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Revisiting the theoretical prediction of the explosive performance found by the Trauzl test

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Revisiting the theoretical prediction of the explosive performance found by the Trauzl test

Abstract

The Trauzl lead block test allows the determination of the approximate performance of explosives in blasting applications by measuring the volume increase (expansion) that is produced by the detonation of an explosive charge in the cavity of a lead block. In this paper, we reconsider the possibility of interpreting the Trauzl test results in terms of detonation parameters or quantities. The detonation parameters used in the analysis are calculated using the thermochemical code EXPLO5, while the hydrocode AUTODYN is used to simulate the effect of explosive charge density and reaction rate on the results of the Trauzl test. The increase in the volume of the lead block cavity was found to correlate best with the product of the detonation heat and the root of the volume of detonation products. Hydrocode simulation showed that the density of explosive charge and the rate of explosive decomposition affect the dynamics of the interaction of the detonation product and the lead block, and consequently the lead block cavity volume increase.

Keywords: Trauzl lead block test; Performance of explosives; EXPLO5; AUTODYN; Detonation heat

Abbreviations

V_T	Net volume increase of the cavity (cm^3)
Q	Detonation heat ($\text{MJ}\cdot\text{kg}^{-1}$)
V_0	Volume of detonation products at standard state ($\text{L}\cdot\text{kg}^{-1}$)
E_0	Detonation energy at infinite volume ($\text{kJ}\cdot\text{cm}^{-3}$)
f	Specific force ($\text{MJ}\cdot\text{kg}^{-1}$)
p_{CJ}	Chapman-Jouguet pressure (GPa)
D	Detonation velocity ($\text{m}\cdot\text{s}^{-1}$)
P_{EM}	Specified detonation parameter or quantity
$a_0, m, \text{ and } n$	Constants in Eq. (2)
r	Correlation coefficient
σ	Standard deviation
MAPE	Mean absolute percentage error (%)
ρ_0	Initial density of explosive charge ($\text{g}\cdot\text{cm}^{-3}$)
ρ_{TMD}	Theoretical maximum density of explosive charge ($\text{g}\cdot\text{cm}^{-3}$)
ρ_{GD}	Gravimetric density of explosive charge ($\text{g}\cdot\text{cm}^{-3}$)
$R_{\max}$	Maximum radial displacement of explosive charge/lead interface in the middle of charge height (mm)
$t(R_{\max})$	Time at which maximum displacement was achieved (μs)
t_{sand}	Time at which ejection of sand from the cavity begins (μs)

t_{gas}	Time at which ejection of products from the cavity begins (μs)
F	Reacted fraction of explosive
G	Constant in I&G model (growth term) ($\mu\text{s}^{-1} \cdot \text{GPa}^{-\gamma}$)
I	Constant in I&G model (ignition term) (μs^{-1})
$a, b, c, d, x, \text{ and } y$	Constants in I&G model
$A \text{ and } B$	Constants in JWL equation of state (GPa)
$R_1, R_2, \text{ and } \omega$	Constants in JWL equation of state
t_{CRZ}	Duration time of reactions (μs)
ID HE	Ideal high explosive
NID HE	Non-ideal high explosive
Primary HE	Primary high explosives
CJD at ρ_{GD}	Chapman-Jouguet detonation at ρ_{GD}
CJD at ρ_{TMD}	Chapman-Jouguet detonation at ρ_{TMD}
CVE at ρ_{GD}	Constant volume explosion at ρ_{GD}

1. Introduction

The performance of explosives (“strength” or “power”) is usually estimated based on the values of the detonation parameters [1, 2]. However, such an approach often does not give the same explosive ranking order. For illustration, when explosives perform strong disintegration work, the most relevant parameters are detonation velocity and pressure. However, for blasting work, the heat of detonation and the amount of gas products are relevant parameters, while the detonation velocity does not play an important role [3]. Thus, the performance of an explosive should be related to the type of work performed by the explosive, and it cannot be judged on a single detonation parameter.

In practice, various experimental tests have been developed to mimic a particular application of explosives. One of such tests is the lead block test, also known as the Trauzl test, which allows the determination of the approximate relative strength of explosives in blasting applications [3,4]. The test was proposed in the 1880s by Isidor Trauzl, while the standard conditions for performing the test were established in 1930 [3,5]. The test consists in firing 10 g of an explosive charge mounted in a cavity ($\Phi 2.5 \times 12.5$ cm), drilled along the block axis) within a lead block ($\Phi 20 \times 20$ cm). After the explosive charge is inserted, the cavity is tamped with quartz sand. The increase in cavity volume (ΔV_T) after charge detonation serves as a measure of explosive strength. One of the key features of the lead block test is that it mimics the conditions fairly closely in a borehole, however, the weakness of the test is that it uses a small explosive charge mass [3,4]. According to Marshall [3], the lead block test can only give satisfactory comparative results for the same class of explosives, i.e., explosives that behave in the same way. If, for example, the pressure growth rates of the two explosives are very different, then the results of the tests are no

longer comparable. Afanasenkov [6] stated that the experimental ΔV_T values for ideal explosives were satisfactorily correlated with the product of the heat of detonation and the amount of gases, while the correlation for explosives detonating at low velocities is significantly poorer. The author assumed that a small amount of explosive charge used in the Trauzl test does not allow establishing the steady-state detonation process in such explosives (non-ideal), which results in a poorer correlation. Mayer et al. [4] also thought that reliable Trauzl test results can only be obtained for ideal high explosives.

The results of the lead block test are affected by various factors, for example, the mechanical properties of the lead block, the uniformity of the temperature of the lead block before the test [3-5], the uniformity of the tamping, and the type of tamping material [7]. Consequently, the results of the test are not highly reproducible [8, 9]. The weakness related to standardised Trauzl tests is that it is not required to record the density of the explosive charge [10]. The reason for this should perhaps be sought in the work of Kast and Dautriche [3] who found that the results of the lead block test are not affected by considerable variations in the explosive charge density. Based on research results published until 1955, Gordon et al. [5] concluded that the density of explosive charge, the fineness of the sand used for the tamping, and the temperature of the lead casting do not have a pronounced effect on the test results. However, the temperature of the lead block before the test has a significant effect on the results. In contrast, Ahrens [11] argues that the results of the Trauzl test are decisively dependent on the density of the explosive charge. Unfortunately, no newer research results have been published to confirm or disprove these two contradictory claims.

Several researchers have tried to interpret the results of the Trauzl test in terms of certain explosive detonation properties. Some of them correlated the results of the Trauzl test with a quantity called "specific pressure", while others considered a quantity that involved density, detonation velocity, and temperature [5]. Berthelot [12] was the first to introduce the term "characteristic products" (QV_0/c , where V_0 is the specific volume of the detonation gas products, Q is the heat and c is the specific heat capacity of the products) and used it to compare the performance of different explosives. Marshall et al. [3] have shown that in the case of fairly low explosive density (so that the perfect gas equation of state is applicable), Berthelot's characteristic product can be transformed into a specific force or a specific pressure ($f = nRT = QV_0/c$, where n is the number of moles of product gases for the unit weight of the explosive, R is the gas constant, and T is the temperature reached in a constant volume explosion). Due to the difficulty in determining the value of c , the product QV_0 is often used instead of QV_0/c (that is, c is assumed to be constant).

According to Mayer et al. [4], the specific force (or energy) is the most relevant thermodynamically calculable parameter with respect to the strength of explosives. It represents the amount of energy that is released when the gaseous products (assumed to occupy the initial volume of the explosive) expand to the surrounding performing mechanical work. The authors state that the results of the specific energy and lead block test correlate well, with this correlation not being linear. Gordon et al. [5], however, have found a good linear correlation between f and

ΔV_T .

In the last two decades, several researchers have reported on the correlation between the results of the lead block test and the different explosive detonation parameters. Afanasenkov [6] proposed the correlation between the ΔV_T and the quantity $Q^{0.75} V_0^{0.25}$. Keshavarz et al. [9] correlated ΔV_T and Q , whereby Q for CHNO explosives is calculated using the empirical equation of Kamlet and Jacobs. The authors found a linear relationship between ΔV_T and Q . Jafari et al. [13] applied the approach applicable to $C_aH_bN_cO_d$ explosives, which uses the ratios of a/d and b/d and some structural parameters to establish a correlation with ΔV_T . A good overview of the possibility of correlation of ΔV_T (and relative strength of explosives) and individual detonation parameters is given in the work of Locking [10]. The author has found that ΔV_T correlates the best with the QV_0 product. There is a somewhat poorer correlation with Q only, whereas the detonation pressure and velocity do not correlate at all with ΔV_T . Wahler and Klapotke [14] considered the explosive charge (ρ_0) and proposed the correlation between the ΔV_T and the quantity $Q^3 V_0 \rho^{1/9}$.

