lower bound (95 %) = The lower bond of a 95 % confidence interval; e) Upper bound (95 %) = The upper bond of a 95 % confidence interval.

of explosive mixtures, Equation (1) can be easily calculated. Table 3 shows the calculated values of $Bris_{relTNT}$ of Equation (1) for some explosive formulations.

Experimental data for some aluminized explosives are given in Table 4. Since aluminum can interact with the detonation products, the partial equilibrium prediction gives better results than full equilibrium condition, obtained by computer codes using an equation of state. However, the study has shown that an extra term can be added to distribution of oxygen atoms between carbon and hydrogen atoms in order to consider the effect of aluminum in aluminized explosives with general formula $C_aH_bN_cO_dAl_e$ as:

$$Bris_{relTNT,Al} = -42.87(d-a-b/2) + 146.71e \qquad (2)$$

where $Bris_{relTNT,Al}$ is the relative brisance with respect to TNT for aluminized explosives. The correlation coefficient of Equation (2) is relatively good with a value of 0.90 [9]. The values of $Bris^+$ and $Bris^-$ equal zero for aluminized explosives. In Table 4, the calculated values of Equation (2) are compared with the measured values of $Bris_{relTNT,Al}$ for several aluminized explosives.

3.3 Statistical Parameters and Comparison of Different Models

Table 5 displays statistical parameters of Equation (1), which contain standard error, the *p*-value, as well as the upper and lower bounds of a 95 % confidence interval. For assessment of the brisance with Equation (1), five general statistical parameters were selected to evaluate the predictive ability of the model: (i) *SSR* (sum of squared residuals): for good statistical significance of a correlation, the value of *SSR* has a small value; (ii) *RMSE* (root mean square error): gives the average difference between the predicted and

Table 6. Comparison of statistical parameters of Equations (1) and (2).

Parameter	Equation (1)		Equation (2)
	Table 1	Table 2	Table 3
SSR[a)]	4319	3254	1267
RMSE[b)]	10	10	11
PRE[c)]	10	9	10
SEP[d)]	10	10	12
MAPE[e)]	8	8	7

a) *SSR*: sum of squared residuals ($SSR = \sum_{j=1}^{n} [(Bris)_{pred,j} - (Bris)_{meas,j}]^2$; where $(Bris)_{pred,j}$ and $(Bris)_{meas,j}$ are the predicted and the measured brisance by sand crush test, respectively; *n* is the total number of compounds used in the prediction set); b) *RMSE*: root mean square error ($RMSE = (SSR/n)^{0.5}$); c) *PRE:* percent relative error ($PRE = (100/Bris_{mean})(SSR/n)^{0.5}$, where $Bris_{mean}$ is the mean of experimental values); d) *SEP:* standard error of prediction ($SEP = [SSR/(n-1)]^{0.5}$); e) *MAPE*: mean absolute percentage error ($MAPE = \frac{1}{n}\sum_{j=1}^{n} |((Bris)_{pred,j} - (Bris)_{meas,j})/(Bris)_{meas,j}| \times 100$).

measured values; (iii) *PRE* (percent relative error): gives the predictive ability of each component; (iv) *SEP* (standard error of prediction): this parameter can be used to determine whether the model describes the experimental process with adequate precision; (v) *MAPE* (mean absolute percentage error): provides a measure of the accuracy of a method with respect to the prediction.

These statistical results for pure, mixture and aluminized explosives are compared in Table 6. As obvious, the predicted results of Equation (1) and Equation (2) are similar to each other. The molecular formula is the only necessary parameter to evaluate the brisance of aluminized explosives. The reliability of the predicted results on the basis of $Bris_{core}$ in Equation (1) can be improved by considering the effects of $Bris^{+}$ and $Bris^{-}$.

4 Conclusions

In this paper, an easy to handle method to predict the brisance of pure, mixed and aluminized explosives as measured by sand crushing test is introduced. For pure and mixed energetic compounds, the brisance depends on $Bris_{core}$ as well as on the molecular structure correlated parameters $Bris^{+}$ and $Bris^{-}$. The brisance of aluminized explosives can also be predicted on the basis of their elemental composition. To aid in the calculation of brisance of energetic materials containing aluminized explosives that have not yet been synthesized, Equations (1) and (2) were developed.

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