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An Answer to the Question about the Energetic Performance of TKX-50

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Dedicated to Dr. Vladimir K. Golubev

Abstract: Some of the relevant detonation performance parameters of TKX-50 were re-determined. The enthalpy of formation was obtained from the measured heat of combustion to be $\Delta H°_f$ (TKX-50(s)) = +213.4 ± 1.2 kJ mol^{-1}. The heat of detonation was measured to be 4650 ± 50 kJ kg^{-1}. The detonation velocity of a TKX-50/wax mixture (97 : 3) at a density of 1.74 g cm^{-3} was found experimentally to be 9190 m s^{-1}. Using the experimentally obtained enthalpy of formation for TKX-50 of +213.4 kJ mol^{-1} and the experimentally determined solid-state density at room temperature of 1.887 g cm^{-3} (TMD), the computed performance parameters for TKX-50 at its theoretical maximum density at room temperature was calculated to be as follows: VoD = 9642 m s^{-1}, $p_{C\text{-}J}$ = 37.0 GPa and Q_{det} = 4770 kJ kg^{-1}.

Keywords: TKX-50 · Detonation parameters · Gurney Energy · EXPLO5 calculations · Detonation velocity

1 Introduction

Dihydroxylammonium 5,5′-bitetrazole-1,1′-dioxide (TKX-50), is one of the most exciting new energetic materials to have been developed in recent years. Due to its properties, TKX-50 shows great promise for future application as a secondary explosive in modern weapon systems. Not only does TKX-50 show low IS and FS, it also possesses high thermal stability, density, and detonation velocity. In addition, it is prepared through a facile, inexpensive synthesis, and possesses low toxicity, making it particularly attractive as a future high-performance explosive with increased safety. Although the original report of TKX-50 dates back to only 2012, such has been the large interest in this compound, that its chemical and physical properties have been intensively investigated and reported by groups from all over the world [1–4].

In a recent publication, Sinditskii et al. reported an experimentally determined enthalpy of formation for TKX-50 of +194.1 kJ mol^{-1} and a calculated detonation velocity at a density of 1.8 g cm^{-3} of 9037 m s^{-1} [5]. Graswald et al. reported a measured detonation velocity for a TKX-50/wax/graphite formulation (94.5/4.5/1) of 9020 m s^{-1} at a formulation density of 1.776 g cm^{-3} [6]. The same authors reported that a TKX-50/HTPB (85/15) PBX formulation resulted in a detonation velocity of 8120 m s^{-1}, outperforming that of the corresponding HMX formulation (7310 m s^{-1}) [6]. In another study, Gottfried et al. reported an experimentally measured (LASEM method) detonation velocity of a single crystal of TKX-50 at TMD (1.887 g cm^{-3}) of 9560 ± 280 m s^{-1} [7]. The high values consistently reported for the detonation velocity of TKX-50 prompted us to re-determine the enthalpy of formation experimentally and to measure the detonation velocity. The results are reported in this paper.

2 Experimental Section

***Caution**! TKX-50 is an energetic material and should be handled accordingly, remembering that energetic materials can show unexpected sensitivities towards various stimuli (e.g. elevated temperature). Although no hazards occurred, proper security precautions (safety glasses, face shield, earthed equipment and shoes, leather jacket, Kevlar sleeves, and earplugs) have to be worn while synthesizing and handling the described compounds.*

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2.1 Materials

Dihydroxylammonium-5,5′-bistetrazole-1,1′-diolate (TKX-50, $C_2H_8N_{10}O_4$) was synthesized according to our previously published procedure [8].

Attempts to press the crystalline TKX-50 into mechanically strong pellets were unsuccessful, therefore it was necessary to mix it with a binder. An effective solution was to incorporate 3% paraffin into the TKX-50 raw powder. Paraffin (delivered by *ROTH*, Art. No CN49.2) was dissolved in gasoline, and the solution (0.06 g paraffin in 1 cm^3 of gasoline) in the designed ratio, was added to a pre-weighed sample of TKX-50 powder. The resulting putty-like mixture was kneaded/rubbed to obtain a powdery consistency. The TKX-50/Paraffin (97/3) granulate was then left for 24 hours at ambient temperature, in order to ensure that the solvent completely evaporated Figure 1.