When it comes to the correlation of ΔV_T and individual detonation parameters or quantities, it appears that there are quite a bit of imprecisions and that some things have been overlooked in many publications. For example, the experimental ΔV_T values are taken from literature sources without going back to the original sources and without knowing the accuracy of the data used, and without knowing the density of explosive charges used in the analysis. It is not specified to which charge density the values of detonation parameters used in the analysis refer, and it is not clear whether the values of Q refer to the Chapman-Jouguet state (where H_2O is gaseous) or they are determined calorimetrically (H_2O is liquid). The mentioned deficiencies can undoubtedly affect the results of the correlation analysis and may lead to erroneous conclusions. The above mentioned motivated us to revisit the possibilities of correlation of Trauzl test results and individual detonation parameters, with emphasis on researching the impact of the method of calculation of detonation heat and volume of detonation products on the results of the correlation analysis. In addition, the objective of the research was to simulate the impact of the density of the explosive charge and the reaction rate on the Trauzl results and the interaction between the detonation products and the lead block.

2. Materials and methods

To interpret the results of the Trauzl lead block test in terms of explosive detonation properties, two sets of experimental Trauzl test results are used: the first set includes our experimental data for commercial ammonium nitrate(AN)-based explosives (ANFO, emulsion explosives, AN-based powdered explosives), and the second set includes data reported in the literature for various types of explosives. Tests are performed in our Explosives Testing Laboratory in the period 1999-2006 in accordance with the standardized procedure [2, 11], using explosive charges of constant mass (10 g). The charge is wrapped in a trapezoidal piece of tinfoil and then placed into the lead block cavity. The charge is initiated by the standard PETN detonator (0.8 g), which is inserted into the charge. The cavity

is stemmed by dry sand. The expansion of the cavity is measured by the volume of water poured from the graduated cylinder. For each explosive, three (and in some cases two) shots were made. The compositions of the explosives studied were taken from the manufacturer or determined experimentally. The bulk density of the explosive is determined by measuring the volume of the known mass of the sample. Detonation velocities were measured using an electro-optical method. ANFO charges are tested in steel pipes, whereas other explosives are tested in their original cartridges. The experimental data reported in the literature for 138 explosives (secondary explosives, primary explosives, non-ideal, aluminised explosives, etc.) are taken from [4, 6, 13, 15]. A complete list of explosives used in the study is given in Appendix A1. The detonation parameters of the explosives studied (detonation velocity and pressure, detonation heat, volume of detonation products, detonation energy, etc.) are calculated by the thermochemical code EXPLO5 [16] using the Chapman-Jouguet detonation model. The details of the calculations using the thermochemical code EXPLO5 can be found in Refs. [17, 18]. Thermochemical calculations are also performed assuming a constant volume explosion module, which roughly mimics the situation in the Trauzl test, where the sample is confined by a lead block and tampering material. The output of such a calculation is the heat of the explosion, the maximum pressure for a specified density, the volume of the explosion products, etc. AUTODYN hydrocode [19] is used to simulate the impact of explosive charge density and reaction rate on the results of the Trauzl test result. The details of the calculation are given in the Section 3.

3. Results and discussion

3.1. Trauzl test results for AN-based explosives

The experimental results of the Trauzl test for AN-based commercial explosives are given in Table 1. Along with the increase in the cavity volume (ΔV_T), the density of explosive charges (ρ_0) and measured detonation velocities (D) at specified densities are also given. The analysis of the data given in Table 1 shows that the average difference between the minimum and maximum ΔV_T values in three tests is equal to 25.6 cm³, and the average deviation from the mean values is equal to 3.5%. Such deviation is close to the deviation of 20 cm³ allowed by some national standards [6] or by recommendation [11]. In most cases, the deviation from the mean values is below 5% and only for four explosives out of 26 tested, the deviation is between 6% and 11%. This consideration refers to the same explosive with identical properties. A similar analysis is performed on literature reported ΔV_T values for RDX, PETN, and TNT to see how the experimental results taken from the different sources differ. The results of the analysis are given in Table 2.

Table 1

Experimental Trauzl test results for AN-based commercial explosives.

No.	Trade name of explosive	Composition	$\rho_0/(\text{g}\cdot\text{cm}^{-3})$	d_{EM}/mm	$D_{\text{expt.}}/(\text{m}\cdot\text{s}^{-1})$	Cavity expansion volume/ cm^3			
						Test 1	Test 2	Test 3	Mean value
1	AMONEKS 2	AN (80.67%), TNT (14.43%), wood dust (4.9%)	1.05	50	3487	319	295	294	303
2	PERMON 50	AN (50.41%), TNT (49.2%), additives (0.09%)	1.06	65	4187	351	335	342	344
3	AMONAL	AN (81.4%), TNT (15.92%), paraffin (1.58%), wood dust (1.1%)	1.06	60	4528	385	366	370	374
4	POLONOT	AN (81.1%), TNT(17.3%), wood dust (1.6%)	1.02	50	3403	372	382	384	379
5	AMONEX-1	AN (82,2%), TNT (17,8%)	1.07	28	4162	385	366		374
6	ANFO (ELMEX)	AN (94.88%), FO (5.12%)	0.87	67*	2145	319	329	244	298
7			0.88	67*	2728	323	334	248	301
8	ANFO (LAGUN 1)	AN (93.86%), FO (6.14%)	0.87	67*	3211	323	304	314	313
9	ANFO (ELMEX)	AN (94.62%), FO (5.38%)	0.84	67*	3189	325	311	327	321
10	ANFO (ELMEX)	AN (94.88%), FO (5.12%)	0.91	65*	3056	324	315	329	322
11	ANFO (VITANOL P)	AN (94.75%), FO (5.25%)	0.89	65*	3785	343	336	340	339
12	ANFO (ELMEXAL)	AN (91.8%), FO (3.6%), Al (4.6%)	0.87	67*	3486	350	332	326	336
13	ANFO	AN (92.01%), FO (3.57%), Al (4.42%)	0.88	65*	3548	362	329	344	345
15	AN/SN emulsion	AN (72.5%), SN (7.6%), FO +emulsifier (5.9%), water (11.7%), GMB (2.3%)	1.16	65	4049	286	240		263
16	EMSIT 1	AN (64.66%), SN (12.68%), FO (3.72%), emulsifier (2%), water (13.23%), GMB	1.11	50	5098	279	273	269	270
17		(3.71%)	1.12	60	5088	274	274	264	271

18			1.12	38	5096	274	273	264	271
19	ELMULEX P	AN (75.8 %), SN (9.8%), FO (2.1%), emulsifier (1.3%), paraffin (3.1%), water (8.7%)	1.06	45	3619	273	283	273	276
20	Kamniktit E3	AN (75.5%), SN (6.3%), FO +emulsifier (5.6%), water (12.6%)	1.16	40	4828	294	289		292
21	LAMBREX 1	AN (68.8%), SN (12.9%), FO +emulsifier (5.1%), water (13.2%)	1.11	30	3068	322	337	322	326
23	EMULGIT 82 G	AN (74%), SN (8%), FO +emulsifier (8%), water (10%)	1.15	65	4629	364	371		367
22	EMULGIT 42 G	AN (75%), SN (8%), FO (6%), water (11%)	1.21	65	4563	359	350		354
13	EMUNIT	AN (82%), SN (5%), FO (5%), water (6%), GMB (2%)	1.20	60	4862	329	362	344	345
24	ELMULEXAL	AN (73.2 %), SN (9.3%), FO (3.6%), emulsifier (0.9%), GMB (1.4%), Al(3.2%), water (8.4%)	1.17	60	5698	329	261		295
25	ELMULEXAL	AN (68.9%), SN (7.0%), FO +emulsifier (5.7%), water (11.1%), GMB (2.3%), Al (2.3%)	1.16	65	5444	284	320		302
26	ELMULEXAL	AN (70.6%), SN (7.4%), FO +emulsifier (4.8), water (10.6%), GMB (1.6%), Al (5.0%)	1.16	38	3969	307	302	277	296

Note: AN- ammonium nitrate, SN-sodium nitrate, FO-fuel oil, GMB-glass micro balloons, ρ_0 – density of explosive charge, d_{EM} – charge diameter, D_{expt} – measured detonation velocity at ρ_0 , ΔV_T – net volume increase of the cavity.

*The detonation velocity of ANFO explosives is measured in steel pipes with a wall thickness of 2 mm; other explosives in the original cartridge.

Table 2

Reproducibility of Trauzl test results.

Explosive	Number of data	$\Delta V_{T,min}/\text{cm}^3$	$\Delta V_{T,max}/\text{cm}^3$	$\Delta V_{T,mean}/\text{cm}^3$	$\Delta V_{T,max}$ $\Delta V_{T,min}/\text{cm}^3$	Standard deviation, σ/cm^3	Average deviation, $\sigma_{mean}/\text{cm}^3$
ANFO	9	298	345	322	47	15.3	12.3 cm ³
	(This work)	(7.5%)	(7.09%)				(3.82 %)
PETN	8	480	523	505	43	15.1	14.0 cm ³
	[4,6,13,15]	(5.0%)	(3.51%)				(2.77 %)
RDX	5	465	520	479	55	18.9	10.3 cm ³
	[4,6,13,15]	(3.57%)	(7.84%)				(2.87 %)
TNT	8	285	310	295	25	16.5	8.6 cm ³
	[4,6,13,15]	(3.39%)	(5.08%)				(2.9 %)

Note: PETN - pentaerythritol tetranitrate, RDX - 1,3,5-Trinitro-1,3,5-triazinane, TNT - 2,4,6-trinitrotoluene.

