Computerized simulations and modelling for evaluation of ballistic and security parameters of explosives for civil use

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Abstract. Explosive**s** are chemical compounds - substances or mixtures of substances that have a large amount of energy and which under the influence of external actions decompose suddenly, violently with the release of heat and the formation of gases capable of performing a mechanical work. Due to their specific characteristics, these products are used, both in the civil field and in industry, for the execution of works such as: extraction from the massif, in mines or quarries of useful rocks, execution of mining works (galleries) for opening and preparing deposits for exploitation, tunnels, wells, road constructions, railways, canals, demolition of foundations / civil / industrial buildings that have become unusable, geophysical-seism metric surveys, etc. Research in the field of use of explosives for civil use in various industrial and civil applications requires in-depth knowledge of areas such as the phenomenology of explosion, the behaviour of materials in shock waves, the dynamics of structures, seismic engineering, etc. The design of these types of processes requires the consideration, with a relative approximation, of the degree of danger due to the design of fragments resulting from detonation, vibrations, pressures, tensions created in the space affected by the explosion, generation of explosion gases, etc. legislation in force, being an important indicator regarding the classification, handling, storage and transport in the assessment and management of the risks related to these operations. The paper presents a series of computer simulations, both of the ballistic parameter regarding the working capacity of the explosives, and of the security parameter regarding the impact sensitivity.

1 Introduction

Research in the field of use of explosives for civil use in various industrial and civil applications requires an in-depth knowledge of areas such as explosion phenomenology, behaviour of materials in shock waves, structure dynamics, seismic engineering, etc. The

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design of these types of processes requires the consideration, with a relative approximation, of the degree of danger due to the design of fragments resulting from detonation, vibrations, pressures, tensions created in the space affected by the explosion, generation of explosion gases, etc. Estimating the maximum values of the induced demands being of essential importance, the implementation of IT solutions for a priori experimentation allows the study of a large number of scenarios, the limit being mainly dependent on the time allocated to computer simulations. In this context, research in the field, the acquisition of experience and knowledge as well as the validation of results by comparison with previous practical experiments and those specified in the literature, become relevant and necessary requirements. Starting from these theoretical and practical considerations, it becomes imperative to focus research on the development of conceptual and experimental models, the likelihood of which is guaranteed by a whole series of scientific solutions characterized by validated results through numerical modelling and simulations. The methods used for the determination of ballistic and safety parameters, analysed by classical and computer means are relevant for the interpretation of the nature of explosive materials in terms of their classification in terms of the effect they may have on the use environment in case of explosion according to legislation in force, being an important indicator regarding the classification, handling, storage and transport in the assessment and management of the risks related to these operations. The following is a series of computer simulations, both of the ballistic parameter on the working capacity of explosives and of the safety parameters (sensitivity to friction and impact) [1, 2].

2 Materials and methods

2.1 Determination of the working capacity of explosives

Determination of the working capacity of explosives (materials and articles considered as explosives by the United Nations Recommendations on the Transport of Dangerous Goods and falling within Class 1 of these Recommendations), by the TRAUZL method, in order to verify compliance with the requirements of Directive 2014/28 / EU, involves performing this test [3 - 5].

The test method consists in detonating an explosive sample in a cylindrical lead block with a hole 125 mm (2 ± 2 mm) long and one diameter (25 ± 0.5) mm and measuring the volume of its cavity before and after the explosion. To admit the conformity of the cylinder, both the bases and its cavities are machined so that they are smooth and perpendicular to the vertical axis of the cylinder, not allowing visible gaps and cracks. Before making the determination, the cylinder must be kept for at least 24 hours at a temperature of $20 \div 25$ ^{0}C, which is the specified working temperature. The verification of the quality of the cylinders is done with standard explosive substance, respectively TROTIL recrystallized in alcohol, having the solidification temperature (80.4 ± 0.1) ^{0}C. A cartridge is prepared from the standard substance according to the procedure: from the sample for checking the quality of the explosive weigh (to the nearest 0.01kg) 10 g of explosive which is inserted into a cartridge with an inside diameter of 24+0.1 mm, made of foil of tin in the form of a truncated cone with approximate dimensions (having a large base of approximately 24 mm, a small base of 8 mm and a height of 62 mm). The explosive substance is pressed into the cartridge until a density approximately equal to that provided in the standard of the explosive to be determined is obtained. A detonating staple is inserted at the free end of the cartridge. The detonating staple is placed in the middle of the cartridge so that the cartridge does not deform with explosive, and the tin foil at the free end of the cartridge is melded