The compatibility of TKX-50 against Paraffin (97/3 and 95/5) was established by DTA and DSC. In both methods, Paraffin melts at 60 °C and TKX-50 decomposes at 221 °C (onset) (pure TKX-50: 221 °C). Also, the impact and friction sensitivities of a TKX-50/Paraffin 97/3 mixture were measured: IS = 18 J, FS = 240 N (pure TKX-50: IS = 18–20 J, FS = 120 N). Therefore it can be stated that TKX-50 is compatible with Paraffin and the sensitivities are lower than for pure TKX-50.

Figure 1. TKX-50/Paraffin 97/3 granulate before drying.

Figure 2. A set of pressed TKX-50/paraffin (97/3) pellets.

For the detonation velocity measurements, as well as for cylinder test (CT), the powdery samples were pressed (at 300 MPa) into cylindrical pellets of 25, 30, 40, and 50 mm diameter, Figure 2.

The heights of the 25 mm and 30 mm pellets were approximately equal to their diameters, while the pellets with a diameter of 40 or 50 mm had heights of approximately half their diameter. All of the pellets were individually weighed (accuracy of ±0.1 mg) and measured (accuracy of ±0.02 mm) in order to calculate their density. Composition, diameters and average densities of the tested charges are presented in Table 1.

The samples which were used in measurements to determine the heat of combustion and heat of detonation of TKX-50 were pressed samples consisting of pure TKX-50 with 13 mm or 25 mm diameter and masses of approximately 4.0 g and 25.0 g, respectively.

2.2 Calorimetric Measurements

2.2.1 Heat of Combustion

A cylindrical stainless-steel bomb with an internal volume of 0.35 dm^3 was the main component of the water calorimeter used for the measurements. The bomb was placed in a polished stainless-steel calorimeter bucket that held 2750 ± 0.1 g of water. The bucket was surrounded by a constant-temperature jacket, the temperature of which was maintained at 20.0 ± 0.1 °C. The thermal equivalent of the instrument, determined by burning certified samples of benzoic acid with purified oxygen at a pressure of 2.0 MPa, was found to be 12.60 ± 0.05 kJ/K. The error of ±0.40% indicates the ultimate precision of the instrument. Approximately 4.0 g samples of pressed TKX-50 (pure samples without added paraffin) were ignited with an electrically heated resistive wire and burned in the bomb, which was filled with oxygen to an initial pressure of 2.0 MPa. Three measurements were performed, and the results (in J/g), were averaged and rounded to the nearest ten.

Table 1. Composition, diameter, and average density of the tested charges of TKX-50/paraffin (97/3).

Explosive [%]	Charge diameter [mm]	Average density [g/cm^3]
TKX-50/Paraffin (97/3)	25.07	1.727 ± 0.003
	30.13	1.735 ± 0.003
	40.16	1.737 ± 0.003
	50.19	1.748 ± 0.003

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2.2.2 Heat of Detonation

Aspherical steel bomb with an internal volume of 5.6 dm^3 was the main component of the water calorimeter used for the measurements. The bomb was placed in a polished stainless-steel calorimeter bucket that held 27000 ± 1 g of water. The bucket was surrounded by a constant-temperature jacket, the temperature of which was maintained at 20.0 ± 0.1 °C. The thermal equivalent of the instrument, determined by burning certified samples of benzoic acid with purified oxygen at a pressure of 2.0 MPa, was found to be 163.7 ± 1.2 kJ/K. The error of ± 0.73 % indicates the ultimate precision of the instrument.

The 25.0 g TKX-50 charges were detonated in the calorimetric bomb which was filled with argon to a pressure of 2.0 MPa. Standard military detonators were used to instigate detonation. The detonator consisted of primary and secondary explosives enclosed in an aluminum cup with the mass of approximately 1.6 g. To estimate the energy released by the detonator, TNT charges of different masses were detonated in the argon-filled bomb. Assuming that the heat of detonation of the fuse does not depend on the mass of the TNT charge (i. e. the degree of reaction that occurs between aluminum and the detonator explosion products with the gaseous products of TNT is independent of the TNT mass), the dependence of the total heat effect on the TNT mass should be linear. This assumption enabled the heat released by the fuse to be determined as being 11.4 ± 0.45 kJ. To calculate the heat of detonation of an explosive, the difference between the measured total heat effect and the heat released by the fuse was divided by the mass of the tested charge. Three measurements were performed, and the results (J/g) were averaged and rounded to the nearest ten.