Standard deviation is calculated by equation: $\sigma = \sqrt{\frac{\sum(x_i - \bar{x})^2}{n-1}}$ and average deviation by equation:

$\sigma_{mean} = \frac{1}{n} \sum |x_i - \bar{x}|$, where n is number of data and $\bar{x}$ is mean of all x_i values.

As visible in Table 2, the minimum and maximum values of ΔV_T differ from 25 to 55 cm³, that is, up to 7.5%. The average deviation from the mean value ranges from 2.8% to 3.82%, which is close to the average deviation obtained for ANFO in our experiments (3.5%). Therefore, based on this analysis it follows that the average deviation of the experimental Trauzl test results from different sources ranges between 3% and 4%. It should be mentioned that the results for ANFO are obtained with samples from different manufacturers, so the type of fuel oil and the exact composition of the mixture are somewhat different and affect the results to some extent. The data for RDX, TNT, and PETN are taken from various literature sources, and no information is available on details of explosive charges (e.g., density, purity, etc.), or on the measurement uncertainties.

3.2. Correlation of the Trauzl test results and detonation parameters

As mentioned above, most of the literature reported Trauzl test results do not contain information on the density of explosive charges, so it is not clear which density of the charge that the values of detonation parameters used in the correlation analysis refers to. It is well known that the detonation parameters are density dependent and therefore the use of inappropriate charge densities for the calculation of the detonation parameters will undoubtedly affect the results of the correlation analysis.

The correlation analysis in this work is done using the values of the detonation parameters calculated by thermochemical code EXPLO5, applying the Chapman-Jouguet (CJ) detonation model. The calculation is done for two densities of explosive charges: the theoretical maximum density (ρ_{TMD}) and gravimetric density (ρ_{GD}). The gravimetric density was chosen because it is assumed that the density of powdered explosives used in the Trauzl

tests is approximately equal to the gravimetric density. For commercial AN-based explosives, the gravimetric density is taken to be equal to the actual density of the cartridges (from the manufacturer's documents). For powdered high explosives it is assumed that the gravimetric density is equal to 65% of the theoretically maximum ($\rho_{GD} = 65\% \rho_{TMD}$). In addition to the ideal detonation calculation, the constant-volume explosion calculation is also done since it mimics quite well the situation where an explosive charge is confined by a casing or other confining environment. The calculation assumes that the casing holds for the timescale of chemical equilibration. In other words, the confinement should last enough for the sound to propagate across the explosive charge at least once [20]. The output result of the calculations is the maximum pressure, temperature, and force at a specified loading density. The experimental results of the Trauzl test are correlated with the detonation parameters calculated as previously described. The increase in cavity volume is expressed as a function of a detonation property or quantity: $\Delta V_T = f(P_{EM})$, where P_{EM} is the detonation parameter considered. The correlation analysis is performed in two steps. In the first step, the experimental detonation parameters for ideal high explosives are analysed (Fig. 1 and Table 3), and in the second step for non-ideal explosives (Fig. 2 and Table 4). By this, we wanted to determine whether the correlation is valid for different types of high explosives, considering that some researchers claim that the correlation is poor for non-ideal low-detonation velocities explosives [6], while others claim that the test is not applicable for modern higher-power explosives (since they can rupture the lead block) [10]. After a preliminary analysis, and taking into account the results of the correlation of other researchers (e.g., Locking [10], Afanaskov [6], Keshavarz et al. [9]), it was found that a linear relationship, having a zero intercept, is the most appropriate to describe $\Delta V_T = f(P_{EM})$ dependence:

$$\Delta V_T = a_0 \cdot P_{EM} \quad (1)$$

where a_0 is the fitting constant and P_{EM} is the detonation parameter (or quantity) considered.

The fitting of $\Delta V_T - f(P_{EM})$ data to Eq. (1) is done in Excel, where the correlation coefficient (r) and the standard deviation (σ) are calculated by equations:

$$r = \frac{n(\sum x_i y_i) - (\sum x_i)(\sum y_i)}{\sqrt{[n \sum x_i^2 - (\sum x_i)^2][n \sum y_i^2 - (\sum y_i)^2]}} \quad (2)$$

$$\sigma = \sqrt{\frac{\sum (x_i - y_i)^2}{n-1}} \quad (3)$$

where x_i and y_i are experimental and predicted values of ΔV_T , respectively, and n is number of data points.

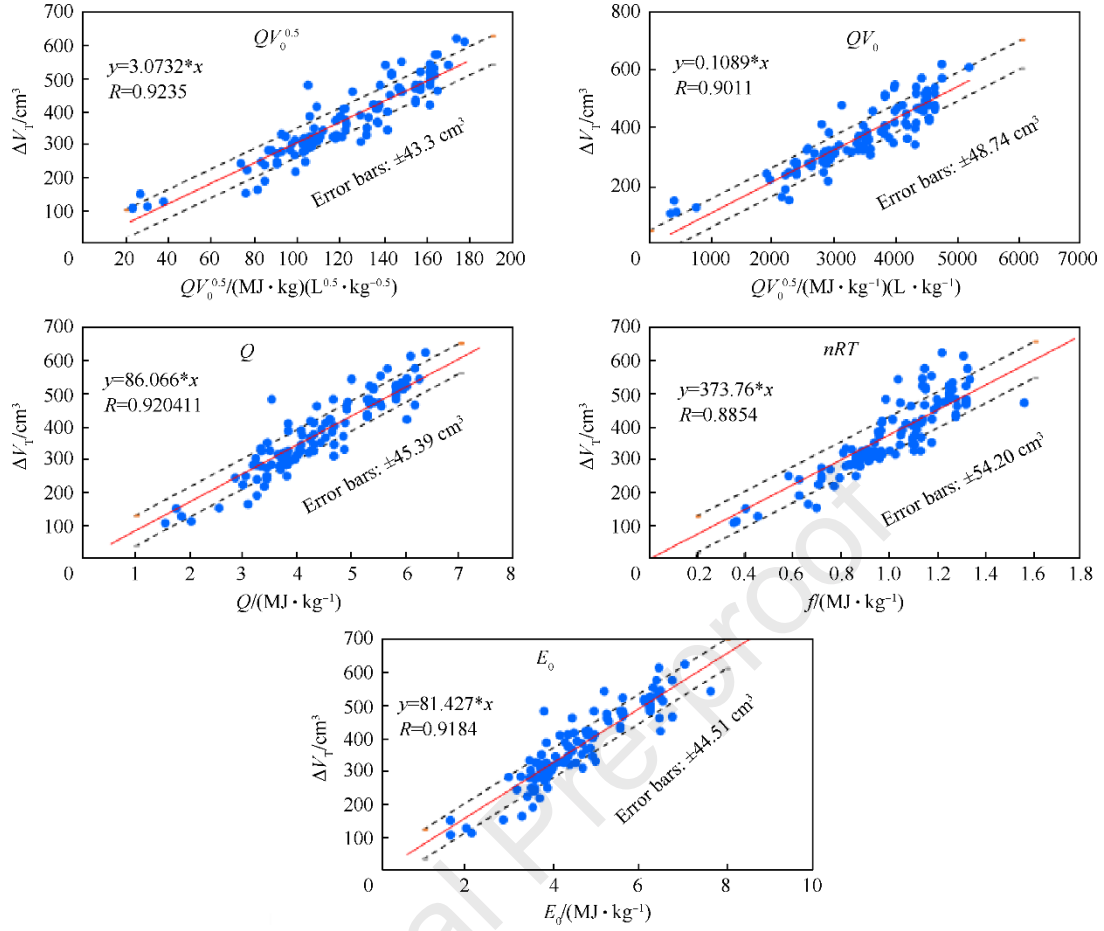


Fig. 1. Correlation of cavity volume increase and detonation parameters for ideal explosives (Note: Detonation parameters calculated at gravimetric densities, error bars represent standard deviation).

It is visible from Table 3 that ΔV_T does not correlate satisfactory with D , p_{cl} , $p_{cl}V$ ($0.42 < r < 0.77$, $72 < \sigma < 113$). There is a somewhat better correlation with E_0 ($0.77 < r < 0.92$, $44 < \sigma < 73$), while the best correlation exists with Q , QV_0 , and $QV_0^{0.5}$ ($0.89 < r < 0.93$, $42 < \sigma < 54$). The fact that the quantity QV_0 correlates very well with ΔV_T is not surprising since it has been known since Berthelot's work [12] that Q and V_0 are the most relevant parameters when it comes to the blasting work of an explosive.