around the staple and fixed with adhesive tape or other suitable means. Also, the density of the TROTIL in the cartridge must be achieved at (1 ± 0.1) g / cm^3 (Figure 1) [6 - 9].

Fig. 1. Cylindrical lead block, TNT explosive assembled in cartridge and primed with detonating electric detonator.

2.2 Determination of the sensitivity to impact

Attach the corresponding ground hammer and trigger to the required drop height, then tighten the trigger to the guides [10 - 13].

Place the impactor in the retaining sleeve on the intermediate anvil without the upper steel cylinder (Figure 2).

Fig. 2. Placement of the test sample in the impactor

Place the samples of explosive substance, prepared according to the working procedure, in the open impactor (Figure 3).

Fig. 3. Placement of the impact device filled with the explosive substance sample in the impact test equipment.

3 Results and discussions

3.1 The working capacity of explosives

Measure the initial volume of the control sample cavity - lead cylinder, which before the determination must be maintained for at least 24 hours at a temperature of $20 \div 25$ ^{0}C, (this being the specified working temperature) by measuring with metered water from a graduated cylinder with a minimum capacity (500 ± 0.2) cm^3. Also, when priming the explosive cartridge, it is inserted into the cavity of the lead cylinder in such a way that it reaches its base in firm contact with the flat surface. The priming wick or rheophore is placed centrally and coaxially in the cylinder cavity and the free space is filled with quartz sand, up to the upper extremity, without being pressed. After preparing the assembly, the primer is initiated and the test results are checked. After the explosion, clean the cavity with a brush for cylindrical cavities and remove the contents after overturning the cylinder, and then measure the volume of the lead cylinder cavity again with water from the graduated cylinder (Figures 4 and 5) [14].
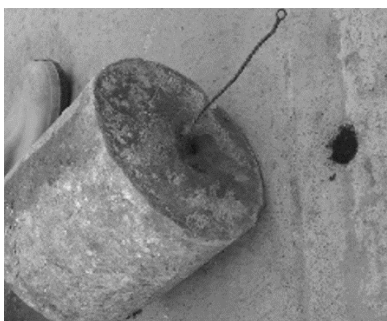

Fig. 4. Cleaning of debris of the control cylinder after blasting.

Fig. 5. Lead cylinder sectioned after Trauzl test with explosion results.

3.2 Calculation, expression and evaluation of results

In order to record and interpret the results, the working capacity of the explosive tested must be taken into account, taking into account the following parameters:
- ability to work in cm^3:

$$V = V_1 - V_o \ [cm^3] \tag{1}$$

where: V_1-volume of the lead cylinder cavity; V_0 -initial volume of the lead cylinder cavity.
    Following the experiment, the following results were recorded:
- the volume of the cavity created following the detonation of 10 grams of TNT, explosive initiated with detonating electric detonator, with a breaking charge of 0.6 grams PETN, V_1 = 385 cm^3;

- working capacity V = 315 cm^3 (initial volume of the cavity V_0 = 70 cm^3).

Determining the impact sensitivity of explosives and detonating wicks in order to ensure the continuous satisfaction of the requirements of Directive 2014/28 / EU transposed at national level by GD 197/2016 and the Technical Norms to Law no. 126/1995 with subsequent amendments and completions, as well as from the normative document of the product, implies the realization of this test. The method consists in dropping a hammer of a specified mass, from a set height, on the explosive sample subjected to the test and calculating the minimum impact energy at which a reaction of at least six tests is obtained.