2.3 Detonation Velocity Measurements

The detonation velocity was measured using short-circuit sensors (shock collapsible sensors) manufactured from two twisted copper wires (50 μm diameter) covered with a thick layer of lacquer. Three measuring distances were used, which were approximately equal to the diameter of the tested charge. The first sensor was fixed at a distance of about 50 mm from the RDX/wax booster. The next sensors were located between consecutive pellets, Figure 3.

The sensors switch a three-channel digital timer of resolution 10 ns. The distance between sensors was measured with an accuracy of ± 0.1 mm.

2.4 Cylinder Expansion Test

A cylinder expansion test (CT) was performed in order to estimate the acceleration capability of the TKX-50/paraffin formulation. The charge was composed of ten pellets,

Figure 3. A set of test samples which were used for measuring the detonation velocity.

which were placed inside a copper tube 250 mm long with an inner diameter of 25 mm and a wall thickness of 2.5 mm. The copper tube was placed at a distance of about 2.7 m from the X-ray impulse source and at a distance of 0.5 m from the film cassette, Figure 4.

The expansion of the tube, which is driven by the detonation products, was recorded using a SANDIFLASH X-ray apparatus. An image was recorded when the detonation front was 15 mm from the end of the charge. One test was performed for a charge having an average density of 1.750 ± 0.003 g/cm^3. The detonation velocity of the charge was simultaneously measured using short circuit sensors. The measuring distance was 130 mm long. After scanning the X-ray image showing the shape of the expanded tube, the position of the points on the profile of the outer surface of the tube was measured (using an appropriate graphic program) and the dependence of the outer radius of the tube on the axial coordinate was obtained. The results were then scaled to real values, as the X-ray image was enlarged. For further analysis, the range of the axial coordinate from the cross-section with the sensor triggering the X-ray source to the cross-section in which the tube volume was 10 times greater than the initial volume was selected.

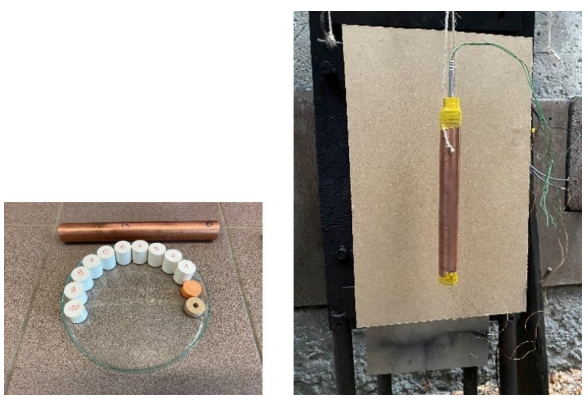

Figure 4. Pellets of the tested explosive, RDX booster, copper tube and the pre-test assembly used to perform the CT.

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2.5 Calculations

The calculations were carried out with the EXPLO5 computer code, version V6.06.01 [9], and the Cheetah 2.0 code [10] using the BKWS product database [11].

3 Results and Discussion

3.1 Heat of Combustion Results and Enthalpy of Formation

Table 2 summarizes the measured individual heats of combustion ($Q_{exp.}$) for the three charges of pure TKX-50. The average result equals to -9130 ± 50 J/g, so that the molar heat of combustion (Q_M) is 2156 ± 12 kJ/mol. This value was used to calculate the molar enthalpy of formation for TKX-50 ($\Delta_f H^0$).

The enthalpy of formation of an energetic material is governed by its molecular structure. TKX-50 contains a highly endothermic 5,5′-bitetrazole moiety, however, it is also an ionic compound with high lattice energy which stabilizes its structure, i.e. reduces the enthalpy of formation. The experimentally determined value for the enthalpy of formation of TKX-50 of 213.4 kJ/mol confirms the stabilizing role that the ionic interactions play and the extensive network of hydrogen bonds that is present in this nitrogen-rich energetic salt.

Table 2. Combustion calorimetry results for TKX-50 performed under a 2 MPa oxygen atmosphere.

Explosive	$Q_{exp.}$ [J/g]	Q_M [kJ/mol]	$\Delta_f H^0$ [kJ/mol]
TKX-50	−9099 −9187 −9113	-2156 ± 12	213.4 ± 1.2

The value of $\Delta_f H^0$ was calculated from a Hess thermochemical cycle according to reaction: $C_2H_8O_4N_{10} + 2\ O_2 \rightarrow 2\ CO_2 + 4\ H_2O + 5\ N_2$, which gives: $\Delta_f H^0 = 2\times(-393.5) + 4\times(-285.8) - (-2156) - (5\times 8.314\times 298.15)/1000 = 213.4$ kJ/mol.