By fitting the $\Delta V_T - (Q, V_0)$ dependence to the equation:

$$\Delta V_T = a_0 Q^m V_0^n \quad (4)$$

(which is similar to the one proposed by by Afanasenkov [6]), it was found that for ideal explosives (without primary) the constant m equals 1.14 and the constant n equals 0.47, with the correlation coefficient (r) of 0.9131. Taking $m = 1$ (as is the case in the work of Berthelot and most subsequent studies) and rounding the value of n to 0.5, the correlation coefficient changes only slightly from 0.9131 to 0.9120. Further analysis done on all studied explosives confirmed that $m = 1$ and $n = 0.5$, (i.e., $\Delta V_T = a_0 \cdot QV_0^{0.5}$ relationship) describes very well Trauzl test results for different explosives (Table 4), with an almost constant value of the constant a_0 regardless of which explosive charge density is used for the calculation of the detonation parameters and regardless the type of

explosive. Using this correlation ΔV_T can be predicted with the mean average percentage error (MAPE) of 9.3%–10.5% and standard deviation of 42–44 cm³. This error is significantly higher compared to the experimental error (MAPE 3%–4% and standard deviation 9–14 cm³, Table 2).

Table 3

Statistical parameters of correlation analysis for ideal explosives.

Parameter/quantity	Method of calculation	Fitting constant a_0	$\sigma/(\text{cm}^3)$	MAPE/%	r	Strength of correlation
$QV_0^{0.5}/(\text{MJ}\cdot\text{kg}^{-1})(\text{L}\cdot\text{kg}^{-1})^{0.5}$	CJD at ρ_{GD}	3.0732	43.253	9.8872	0.9235	Very strong
	CJD at ρ_{TMD}	3.0399	43.813	10.547	0.9243	Very strong
	CVE at ρ_{GD}	3.0856	42.001	9.322	0.9271	Very strong
$Q^{(a)}/(\text{MJ}\cdot\text{kg}^{-1})$	CJD at ρ_{GD}	86,066	45.391	10.691	0.9203	Very strong
	CJD at ρ_{TMD}	79.369	53.797	13.573	0.8957	Very strong
	CVE at ρ_{GD}	88.402	42.564	9.671	0.9249	Very strong
$QV_0/(\text{MJ}\cdot\text{kg}^{-1})(\text{L}\cdot\text{kg}^{-1})$	CJD at ρ_{GD}	0.1089	48.743	11.369	0.9011	Very strong
	CJD at ρ_{TMD}	0.1149	47.107	10.999	0.9088	Very strong
	CVE at ρ_{GD}	0.1068	50.416	11.737	0.8971	Very strong
$E_0/(\text{MJ}\cdot\text{kg}^{-1})$	CJD at ρ_{GD}	81.427	44.513	10.405	0.9184	Very strong
	CJD at ρ_{TMD}	76.678	72.687	16.203	0.7668	Strong
	CVE at ρ_{GD}					
$f/(\text{MJ}\cdot\text{kg}^{-1})$	CJD at ρ_{GD}	373.76	54.197	12.213	0.8854	Very strong
	CJD at ρ_{TMD}	442.60	46.878	10.817	0.9167	Very strong
	CVE at ρ_{GD}	408.30	51.341	11.393	0.8948	Very strong
$p_{\text{Cl}}V/(\text{GPa}\cdot\text{cm}^3\cdot\text{g}^{-1})$	CJD at ρ_{GD}	39.61	78.171	15.624	0.7275	Strong
	CJD at ρ_{TMD}	27.14	75.640	16.797	0.7375	Strong
	CVE at ρ_{GD}	87.302	72.069	14.408	0.7696	Strong
$D/(\text{m}\cdot\text{s}^{-1})$	CJD at ρ_{GD}	0.0634	85.321	21.867	0.6801	Strong
	CJD at ρ_{TMD}	0.0506	89.490	23.638	0.6367	Strong
	CVE at ρ_{GD}					
$p_{\text{Cl}}^{(b)}/\text{GPa}$	CJD at ρ_{GD}	31.279	112.860	25.631	0.5521	Moderate
	CJD at ρ_{TMD}	15.366	110.969	25.799	0.4191	Moderate
	CVE at ρ_{GD}	69.175	107.764	23.864	0.5843	Moderate

Legend: Strength of the correlation determined according to suggestion of Evans [21]; CJD at ρ_{GD} - the CJ detonation at ρ_{GD} , CJD at ρ_{TMD} -the CJ detonation at ρ_{TMD} , CVE at ρ_{GD} -constant volume explosion at ρ_{GD} ; E_0 - detonation energy at infinite volume, f -force ($f = nRT$), σ - standard deviation, MAPE – mean absolute percentage

error calculated by equation $MAPE = \frac{1}{n} \sum \frac{|x_i - y_i|}{x_i} \cdot 100$, r – correlation coefficient; a) in the case of detonation Q represents heat of detonation at the CJ point, while in the case of constant volume explosion Q is explosion heat, b) in the case of detonation p is pressure at the CJ point, while in the case of constant volume explosion p is maximum pressure.

The data from Table 3 shows that ΔV_T correlates the best with Q and V_0 calculated using a constant volume explosion module, while the worst correlation exists with detonation heat at theoretical maximum density. This suggests that the correlation should be done using the values Q and V_0 at the actual density of the explosive charge. The effect of charge density is also manifested in the fact that the fitting constant a_0 in the relationship $\Delta V_T = a_0 Q$ and $\Delta V_T = a_0 Q V_0$ changes for 8.4% and 5.2% respectively, when the density changes from ρ_{TMD} to ρ_{GD} . At the same time the fitting constants in relationship $\Delta V_T = a_0 Q V_0^{0.5}$ differ only 1.1%. This will be commented in more detail below.

In the second part of the correlation analysis, the ΔV_T values for 51 non-ideal explosives (AN-based, aluminized, and other slightly non-ideal high explosives) are correlated with $Q V_0^{0.5}$, $Q V_0$, Q , E_0 , and f , which were previously found to correlate very well with ΔV_T values for ideal explosives. The statistical parameters of the correlation analysis for different types of explosives are summarized in Table 4, while the comparison of calculated and experimental ΔV_T values is given in Fig. 2.

Table 4

Statistical parameters of correlation analysis for ideal and non-ideal explosives.

Parameter	Method	Ideal explosives			Non-ideal explosives			All explosives		
		a_0	σ/cm^3	r	a_0	σ/cm^3	r	a_0	σ/cm^3	r
$Q V_0^{0.5}/(\text{MJ} \cdot \text{kg}^{-1})(\text{L} \cdot \text{kg}^{-1})^{0.5}$	CJD at ρ_{GD}	3.073	43.25	0.9235	3.066	56.87	0.6947	3.072	48.21	0.8886
	CVE at ρ_{GD}	3.086	42.00	0.9271	3.081	52.74	0.7580	3.095	45.81	0.9035
$Q V_0/(\text{MJ} \cdot \text{kg}^{-1})(\text{L} \cdot \text{kg}^{-1})$	CJD at ρ_{GD}	0.1089	48.74	0.9011	0.104	64.61	0.6272	0.108	54.96	0.8583
	CVE at ρ_{GD}	0.1068	50.42	0.8971	0.104	56.47	0.7345	0.107	50.42	0.8971
$Q/(\text{MJ} \cdot \text{kg}^{-1})$	CJD at ρ_{GD}	86.07	45.39	0.9203	88.1	61.75	0.6754	86.49	51.61	0.8712
	CVE at ρ_{GD}	88.40	42.56	0.9249	89.4	60.50	0.7063	89.40	49.62	0.8881
$f/(\text{MJ} \cdot \text{kg}^{-1})$	CJD at ρ_{GD}	373.8	54.20	0.8854	364.3	60.38	0.5840	371.7	56.57	0.8427
	CVE at ρ_{GD}	408.3	51.34	0.8948	405.9	52.10	0.7064	407.8	51.80	0.8694
$E_0/(\text{MJ} \cdot \text{kg}^{-1})$	CJD at ρ_{GD}	81.44	44.51	0.9184	78.73	73.57	0.5622	80.77	55.85	0.8494

One may note from Table 4 that the fitting constants a have almost the same value for ideal and non-ideal explosives, while the correlation coefficient is lower, and the scattering of results is significantly higher for non-ideal explosives ($\sigma = 42\text{--}54 \text{ cm}^3$ for ideal and $\sigma = 52\text{--}74 \text{ cm}^3$ for non-ideal). Since most of the non-ideal explosives

studied belong to the group of AN-based commercial explosives, a large scattering can be partly attributed to differences in the properties of ingredients (AN prills, fuel oil, etc.) used by different manufacturers.