To determine the sensitivity to impact, the test was performed with a granular explosive consisting of a mixture of porous ammonium nitrate and diesel fuel type AUSTINITE, manufactured by Austin Powder. The granular powder was passed through a 0.5 mm sieve, using the fraction passed through this sieve for testing. For each test, a sample of the substance prepared according to the working procedure was taken with a cylindrical measurement of 40 mm^3 capacity (3.7 mm diameter and 3.7 mm length) (Figure 2). The scope of the test method is in the range -30 ÷ +80 ^{0}C, so no special environmental conditions are required.

3.3 Computer simulation of the Trauzl test

Thus, by using the Geometry module within the ANSYS Multiphysics package, the geometry of the lead block and of the explosive charge located in the central channel, and of the borehole was made (Figure 6) [15].
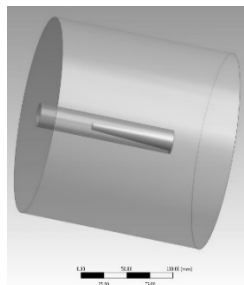

Fig. 6. Geometry of Lead block and explosive charge.

Through the ANSYS Workbench platform, the connection between the Geometry module and the Explicit Dynamics application was made, in which the discretization network for the entire virtual model was configured in order to perform the numerical simulation of the working capacity of the TNT type explosive (Figure 7), resulting in a number of 400,113 finite elements comprising 71,956 nodes.
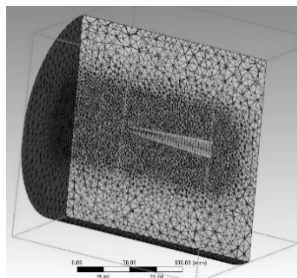

Fig. 7. Discretization for the elements of the model.

As can be seen from the figure, the discretization is much refined in the area of interest, respectively the central channel, in order to obtain qualitative and quantitative results with increased accuracy. At the same time, the contact surfaces between the interacting elements were defined: explosive, borehole and lead body, as well as the defining characteristics of these elements: TNT, quartz sand - borehole and lead (masses, densities, volumes, etc.).

Following the setting of the main characteristics of the virtual model elements, respecting the values used to perform the physical experiment - Trauzl test and initiation of TNT explosive with a predefined point source, running the Explicit Dynamics application using the Slovenian AUTODYN consisted of 1,829 calculation cycles, on a 12-processor workstation (CORES). The obtained result, respectively the internal deformation of the lead block by detonating the 10 grams of TNT, is presented in figure 8.
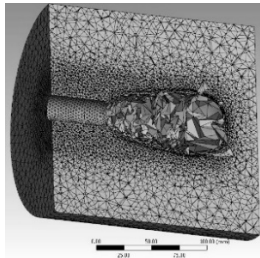

Fig. 8. Internal deformation of the lead block following TNT detonation.

For the calculation of the free interior volume obtained following the virtual simulation of the Trauzl test for TNT, a geometric transposition of the deformation was used, using the facilities of the AUTOCAD program. The volume thus determined was 384.989 cm^3, which means a working capacity of TNT of 314.849 cm3 (decreasing the initial volume of the central channel). This result is very close to the value obtained in the case of the physical experiment (315 cm^3), which demonstrates the usefulness of computer simulations using the ANSYS Multiphysics package in the field of explosives for civil use to determine the operating / working parameters. ANSYS Multiphysics used in the field of explosives for civil use to determine the operating / working parameters is highlighted in figure 9.
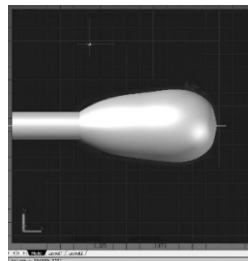

Fig. 9. Determining the volume of internal deformation.

3.4 The sensitivity to impact

Place the upper steel cylinder in the impactor and press lightly until it reaches the sample which can be felt due to a slight resistance, avoiding compaction of the sample[16].