Table 3. Average results for the detonation calorimetry measurements which were performed under a 2 MPa argon atmosphere.

Explosive	Test No	Measured detonation heat [J/g]	Average detonation heat [J/g]
TKX-50	1	4699	4650 ± 50
	2	4602	
	3	4655	

3.2 Heat of Detonation Results

The results of the measurements undertaken to determine the heat of detonation are given in Table 3.

TKX-50 is a nitrogen-rich endothermic compound with a low oxygen and carbon content, and therefore, its detonation energy is mainly derived from its enthalpy of formation, rather than from the heat of internal combustion. Since the current investigations show that the enthalpy of formation is not particularly high, it is understandable why the heat of detonation of TKX-50 is comparable to that of TNT.

3.3 Detonation Velocity Results

Table 4 summarizes the experimentally ($D_{exp.}$) and theoretically ($D_{calc.}$) determined detonation velocities for the tested charges containing pellets of TKX-50/Paraffin with the ratio 97/3 and with diameters of 25 mm, 30 mm, 40 mm, and 50 mm. Calculations were performed using the Cheetah 2.0 code. The input data which was used were the measured charge densities, as well as the enthalpy of formation of TKX-50 which was determined in this study (213.4 kJ/mol).

As expected, the calculated detonation velocities are higher than the corresponding measured values. Furthermore, the difference between the calculated and measured values decreases as the value for the charge diameter increases. The increase in the calculated detonation velocity as a result of the increase in the charge density from 1.727 g/cm^3 to 1.748 g/cm^3 corresponds to approximately 100 m/s. This value was used to correct the dependence of the detonation velocity on the diameter of the charges, Figure 5.

The diameter of the TKX-50/Paraffin charge above which no increase in the detonation velocity is observed corresponds to values above 50 mm. However, if the effect of the changes in density is taken into account, it can be expected that this value actually corresponds to diameters of 60–65 mm.

The detonation velocity decreases linearly with the reciprocal of the charge diameter (Figure 5, below). By extrapolating this relationship to the *y* axis where the reciprocal diameter equals zero ($1/d = 0$), it is possible to determine the detonation velocity for infinitely large diame-

Table 4. Results of the measured and calculated detonation velocities.

Explosive	Diameter [mm]	Density [g/cm^3]	$D_{exp.}$ [m/s]	$D_{calc.}$ [m/s]
TKX-50/Paraffin	25	1.727	8540 ± 30	8831
	30	1.735	8660 ± 50	8867
	40	1.737	8780 ± 10	8887
	50	1.748	8870 ± 60	8933

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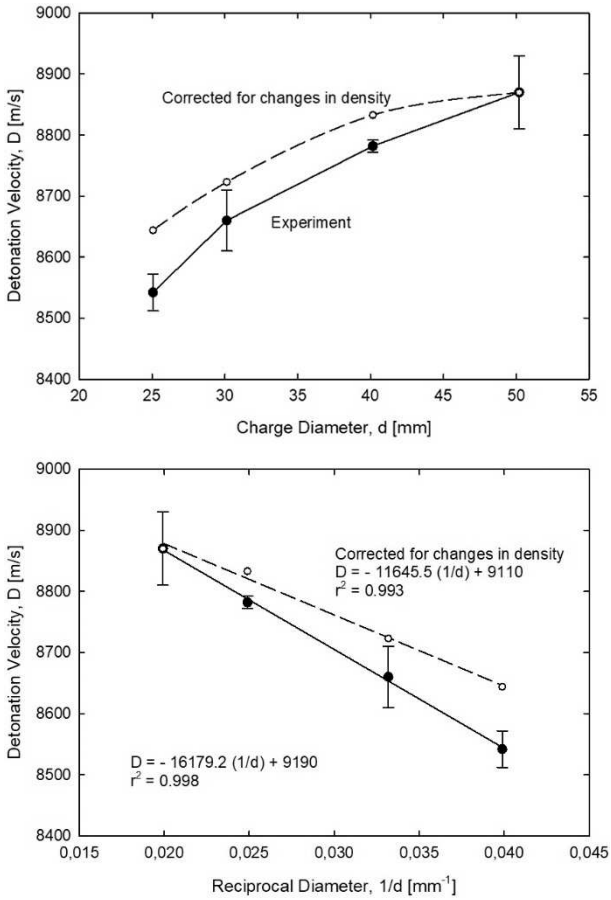

Figure 5. Plot of the detonation velocity of TKX-50/Paraffin versus the charge diameter (above), and versus the reciprocal of the charge diameter (below).

ter (D_∞). For the TKX-50/paraffin (97/3) charges with an average density of approx. 1.74 g/cm^3, this value equals 9190 m/s. After correcting the dependence due to the difference in the densities of the charges, the value is 80 m/s lower.