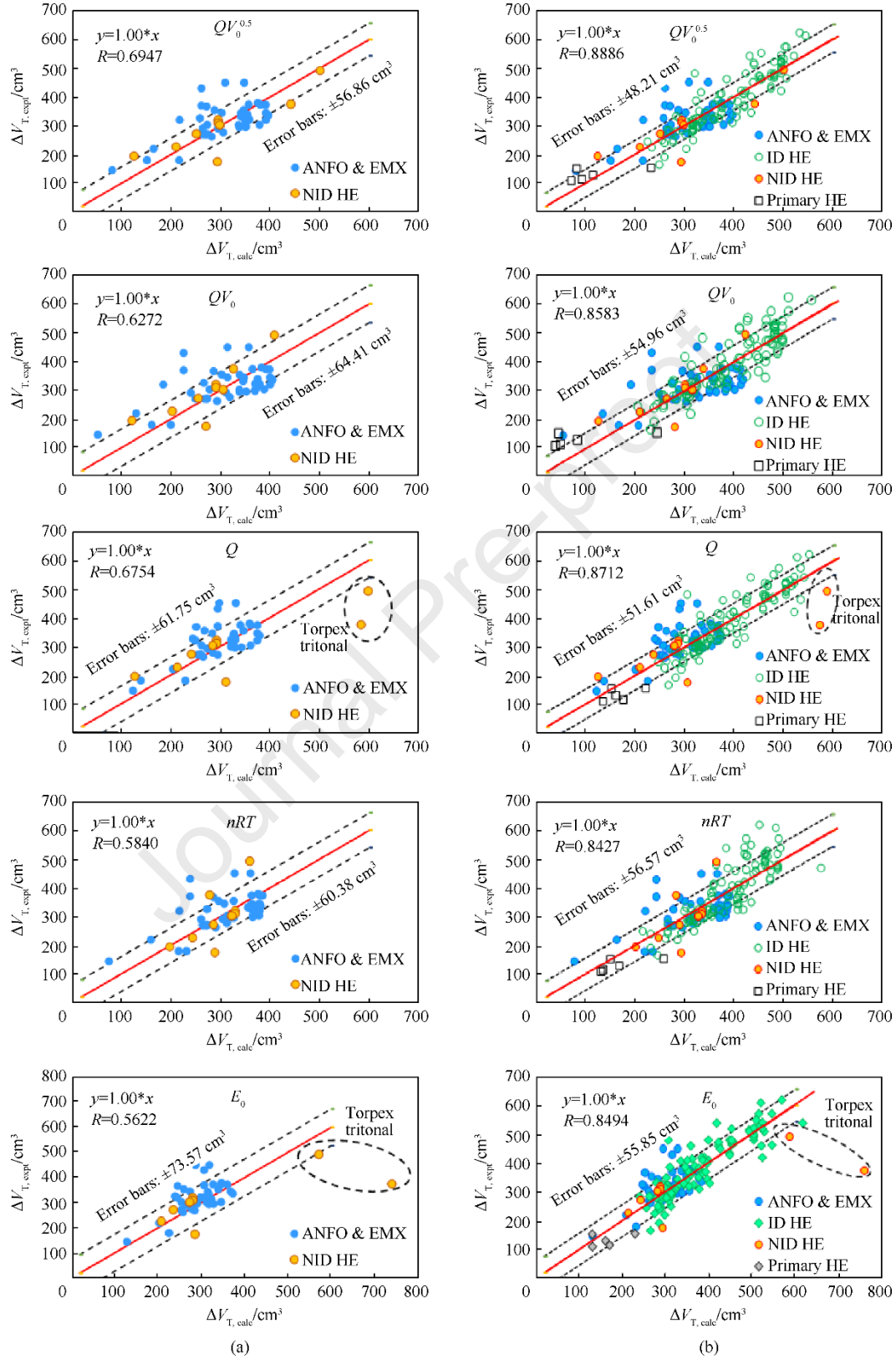


Fig. 2. Comparison of calculated and experimental cavity volume expansion for (a) non-ideal and (b) for all studied explosives. (Note: ID HE – ideal explosive, NID HE-non-ideal explosive, Primary HE – primary explosives, error bars

represent standard deviation).

A large scattering of results for low-velocity detonating explosives was also reported by Afanasenkov [6], who attributed it to the non-ideal behaviour of such explosives. The author even thinks that the Trauzl test is not applicable to low-sensitive ANFO and emulsion explosives since they have large critical diameters, so the steady-state detonation cannot be reached in small charges used in the test. For non-ideal ANFO and emulsion explosives correlation between ΔV_T and the quantity $QV_0^{0.5}$ is significantly poorer than for the ideal high explosives ($r = 0.758$, $\sigma = 52.7 \text{ cm}^3$, calculated using the constant volume explosion module). However, according to Evans' [21] recommendation regarding the strength of the correlation, $r = 0.758$ indicates existence of a strong correlation between ΔV_T and $QV_0^{0.5}$. Such strong correlation may point to the conclusion that the decomposition of these explosives into gaseous products (and the release of heat energy) is completed before the sand and products are discharged from the cavity. However, it is quite certain that the rates of reactions, the dynamics of pressure rise, and the rate of heat energy release, are different in the case of ideal and highly non-ideal explosives. This will be analysed later using hydro-code simulation (Subsection 3.4).

It is important to note that $\Delta V_T - Q$ and $\Delta V_T - E_0$ correlations are not applicable for explosives containing large amount of aluminium (e.g., Torpex and Tritonal) – a large heat of detonation of such explosives does not correspond to a proportionally large volume of the cavity. However, $\Delta V_T - QV_0$ and $\Delta V_T - QV_0^{0.5}$ correlations give satisfactory results for these explosives as well.

3.3. Effect of density on heat of detonation and volume of detonation products

The detonation parameters, including Q and V_0 , change with explosive density. However, change of Q and V_0 with density does not follow the same rule for all explosives. For example, in the case of explosives having a positive oxygen balance (OB), Q and V_0 do not change with density, for explosives having slightly negative OB (e.g., ANFO, PETN, etc.), Q increases slightly with density, while V_0 decreases. In the case of explosives that have a very negative OB (below -45%), Q increases up to 20% with density while V_0 decreases up to 25% (e.g., TNT, PA, etc.) when density changes from ρ_{GD} to ρ_{TMD} . With that in mind, it is clear that the density of explosive charge in the Trauzl test must be considered when performing the correlation analysis.

The change in Q and V_0 with density is related to the fact that the detonation pressure and temperature change with explosive density, which in turn affects the composition of the detonation products and, consequently, the values of Q and V_0 . Generally, a higher density results in a higher detonation pressure, which favors the formation of more C(s) and CO_2 . The increase in CO_2 and C(s) results in an increase in Q and a decrease in V_0 . To determine the impact of density on Q and V_0 (and thus on the $\Delta V_T - QV_0$ correlation), the detonation parameters are calculated at two densities, ρ_{GD} and ρ_{TMD} , for a series of explosives. The comparison of Q and V_0 for these two densities is given in Fig. 3.

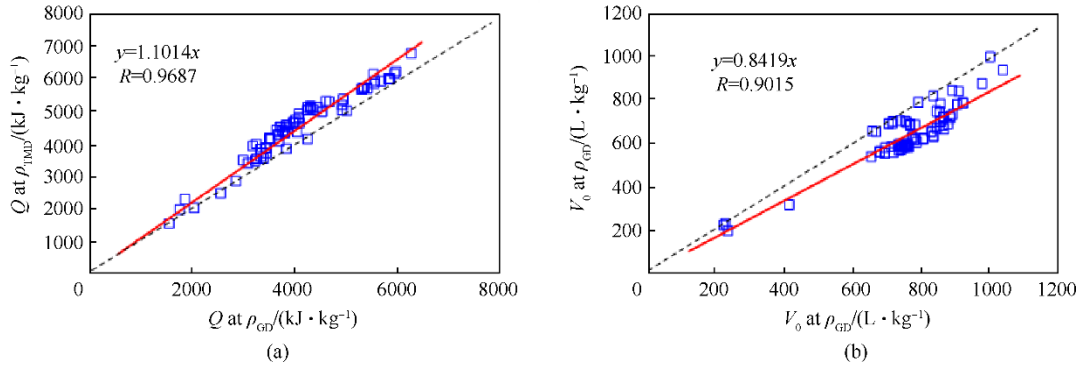


Fig. 3. Comparison of calculated (a) heats of detonation and (b) volume of detonation products at gravimetric and theoretical maximum densities.

The mean value of the heat of detonation of explosives studied increases by 10%, while the volume of detonation products decreases by 16% when the density increases from ρ_{GD} to ρ_{TMD} . At the same time, the fitting constant a_0 in $\Delta V_T = a_0 Q$ changes by 8.4%. For the sake of illustration, this means that ΔV_T value predicted using $\Delta V_T = a_0 Q$ correlation and the constant a_0 determined using $Q(\rho_{GD})$ values, will differ for 8.4% (approximately 25 cm^3 in the case of TNT) if one use $Q(\rho_{TMD})$ instead of $Q(\rho_{GD})$. The fitting constants a_0 in relationship $\Delta V_T = a_0 Q V_0^{0.5}$ differ only 1.1% when density changes from ρ_{TMD} and ρ_{GD} . This is related to the fact that Q increases while V_0 decreases with increasing density, which ultimately results in almost the same value of a_0 for both densities. This is not the case for the ΔV_T - $Q V_0$ correlation (the difference is 5.2%), although the constant a_0 varies less than in the case of the ΔV_T - Q correlation. The above means that in ΔV_T - $a Q V_0^{0.5}$ correlation, Q and V_0 can be calculated either at ρ_{GD} to ρ_{TMD} with an error of 1.1%.