After placing the impactor filled with explosive material so that it is centred on the intermediate anvil, close the protective case of the impact test equipment (Figure 2). The test is started with an impact energy of 10 J (5 kg hammer, drop height 20 cm). The hammer is released following the behaviour of the sample and the classification of the

manifestation in one of the following categories: with reaction (R) and without reaction (FR).

As no reaction to the explosive sample (FR) was detected, the test was repeated 5 more times using the same falling mass (5 kg hammer) under conditions of increasing the falling height by 10 cm, obtaining the following impact energies: 15 J (h = 30 cm), 20 J (h = 40 cm), 25 J (h = 50 cm), 30 J (h = 60 cm) and 35 J (h = 70 cm).

Given that a reaction (R) was found for the impact energy of 35 J, then the test was repeated for a lower impact energy (32.5 J at a drop height of 65 cm), in which case which was also found to have a reaction (R).

In a completely similar way, the test was repeated 6 times for a lower impact energy (30 J at a drop height of 60 cm), in which case no reaction to the explosive sample (FR) was found. These results are summarized in Table 1.

Impact sensitivity S_i (in J) is the product of the mass of the hammer M (in kg), the drop height h (in m) and the gravitational acceleration g (value 10 m /s^2) at which at least one reaction in 6 tests is obtained.

$$Si = M \cdot h \cdot g \text{ (J)} \tag{2}$$

The test method does not involve a calculation of uncertainty as the result is of a qualitative type, ie ″ with reaction ″ (R) or ″ without reaction ″ (FR).

The test to determine the impact sensitivity of the granular explosive consisting of a mixture of porous ammonium nitrate and AUSTINITE type diesel resulted in a minimum impact energy of 32.5 J.

Table 1. Results of the tests.

No.	Hammer Mass M [kg]	The height of drop h [m]	Temperature room [^{0}C]	Result: R – reaction; FR – no reaction	Impact sensitivity S_i=M·h·g [J]
1.	5	0,20	18	FR	10,0
2.	5	0,30	18	FR	15,0
3.	5	0,40	18	FR	20,0
4.	5	0,50	18	FR	25,0
5.	5	0,60	18	FR	30,0
6.	5	**0,70**	18	**R**	**35,0**
7.	5	**0,65**	18	**R**	**32,5**
8.	5	0,60	18	FR	30,0
9.	5	0,60	18	FR	30,0
10.	5	0,60	18	FR	30,0
11.	5	0,60	18	FR	30,0
12.	5	0,60	18	FR	30,0
13.	5	0,60	18	FR	30,0

3.5 Computer simulation of the sensitivity to impact test

Thus, by using the Geometry module within the ANSYS Multiphysics package, the geometry of the impact device and of the explosive charge placed within it were realized [17].

Determining the sensitivity to impact of explosives and detonating cord in order to ensure the continuous fulfilment of the requirements of the Directive 2014/28/EU

transposed at national level by GD 197/2016 and the Technical Norms to the Law no 126/1995 with the subsequent modifications and completions, as well as from the normative document of the product, involves performing this test.

The method consists in dropping of a specified mass hammer, from a set height, on the explosive sample subjected to the test and calculating the minimum impact energy to which at least one reaction from six tests is obtained. In order to determine the sensitivity to impact, the test was performed with a granular explosive consisting of a mixture of porous ammonium nitrate and diesel AUSTINITE type, manufactured by Austin Powder. The granular powdery substance was passed through a sieve with 0.5 mm mesh, for test was using the fraction that passed through this sieve. For each test, capacity (3.7 mm diameter and 3.7 mm long) was taken a sample of the substance, cylindrical measure of 40 mm^3, prepared according to the working procedure. The scope of the test method is in the range - 30 ÷ +80^{0}C, so no special environmental conditions are required. Thus, by using the Geometry module within the ANSYS Multiphysics package, the geometry of the impact device was realized and the explosive load was placed within it.