3.4 Cylinder Expansion Test Results

The results of the cylinder test are the detonation velocity of the tested explosive and the shape of the copper tube when the detonation front approaches the end of the charge. Figure 6 shows the X-ray image of the tube-driven by the TKX-50/Paraffin detonation products. The detonation velocity measured in the cylinder tests was 8810 m/s. The calculated (with the Cheetah code) detonation velocity for the tested explosive at a density of 1.75 g/cm^3 equals to 8936 m/s and is therefore slightly higher than the detonation velocity measured in the cylinder test.

The dependence of the external tube radius (r_e) on the axial coordinate (x) is shown in Figure 7.

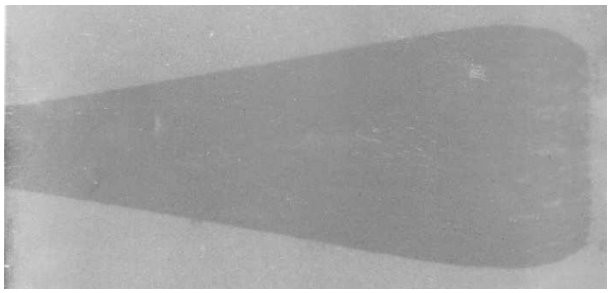

Figure 6. Inverse radiograph of the copper tube driven by the detonation products of a TKX-50/Paraffin (97/3) test sample.

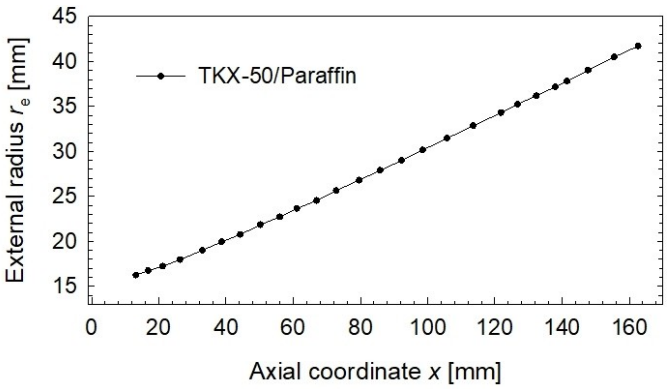

Figure 7. Radius of the external tube versus axial co-ordinate for the tested explosive.

The ability of the detonation products of an explosive to accelerate is given by the so-called Gurney energy (E_G). This corresponds to the sum of the kinetic energy of the driven tube (plate) and the detonation products following it. In the case of cylindrical envelopes (tubes), it is expressed by the following relation:

$$E_G = \left(\mu + \frac{1}{2}\right)\frac{u_L^2}{2} \tag{1}$$

where u_L is the velocity of the tube and μ denotes the ratio of tube mass to explosive mass.

The method used for determining the Gurney energy is described in detail in [12]. In the model which was used, it is assumed that the detonation process of the copper tube is stationary in the analyzed range of the axial coordinate. The x axis coordinate and time t are uniquely related by the linear relationship $x = D\,t$, where D is the detonation velocity. This makes it possible to swap the dependence of the tube radius on the axial coordinate with the dependence of the radius on time. The tube velocity u_L is obtained from the latter by differentiation and the Gurney energy from Eq. (1).

The tube velocity as a function of the relative volume of the tube-driven by the detonation products of TKX-50/Par-

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affin is shown in Figure 8. For comparison, the velocities of a standard tube (25.4 mm diameter, 2.54 mm thick) calculated for three relative volumes using the Ceetah code are also presented in Figure 8.

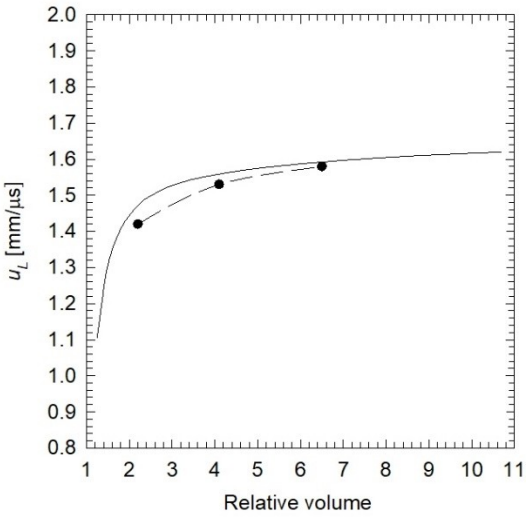

Figure 8. Tube velocity as a function of the relative volume for TKX-50/Paraffin samples.