3.4. AUTODYN simulation

To get a more detailed insight into the dynamics of the interaction between the detonation products and the lead block, as well as the dependence of the Trauzl test results on density of explosive charge and rate of explosive decomposition, the numerical simulation of the Trauzl test is performed using the AUTODYN hydro-code. The simulation is carried out using 2D axisymmetric Euler formulation (Fig. 4). The size of the element (axial $\times$ radial) was 1×1 mm for all calculations. The lead block is modelled using the material properties of lead taken from the AUTODYN material library [26]. The dynamic behaviour of lead was modelled using the von Mises strength model ($G_s = 11.13$ GPa, $\sigma_y = 30$ MPa) and Shock EOS ($\rho_0 = 11.43$ g/cm^3 , $\gamma = 2.0$, $S = 2.09$ $\text{mm}/\mu\text{s}$, $C_0 = 1.452$). The material properties of sand are taken from the AUTODYN material library, where dynamic properties are modelled by the MO Granular strength model, Hydro (P_{min}) failure model, and Compaction EOS.

The explosive charges are initiated by 1 g PETN detonator. The parameters in the Jones-Wilkins-Lee EOS (JWL parameters) for PETN detonator (1.5 g/cm^3 density) are taken from the AUTODYN built-in material library. Moving gauges are placed within the explosive charge and lead block to register the pressure and displacement of material in the individual elements.

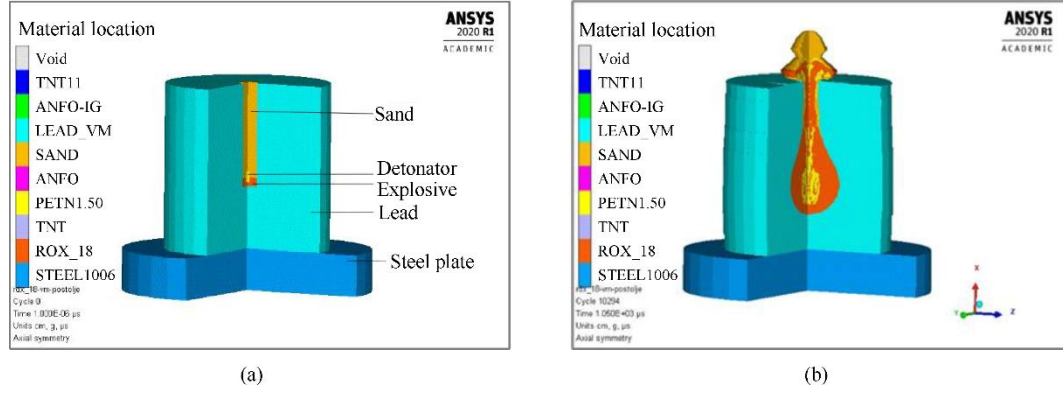


Fig. 4. AUTODYN numerical model of Trauzl lead block test: (a) Before and (b) after detonation of explosive charge.

The increase in cavity volume is determined in the following way. From the image of the longitudinal cross section of the block, taken at the end of the cavity expansion, axial and radial positions of the lead/detonation products interface are determined at about 50 sections along the cavity height. This is done using open-source Engauge Digitiser Software [22]. The volume of the cavity was calculated as the sum of volumes of individual sections, where the shape of the sections is approximated by a truncated cone.

To validate the model, we compared the calculated cavity volume increase produced by TNT charge ($\rho_0 = 1.1 \text{ g/cm}^3$) with those obtained experimentally. The parameters in the Jones-Wilkins-Lee EOS for TNT are calculated by EXPLO5 code ($A = 156.450 \text{ GPa}$, $B = 3.123 \text{ GPa}$, $R_1 = 4.4746$, $R_2 = 1.0448$, $\omega = 0.3146$, $D = 5.4 \text{ km/s}$, $p = 8.4 \text{ GPa}$, $E_0 = 4.26 \text{ kJ/cm}^3$). The calculated increase in the volume of the cavity of TNT ($\rho_0 = 1.1 \text{ g/cm}^3$) is 20% smaller than experimentally determined, which is mainly related to the EOS and the dynamic properties of lead and sand used in the simulation. To obtain ΔV_T values equal to those determined experimentally, the calculated ΔV_T is multiplied by the correction factor k_f that represents the relationship between the calculated and the volume of the experimental cavity volume for TNT ($\Delta V_{T \text{ corrected}} = k_f \Delta V_{T \text{ calculated}}$, where $k_f = 300/249 = 1.20$). The correction factor thus determined is applied in all calculations to obtain true cavity volume increase.

3.4.1. Effect of charge density

The effect of charge density on cavity volume increases is analysed using an RDX explosive. The loading density of the RDX charges is varied between 1.8 g/cm^3 and 0.25 g/cm^3 . RDX is modelled by the JWL model, where the detonation parameters and the JWL coefficients of RDX are calculated using the EXPLO5 code [23]. The constant weight of 10 g of explosive charge is used. Charge size was calculated based on loading density and constant weight, taking into account the recess for the detonator (Table 5). The pressure and radial displacement are recorded by the gauges located in the lead block and the explosive charge, near the lead/explosive charge interface, at a height corresponding to half of the charge height. The results of the simulations are summarised in Fig. 5 and Table 5.

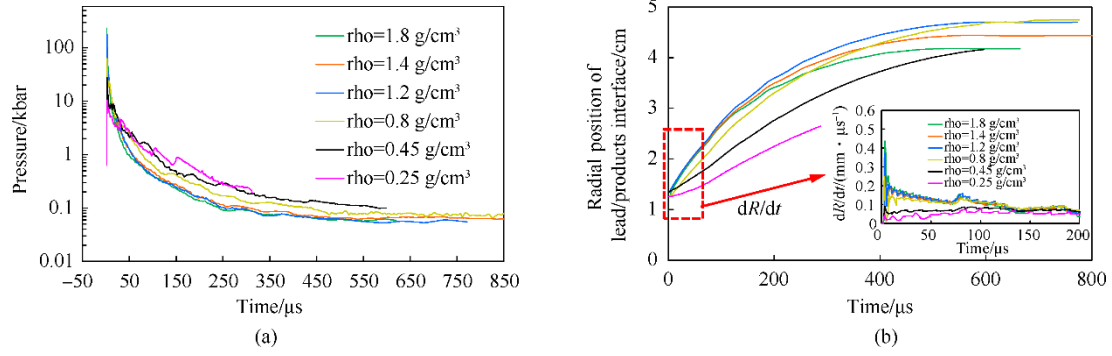


Fig. 5. (a) Pressure-time profile in explosive charge and (b) radial displacement of interface-time for RDX charges as a function of charge loading density.

A rapid pressure jump upon the initiation of explosive charge (Fig. 5(a)), which lasts less than 5 μ s, give rise to a radial acceleration and formation of a shock wave in the lead block. The detonation products expand and plastically deform the lead block. At the same time, part of the energy of the products is spent on heating the lead, a part is spent on giving the velocity of the sand, and a part is lost with the detonation products discharged from the cavity. An increase in the density of explosive charge results in an increase in detonation pressure (Table 5), which in turn leads to a faster increase in the cavity volume at the initial stage, which can be concluded from the slope of radial displacement -time curves (Fig. 5(b)). The effect of the charge density on pressure-time and radial displacement-time curves is clearly visible for densities between 0.25 g/cm³ and 1.2 g/cm³, however an increase of density above 1.2 g/cm³ does not result in a substantial change of pressure-time curves profiles and all the curves are overlapping after initial pressure jump.

For illustration, the time to reach pressure of 200 bar decreases monotonically from 320 to 200 μ s when density changes from 0.25 to 1.2 g/cm³, however for densities between 1.2 and 1.8 g/cm³ it changes only slightly; from 160 to 170 μ s. After approximately 600–700 μ s pressure drops below 100 bar (for $\rho_0 = 0.25$ g/cm³), and 60 bar for $\rho_0 \geq 1.2$ g/cm³ and can no longer deform the lead block.

Table 5

Effect of RDX charge density on the Trauzl test results (charge mass = 10 g).

Density of charge/(g·cm ⁻³)	Detonation pressure/GPa ^(a)	Height of charge/mm	$\Delta V_{TAD}/\text{cm}^3$	R_{max}/mm	$t(R_{max})/\mu\text{s}$	$t_{sand}/\mu\text{s}$	$t_{gas}/\mu\text{s}$
0.25	1.0	75	353	27	>330	90	280
0.45	2.3	44	515	42	>600	130	520
0.60	3.7	33	579	45	680	130	615
0.80	6.3	25	557	47	705	135	760
1.00	9.7	20	504	46	635	135	810
1.20	14.7	16	444	47	610	135	880
1.40	19.9	14	438	44	540	135	870
1.80	34.0	11	416	44	530	135	915

Note: (a) Chapman-Jouguet pressure calculated using the EXPLO5 code, $\Delta V_{r,AD}$ – calculated increase in cavity volume, R_{max} – maximum radial displacement of explosive charge/lead interface in the middle of charge height, $t(R_{max})$ – time at which the maximum displacement was achieved, t_{sand} – time at which the ejection of sand from the cavity begins, t_{gas} – time at which the ejection of products from the cavity begins.