Through the ANSYS Workbench platform, the connection was made between the Geometry module and the Explicit Dynamics application, in which the geometry of the ensemble was realized, the discretization network for the entire virtual model in order to perform the numerical simulation of the impact sensitivity of the explosive consisting of a mixture of porous ammonium nitrate and diesel type AUSTINITE (Figures 10÷13).
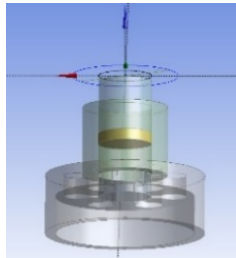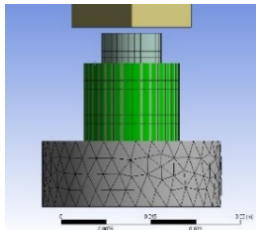

Fig. 10. The geometry of the assembly.

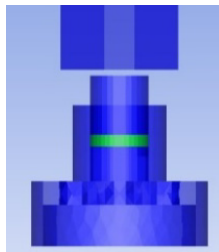**Fig. 11.** Discretization for the elements of the numerical simulation mode.

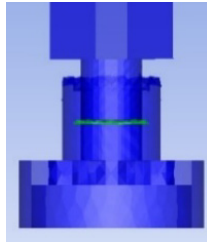**Fig. 12.** Image taken from AUTODYN before the impact triggeri.

Fig. 13. Image taken from AUTODYN after the triggering of the impact.

Further, the diagrams showing the evolution of kinetic energy parameters and the component on the Y axis of the impulse force are highlighted (Figures 14 and 15).
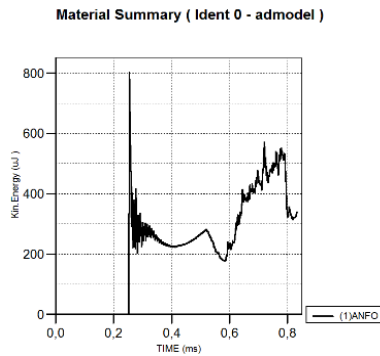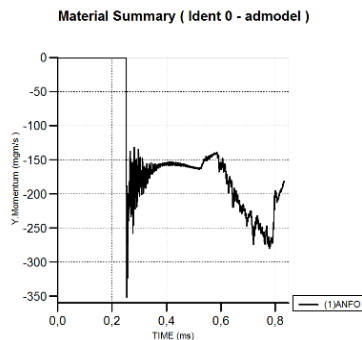

Fig. 14. Impact kinetic energy.

Fig. 15. The component of the impulse force on the y axis.

Figures 14 and 15 show the graph-analytical results of the two characteristics related to the kinetic energy and the force/impulse couple that were obtained following computerized simulations with the ANSYS program, resulting in the evolution over time of the variation of the two parameters.

4 Conclusions

For the calculation of the free interior volume obtained following the virtual simulation of the Trauzl test for TNT, a geometric transposition of the deformation was used, using the facilities of the AUTOCAD program. The volume thus determined was 384,989 cm^3, which means a working capacity of TNT of 314,849 cm^3 (decreasing the initial volume of the central channel). This result is very close to the value obtained in the case of the physical

experiment (315 cm^3), which demonstrates the usefulness of computer simulations using the ANSYS Multiphysics package in the field of explosives for civil use to determine the operating / working parameters

Following the setting of the main characteristics of the elements of the virtual model, respecting the values used to perform the physical experiment ″Determination of impact sensitivity″, running the Explicit Dynamics application using the Slovenian AUTODYN consisted of: computer 1 (33,150 calculation cycles, on one station work with 12 processors - CORES); computer 2 (60,945 computing cycles, on a workstation with 30 processors - CORES). The result obtained did not lead to the detection of any reaction (R) in the mass of explosive substance tested (apart from the deformation by pressing of the quantity of explosive substance tested), as a result of generating an impact energy of approximately 40.0 J corresponding to the fall a mass of 5 kg from a height of 65 cm, taking into account a gravitational acceleration of 10 m /s^2.

This result leads to the idea of continuing research in the field of computer applications to obtain a virtual model capable of reproducing the conditions for determining the safety parameter on the impact sensitivity of explosives for civil use, using the ANSYS Multiphysics package.

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