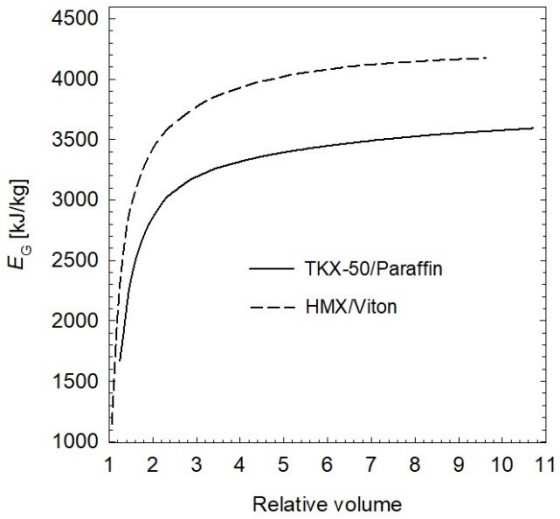

Figure 9. Gurney energy as a function of the relative volume for TKX-50/Paraffin and HMX/Viton.

Figure 9 shows the TKX-50/Paraffin Gurney energy (Eq. 1) as a function of the relative volume. For comparison, the figure also shows this relationship for HMX/Viton 95/5, which was determined under the same conditions.

The Gurney energies reported in the literature are determined for the volume of the tube just prior to its rupture. Table 5 shows the final Gurney energies determined for TKX-50/Paraffin, as well as for other commonly used explosives [13]. Table 5 also includes values for the Gurney constant (velocity) $\sqrt{2\,E_G}$, which is used in formulas for estimating the velocity of objects driven by the detonation products of a given explosive in various geometric systems [14].

The data presented in Table 5 show that although TKX-50/paraffin has the highest detonation velocity, it does not possess the highest acceleration capability. It appears to be the case that this is due to the relatively low heat of detonation of TKX-50.

The velocity of detonation depends not only on the detonation heat of the explosion but also on the composition of detonation products and a number of moles of gaseous products per unit mass of the explosive. Both the parameters affect the value of the isentrope exponent at the CJ point, g. The calculated number of gaseous detonation products of TKX-50/Paraffin (97/3) is 37.3 mol/kg. They contain 18.6 moles of N_2, and 4.3 moles of CO_2 per 1 kg, whereas 1 kg HMX/wax (96/4) produces only 31.8 moles of gases which contain 12.1 moles of N_2 and 8.9 moles of CO_2. As a result, the determined exponent value is 3.49 for TKX-50/Paraffin (97/3), and 3.05 for HMX/wax (96/4). The simplified formula between detonation velocity and detonation heat is as follows

$$D = \sqrt{2(\gamma^2 - 1)Q}$$

where Q denotes the heat of detonation, g is the isentrope exponent at CJ point.

For TKX-50/Paraffin 97/3

$$Q = 4650\ \mathrm{J/g},\ \mathrm{g} = 3.49, D = 10197\ \mathrm{m/s}$$

For HMX/wax 96/4

$$Q = 5850\ \mathrm{J/g},\ \mathrm{g} = 3.05, D = 9856\ \mathrm{m/s}$$

Table 5. Detonation velocity D, Gurney energy E_G and Gurney velocity $\sqrt{2\,E_G}$ for TKX-50 and other selected explosives.

Explosives	Density [g/cm^3]	D [m/s]	E_G [kJ/kg]	$\sqrt{2\,E_G}$[m/s]
TKX-50/Paraffin (97/3)	1.75	8810	3590	2680
HMX/wax (96/4)	1.78	8730	4300	2930
RDX/wax (95/5)	1.65	8390	3740	2730
TNT (100)	1.59	6910	2795	2360

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The data obtained from the cylindrical test, as well as the results from the numerical simulation of the acceleration of a copper tube enable other detonation parameters to be determined, such as the detonation pressure and detonation energy, as well as the determination of the JWL coefficients for the detonation products.