Fig. 5 shows that in the initial stage of interaction of the detonation products and the lead block, for $\rho_0 = 1.8$, 1.2, and 0.8 g/cm³ the initial velocity of the interface jumps to 640, 570, and 250 m/s, respectively, and after 3–5 μ s it drops below 300 m/s. For $\rho_0 = 0.45$ and 0.25 g/cm³ (i.e., $p_{Cl} = 2.3$ and 1.0 GPa) initial interface velocity is below 85 m/s and does not change significantly until 300 μ s, after which it slowly decreases. Such behaviour of higher density charges favours Backofen's two-step detonation-driven propulsion model [24,25], which assumes that the initial motion (first stage) is related to a brisant shock-dominated process while the subsequent motion (second stage, gas-push stage) is related to the action of expanding products which push the lead block/products interface. However, since the first stage lasts a short time, the interface does not travel long distance, and most of the deformation of the lead block is done by expanding detonation products in later stage, which lasts much longer (roughly 400–700 μ s, depending on the charge density). The initial jumpwise interface velocity increase is not pronounced for the charges having lower densities (i.e., for lower detonation pressures) and the deformation of the lead block is entirely related to expansion of the detonation products.

The simulation has also shown that the charge height plays a role when considering the effect of charge density. When the constant charge weight approach is used to model the Trauzl test, then a decrease in the charge density results in an increase in charge height and in the surface of the cavity on which the pressure acts. Because of that, the amount of stemming material decreases, and ejection time decreases (which means that more energy of detonation products is lost with) with a decrease of charge density. This results in different shapes of the cavities obtained with different charge densities (and sizes) (Fig. 6), which is especially evident with charge having a density of 0.25 g/cm³.

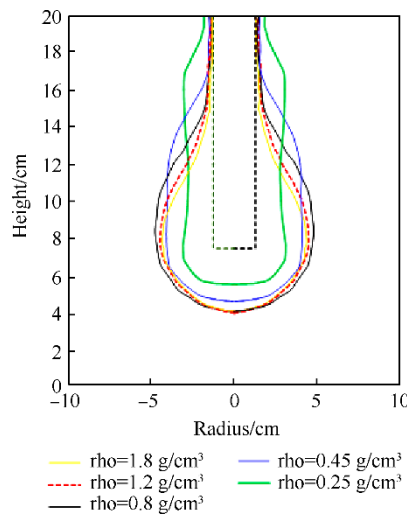


Fig. 6. Shapes of cavity cross section at different RDX charge densities.

It is interesting that the highest ΔV_T value was not obtained for $\rho_0 = 1.8 \text{ g/cm}^3$ (as one might expect) but for $\rho_0 = 0.8 \text{ g/cm}^3$ (557 cm^3). This means that in addition to the detonation pressure (i.e., brisance of explosive) other factors also affect the increase in the cavity volume (e.g., charge size, dynamics of interaction of gas products and lead block, etc.).

The impact of the charge density on the Trauzl test results is also analysed using a constant charge volume approach (10 cm^3) and it turned out that density plays an important role in this case as well. However, in the case of constant charge volume, ΔV_T decreases with density (since the charge mass and detonation pressure decrease too), whereby this change is less pronounced (maximum and minimum values of ΔV_T in the case of RDX differ about 8.3% if density changes from 0.6 to 1.8 g/cm^3). It should be noted that the explosive charges were initiated by 1 g PETN detonator, so the mass of the detonator's explosive charge significantly affects the results for lower charge densities, where the fraction of PETN goes over 10% of the total mass of the explosive (RDX + PETN).

Table 6

Effect of RDX charge density on the Trauzl test results (charge volume = 10 cm^3).

Density of charge/ $(\text{g}\cdot\text{cm}^{-3})$	Detonation pressure/GPa	Mass of charge/g	$\Delta V_{T,AD}/\text{cm}^3$	$R_{\text{max}}/\text{mmt}$	$R_{\text{max}}/(\mu\text{s})$	$t_{\text{sand}}/\mu\text{s}$	$t_{\text{gas}}/\mu\text{s}$
0.6	3.7	6.0	477	45	640	135	780
0.8	6.3	8.0	497	46	640	135	790
1	9.7	10.0	504	46	635	135	810
1.2	14.7	12.0	506	46	630	135	820
1.4	19.9	14.0	517	47	640	135	815
1.8	34	18.0	520	48	650	135	815

3.4.2. Effect of the reaction rate

The impact of the rate of conversion of explosives into products (reaction rate) on the pressure-time history in the Trauzl test is simulated on non-ideal explosive ANFO using AUTODYN. The rate of reactions is described by two terms Lee-Tarver Ignition and Growth (I&G) model [26].

$$\frac{\partial F}{\partial t} = I(1 - F)^b(\mu - a)^x + G(1 - F)^c F^d p^y \quad (5)$$

where F is the reacted fraction (or conversion), p is the pressure, $\mu = [\rho/(\rho_0 - 1)]$ is the compression and I, a, b, c, d, x, y, G are constants.

The equations of state, detonation properties, and rate constants for ANFO are taken from Ref. [27]. The dynamic behaviour of ANFO was modelled using the von Mises strength model ($G_s = 0.3 \text{ GPa}$, $\sigma_y = 0.03 \text{ GPa}$) and JWL EOS ($A = 1454.25 \text{ GPa}$, $B = -0.347 \text{ GPa}$, $R_1 = 21.8866$, $R_2 = 0.7874$, $\omega = 3.4613$, $E_0 = -0.1549 \text{ kJ/cm}^3$). Different conversion rates for simulation purposes are obtained by changing the constant G in Eq. (5), while other constants were kept unchanged. For comparison, the simulation results for ideal explosive PETN are also given. PETN is modelled by the I&G model, where the constants in the model are taken from the AUTODYN library for PETN ($\rho_0 =$

1.75 g/cm³). The results of simulations are summarised in Fig. 7 and Table 7. The dynamic behaviour of PETN was modelled using the von Mises strength model ($G_s = 4.7$ GPa, $\sigma_y = 0.2$ GPa) and JWL EOS ($A = 3745.999$ GPa, $B = -131.30$ GPa, $R_1 = 7.2$, $R_2 = 3.6$, $\omega = 1.173$, $E_0 = 0.0661$ kJ/cm³).

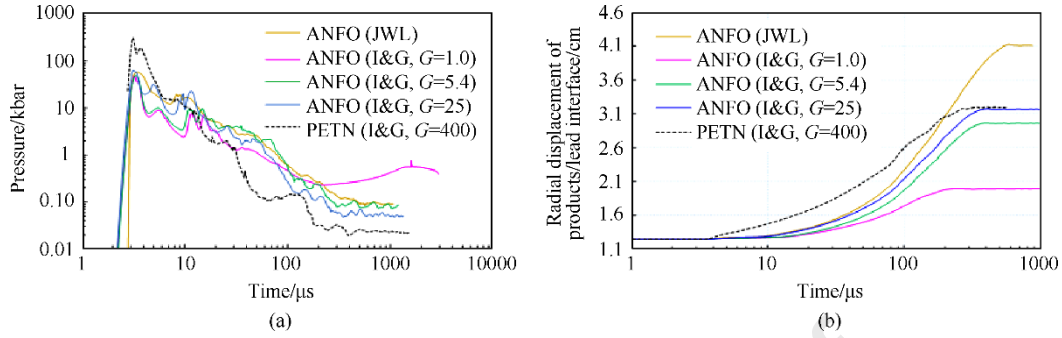


Fig. 7. (a) Pressure-time and (b) radial displacement-time profiles for ANFO charges as a function of reaction rate

Table 7

Effect of reaction rate on Trauzl test results.