Analysis of the exponent of the isentrope of detonation products behind the detonation wave front shows that its value changes only to a small extent [12], and can be assumed to be constant when the change in the relative volume of the products does not exceed a value of 3. In such a case, the physical properties of the detonation products in the initial phase of decompression can be described by the isentrope equation as follows:

$$p = p_{CJ}\left(\frac{v_{CJ}}{v}\right)^{\gamma}, \tag{2}$$

where p_{CJ} and v_{CJ} are the pressure and specific volume at the Chapman-Jouguet (CJ) plane, v is the specific volume, and γ is the isentropic exponent.

The detonation pressure can be calculated using the formula:

$$p_{CJ} = \frac{\rho_0 D^2}{\gamma + 1} \tag{3}$$

The value of the exponent γ was determined by a comparison of the experimental profile of the copper tube with that obtained from the numerical simulation of its expansion. In the numerical model, the isentrope (Eq. 2) was used [15]. The problem of driving the tube is solved numerically for a given value of the exponent γ, and a discrete dependence of the external tube radius on the axial coordinate was obtained. The isentropic exponent value was determined by minimizing the difference between the experimental and theoretical dependences. Such a comparison is shown in Figure 10 for the explosive formulation which was investigated.

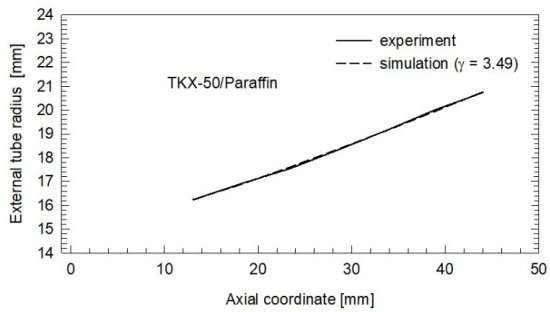

Figure 10. Experimental and calculated profiles of the cooper tube driven by the detonation products of TKX-50/Paraffin (the expansion of the detonation products is described by γ-const isentrope).

The calculated value for the isentropic exponent equals 3.49, therefore, the detonation pressure calculated from Eq. 3 is 30.25 GPa. Calculations using the Cheetah code give $\gamma = 3.55$, and a detonation pressure p_{CJ} of 30.68 GPa.

The detonation energy e_0 of high explosives is defined as being the maximum work done by the detonation products during their expansion from the CJ point to infinite volume minus the shock compression energy. As was shown in [12] and [16], the detonation energy can be estimated from the relation:

$$\frac{e_0}{e_0^{st}} = \frac{\left(\mu + \frac{1}{2}\right)}{\left(\mu^{st} + \frac{1}{2}\right)} \left(\frac{u_L}{u_L^{st}}\right)^2, \tag{4}$$

where e_0 and e_0^{st} denote the detonation energies related to unit mass of the explosive tested and a standard (reference) explosive, respectively, and u_L and u_L^{st} are the velocities of the driven tubes determined for a relative volume of 10.

In order to estimate the detonation energy of the explosive being investigated, RDX/wax (95/5) was chosen as a reference explosive. The density of the RDX/wax sample was 1.63 g/cm^3 and the detonation energy was 5430 J/g [13]. The approximations of the relation $u_L^2 = f(v_0/v)$ were extrapolated to the relative volume $v/v_0 = 10$ and the squares of the tube velocity for this volume were determined (Figure 11).

The detonation energy for TKX-50/Paraffin determined from Eq. 4 is 4840 J/g, and was estimated to be 4780 J/g using the CHEETAH code.

The JWL isentrope of the detonation products has the form:

$$p = A\, e^{-R_1 V} + B\, e^{-R_2 V} + C\, V^{(-1-\omega)} \tag{5}$$

where $V = v/v_0$. Connections between the JWL constants can be established from the conservation laws written for

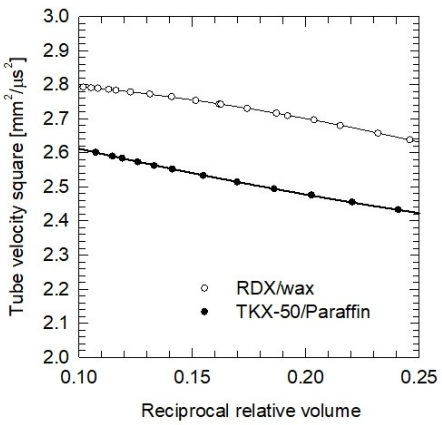

Figure 11. Dependence of the square of the velocity of the copper tube on the reciprocal volume of the detonation products for TKX-50/Paraffin and RDX/wax.