Explosive	Density of charge/(g·cm ⁻³)	Calculation model	Constant $G/(\mu\text{s}^{-1}\cdot\text{Mbar}^{-\gamma})$	dF/dt at $F = 0.5/\mu\text{s}^{-1}$	$t_{\text{CRZ}}/\mu\text{s}$	$\Delta V_{\text{TAD}}/\text{cm}^3$	R_{max}/mm	$t(R_{\text{max}})/\mu\text{s}$	$t_{\text{sand}}/\mu\text{s}$	$t_{\text{gas}}/\mu\text{s}$
ANFO	0.8	JWL model	-	-	-	398	41	570	145	960
		I&G model	25	5.9×10^{-1}	3	207	32	410	190	1250
			5.4	3.3×10^{-2}	55	157	30	400	200	1800
			1.0	5.2×10^{-4}	1960	32	19	255	290	2900
PETN	1.75	I&G model	400	1.7×10^1	0.2	198	34	405	140	1500

Note: The values of reaction rate constants in the I&G model: $l = 10 \mu\text{s}^{-1}$, $a = 0.2$, $b = 0.222$, $x = 4$, $G = 5.4 \mu\text{s}^{-1}\cdot\text{Mbar}^{-\gamma}$, $c = 0.222$, $d = 0.666$, $\gamma = 0.9$, and $F_{\text{igmax}} = 0.3$, reproduce experimental detonation velocity – charge diameter data [27]. Values $G = 25 \mu\text{s}^{-1}\cdot\text{Mbar}^{-\gamma}$ and $G = 1.0 \mu\text{s}^{-1}\cdot\text{Mbar}^{-\gamma}$ are arbitrary chosen to obtain higher and lower reaction rates in the simulation; dF/dt is the rate of reaction at $F = 0.5$ (it is given just for rough estimation of reaction rates at different value of G , t_{CRZ} is the duration time of reactions (values of t_{CRZ} and dF/dt are recorded by the gauge located near explosive/lead interface, at half of the charge height)

As can be seen from Fig. 7, after an initial pressure jump related to the shock wave impact on the adjacent material, the pressure decreases while the radial displacement of the interface (i.e., cavity volume) increases. In fact, two processes are taking place with opposite effects on the pressure – one is the cavity volume increase, which tends to decrease the pressure, and another is gas generation in chemical reactions, which tends to increase pressure. The pressure-time profile will depend on the rates of these two processes. For example, when the reaction rate is higher (e.g., for $G = 25 \mu\text{s}^{-1}\cdot\text{Mbar}^{-\gamma}$), production of gaseous detonation products is faster (for the mentioned G , all explosive is converted in products in 3 μs), the cavity volume increases faster, and consequently pressure drops faster. The opposite of that, when the reactions rate is lower (e.g., for $G = 1 \mu\text{s}^{-1}\cdot\text{Mbar}^{-\gamma}$) it will take longer for the reactions to complete ($t_{\text{CRZ}} = 1960 \mu\text{s}$) and gas generation in the reactions will take longer. As a result of that, the cavity volume increases slower, and pressure remains higher and even increases during the time near

the end of the reactions (at 1960 μs)

The simulation has shown that for the same explosive ΔV_T increases when the rate of reaction increases; from 32 cm^3 at $G = 1 \mu\text{s}^{-1} \cdot \text{Mbar}^\gamma$ to 207 cm^3 at $G = 25 \mu\text{s}^{-1} \cdot \text{Mbar}^\gamma$. This raises the question of whether it is possible to compare the Trauzl test results, i.e., the strength of explosives, if the reaction rates of explosives are very different. Marshal [3], who wrote about this issue back in 2017, claimed that all test methods for determination of explosive strength do not consider an important factor: the time required for pressure growth to its maximum value. He even suggested that the Trauzl test can only give satisfactory comparative results for the same class of explosive, i.e., for explosives which behave in the same manner. In the Trauzl test, a part of energy of the detonation products is spent to deform the lead block, a part is spent on heating the lead, a part is spent on giving the velocity of the sand, and a part is lost with the detonation products discharged from the cavity. It seems very likely that by changing the rate of the reaction, fractions of energy spent on individual kinds of work are changing too, which ultimately results in different ΔV_T .

We noticed that for both ANFO and PETN the value of ΔV_T calculated using JWL model are much higher than the value calculated using I&G model, even using the same EOS of detonation products and very high reaction rates. Possible reasons for this could be the following: a) I&G model considers von Neuman spike while the JWL model neglects it and as the consequence I&G model predicts about 35% higher initial pressure jump, faster initial increase of the cavity volume, and faster pressure decrease - which ultimately results in lower ΔV_T , b) the JWL model assumes the steady-state detonation upon the initiation while the I&G model considers shock-initiation process which results in lower detonation velocity in small explosive charge used in Trauzl test, c) inadequate reaction rate model, d) inadequate EOS and strength model of unreacted explosive.

It is also important to note that for $G = 5.4 \mu\text{s}^{-1} \cdot \text{Mbar}^\gamma$ conversion of ANFO to products takes 55 μs (at a gauge position), the maximum radial displacement is achieved after 398 μs , and the escape of detonation products from the cavity starts after 1800 μs (Table 7, Fig. 7). This means that in the Trauzl test, ANFO completely reacts before the maximum volume of the cavity is reached, and much earlier than the products are discharged from the cavity. In other words, all energy of ANFO has been released, and this explains the fact that $\Delta V_T - QV_0$ correlation for ANFO gives satisfactory results (Fig. 8). However, in the case of rather slow reactions, when an explosive cannot completely react before products start to escape from the cavity, the fraction of explosive will remain unreacted, and the correlation will be poorer.

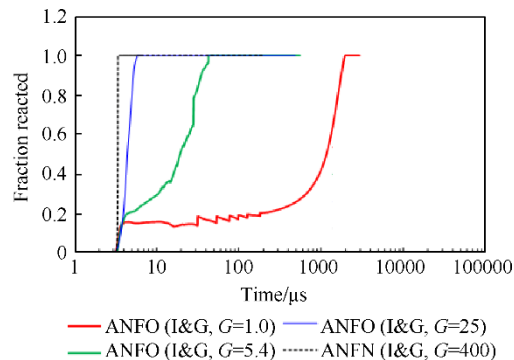


Fig. 8. Fraction reacted vs. time profiles for ANFO charges as a function of reaction rate constant G .

The simulation has shown that more brisant explosives (higher p_{CL} , faster detonation velocity, and faster decomposition reactions) produce two distinct effects on the lead block, the initial brisant effect and the second gas-push effect. The brisant effect decreases with a decrease in explosive density and with a decrease in reaction rate. The result is that for the same explosive with different reaction rates (e.g., when a size of glass micro-balloons in emulsion explosives changes) Trauzl test result will be different. This brings us to Marshall's claim [3]: "Lead block tests can only claim to give satisfactory comparative results when they are performed with the same class of high explosive. If there are great differences in the speed with which the pressure develops, the results are no longer comparable". The presented simulation shows that the same explosive with different reaction rates produces different ΔV_T values. This could explain to some extent the fact that ΔV_T values for EMX (Table 1) differ by about 100 cm³ (i.e., 35%), although systematic experimental research on the influence of charge density and the rate of decomposition on Trauzl test results should be done for a reliable conclusion.

4. Conclusions

In this work we revisited the correlation between the Trauzl lead block test results and the detonation parameters and analysed the effect of the explosive charge density and the rate of conversion of unreacted explosives into detonation products on the test results and dynamics of interaction between the products and the lead block.

(1) The results of the correlation analysis confirmed that the results of the Trauzl test strongly correlate with the heat of the detonation and the volume of the detonation products. It was found that the product $QV_0^{0.5}$, with Q and V_0 calculated with the constant volume explosion method, correlates the best with ΔV_T for a range of tested explosives. Based on this correlation, ΔV_T for studied ideal explosives can be predicted with $r = 0.9271$, $\sigma = 42.0$ cm³, and MAPE = 9.32%, and $r = 0.7580$, $\sigma = 52.74$ cm³, and MAPE=14.52% for non-ideal explosives. Compared to the experimental error, this error is more than two times higher.

(2) It was demonstrated that the heat of detonation and the volume of detonation products of most explosives change with their density, and therefore the detonation heat used in the correlation analysis must be calculated/determined at the actual charge density. It is recommended that the charge density be indicated with the Trauzl test result.

(3) AUTODYN simulations showed that the density of explosive charge has a significant impact on the Trauzl test results when a constant sample mass approach is used. The effect of density can be related to the fact that a change in density results in a change in the detonation pressure, which in turn changes the dynamics of the interaction between the lead block and the detonation products, and ultimately the resulting increase of the cavity volume. The simulation has confirmed the existence of an initial short-term shock-dominated process (brisance) for higher density charges, followed by the subsequent expansion of the detonation products and deformation of

the lead block, which is consistent with the two steps detonation-driven propulsion model of Backofen. However, regardless of the charge density, the cavity volume increase is predominantly a result of the action of expanding detonation products, which push the lead block/detonation product interface.)

(4) The simulation also shed some light on the behaviour of non-ideal explosives and impact of the rate of conversion of explosives to detonation products on the Trauzl test results. The conversion of non-ideal ANFO explosive into detonation products takes place after the CJ point is reached and is finished completely before the maximum radial expansion was reached and before the products started to flow out of the cavity. The cavity volume increases, and the product ejection time decreases with increasing reaction rate. The duration of reactions in ANFO explosives is several hundred times longer than that in ideal explosives.

(5) The simulation implies the conclusion that a reliable comparative analysis of the results of the Trauzl test for very different classes of explosives is questionable, considering the significant influence of the reaction rate on the dynamics of the interaction between the detonation products and the lead block and consequently on the result of the Trauzl test.

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Declaration of interests

☒ The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

☐ The authors declare the following financial interests/personal relationships which may be considered as potential competing interests:

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