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the CJ plane. As a result, constants *A*, *B*, and *C* are expressed as functions of R_1, R_2, ω and ρ_0, *D*, $p_{CJ,}$ and $E_0 = \rho_0 e_0$ [17]. Thus, only the constants R_1, R_2, and ω need to be determined.

These constants were calculated using a method in which the experimental dependence of the radial displacement of the external tube surface on the axial coordinate was compared with that obtained from a numerical simulation [17]. The mathematical model for the process of acceleration of the copper tube by the detonation products used in the computer simulation has been described in detail in [18]. The set of JWL constants was chosen for which, the experimental and simulated displacements were sufficiently close to each other. This comparison for the TKX-50/Paraffin formulation is shown in Figure 12.

The JWL constants for the tested explosive are given in Table 6. The detonation parameters used in the determination of the JWL coefficients are summarized in Table 7.

The JWL isentrope coefficients and detonation parameters can be used in the numerical simulations of explosion phenomena in which the JWL-EOS is applied.

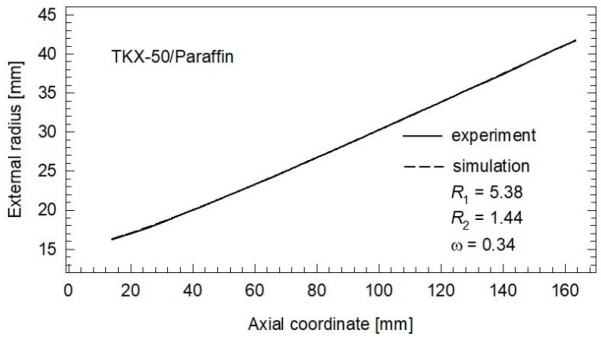

Figure 12. Experimental and calculated profiles for the copper tube driven by the detonation products of TKX-50/Paraffin (the expansion of detonation products is described by the JWL isentrope).

Table 6. JWL constants for the detonation products of TKX-50/Paraffin.

$A = 1525.53$ GPa	$R_1 = 5.38$
$B = 16.087$ GPa	$R_2 = 1.44$
$C = 1.2143$ GPa	$\omega = 0.34$

Table 7. Detonation parameters of TKX-50/Paraffin.

Density [kg/m^3]	*D* [m/s]	p_{CJ} [GPa]	E_0 [GPa]
1750	8810	30.25	8.5

3.5 Computational Results

Using the highly precise enthalpy of formation of TKX-50 of + 213.4 kJ/mol which was obtained experimentally as is described above, and the experimentally determined solid-state density at room temperature of 1.887 g/cm^3 [8], the performance parameters of TKX-50 for various densities were calculated (Table 7) using the EXPLO5 code [9].

It can be concluded from Table 8 that neat TKX-50 exceeds RDX and HMX in terms of detonation velocity, as well as RDX in terms of detonation pressure. The detonation pressures of neat TKX-50 and HMX are essentially the same. The detonation velocity of TKX-50 is slightly lower than that of CL-20, whereas the detonation pressure is significantly lower, which is most likely due to the lower heat of detonation of TKX-50. The calculated detonation velocity for TKX-50 at TMD of 9642 m s^{-1} shows very good agreement with the LASEM measured value of 9560 ± 280 m s^{-1} [7].

4 Conclusion

TKX-50 is a new and very promising secondary explosive with low sensitivities (IS = 20 J, FS = 120 N) and good performance parameters at its theoretical maximum density (1.877 g cm^{-3} at 298 K) such as $D = 9642$ m s^{-1} and $p_{CJ} =$ 37 GPa.

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Table 8. Computed performance parameters for TKX-50 in comparison with RDX, HMX and CL-20.

Density [g/cm^3]	HE/wax	*D* [m s]	p_{CJ} [GPa]	Q_{det} [kJ/kg]
		TKX-50		
1.74	97/3	8911	29.9	4608
1.877 (TMD)	100	9642	37.0	4770
		RDX		
1.74	97/3	8485	30.0	5543
1.82 (TMD)	100	8872	34.3	5730
		HMX		
1.74	97/3	8467	29.9	5485
1.905 (TMD)	100	9188	37.8	5684
		CL-20		
1.74	97/3	8503	31.4	5845
2.038 (TMD)	100	9770	44.7	6223

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