Abstracts of the 27th Seminar on

New Trends in Research of Energetic Materials

Pardubice, April 2–4, 2025

University of Pardubice, Faculty of Chemical Technology
Institute of Energetic Materials

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New Trends in Research of Energetic Materials

Held at the University of Pardubice

Pardubice, Czech Republic
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Intended as a meeting of students, postgraduate students, university teachers, and young research and development workers, concerned from the whole world.

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Contents

Posters

Preface

The International Seminar New Trends in Research of Energetic Materials (NTREM) has traditionally been an international meeting of students and early-career researchers involved in the research, development, technology, or industrial application of energetic materials.

It started as a local meeting organized by Research Institute of Industrial Chemistry in Explosia in 1999 with the aim of teaching the youth scientists to present the results of their work to a professional audience. Students from the Institute of Energetic Materials took part in the event and found it useful to their professional development. Therefore, it was decided to continue with these seminars and hand over their organization to the University of Pardubice.

Under the enthusiastic leadership of Prof. Zeman, this local meeting developed into a well-established international event. Although growing in size, it maintained its original focus and always aimed to give students and newcomers to the field of explosives the ability to present their work even in the early stages of development and to build personal relationships with colleagues from countries all over the world.

The 27th NTREM seminar featured a diverse range of topics while maintaining its traditionally strong emphasis on synthesis. The seminar proceedings contain papers presented at the event either in oral or poster form.

I would like to take this opportunity to express my sincere gratitude to the generous sponsors for their support. Their financial assistance was invaluable in making this event possible and allowed us to keep the registration fee at a minimal level. The seminar was supported by the following:

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I also express my deep gratitude to the members of Scientific Committee, the Organizing Committee, the authors of all the seminar papers and, finally, all the participants of this seminar.

Pardubice, March 5th, 2025 Jiri Pachman

Recent developments of energetic di- and trisubstituted cubanes

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Keywords: energetic material; cubane; UV-reaction; NMR spectroscopy; sensitivities.

Apart from computational studies, there is a lack in literature in regards to direct comparison between the energetic properties of cubane derivatives with varying levels of substitution. Their synthesis is presented as well as characterization by NMR spectroscopy, DSC and sensitivity measurements. The energetic properties of some polysubstituted energetic cubane derivatives were determined and compared. The energetic parameters were calculated using the EXPLO-5 program, utilizing the density derived from X-ray crystallography/pycnometer and the heat of formation calculated with the Gaussian program package.

Mitigating environmental impact of TNT production: Strategies for red water reduction and treatment

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Keywords: literature review; TNT; red water; advanced oxidation processes; integrated wastewater treatment.

The commonly used purification route of 2,4,6-trinitrotoluene (TNT) using a sodium sulfite wash, also called the sellite process, generates significant quantities of red water, a hazardous byproduct containing toxic, carcinogenic, and mutagenic nitroaromatic compounds. This review explores two primary strategies for mitigating red water production associated with the sellite process and its environmental impact: The first approach involves the exploration of alternative synthesis routes, nitration agents such as N2O5, and the use of catalysts such as zeolites, which minimize the generation of asymmetrical derivatives, thereby reducing or eliminating the necessity for the sellite process. Second, if red water production cannot be avoided, advanced red water treatment technologies, especially integrated treatment systems combining physical, chemical, and biological methods, were investigated. Advanced oxidation processes and the use of zero-valent iron offer promising solutions for red water detoxification and treatment. These approaches aim to establish a sustainable and economically viable solution for TNT synthesis that complies with modern environmental standards while addressing the risks involved in handling TNT red water.

LLM-105: achieving different morphologies for different properties

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CEA, DAM, Le Ripault

Keywords: LLM-105 ; morphology.

2,6-Diamino-3,5-dinitropyrazine-1-oxide, known as LLM-105, stands as one of the best safety/performances trade-offs to date in the field of explosives. Its common synthesis involved a 3-steps process from 2,6-dimethoxypyrazine, known as the DMP route. However, a more recent route, consisting in the dinitration of 2,6-diaminopyrazine-1-oxide (DAPO), offers substantial advantages: there is only one step to be carried out in facilities dedicated to explosives, and the product is highly pure, avoiding the issue of residual ANPZ associated with the DMP route. Initial drawbacks of the DAPO pathway were circumvented through optimization of the quench step. Quenching the nitrating mixture in the presence of nitrates yielded LLM-105 samples with enhanced thermostability and particle size. Particle morphology is a critical issue when developing new formulations, and the work focuses here on the relationships between a microscopic feature (particle morphology) and macroscopic properties. Different morphologies were achieved through specific quench conditions or post-synthesis treatments. For example, sonication of as-precipitated LLM-105 resulted in a dramatic change in the morphology: partial fragmentation occurred, and eroded, rounded particles were obtained. Some specific morphologies induced different behaviors in safety characteristics, but also in PBX processing and in detonics experiments. This was particularly evaluated in small-scale corner turning experiments, using cylinders of LLM-105-based PBXs initiated with a slapper detonator.

Synthesis and evaluation of novel TATB-inspired energetic materials

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Keywords: novel synthesis; energetic material.

Energetic materials that balance high-performance with low sensitivity have been heavily utilized in both military and civilian sectors. Among common sensitivities including shock and friction, elevated thermal stability is particularly desirable in these materials as it significantly broadens their potential range of applications. Toward the development of thermally stable energetic materials, we describe the synthesis, characterization, and energetic performance of several TATB-inspired compounds. Additionally, we provide some insight into the influence that small functionality changes can impart on the performance of otherwise structurally-similar systems.

$BKNO_3$ pyrotechnic igniters for SRM: analysis of performance dispersion from development to production

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Keywords: $BKNO_3$ pellet; pyrotechnic igniter; solid rocket motor.

In Solid Rocket Motor, thrust is obtained from the controlled combustion of the propellant grain at high pressure and temperature. This reaction is predictably and repeatably triggered using a system called igniter, which is commonly made of an initiation system and an energy release system. These two components are physically inserted into a series of housings mounted on fixed or temporary (ejected during firing) supports inside the motor. The energy release system represents the core of the igniter and, in case of pyrotechnic igniter, is made of a pyrotechnic charge encapsulated inside a perforated basket. The most common pyrotechnic charge is made in form of pellets composed of BKNO3. In the development phase, different configurations are investigated to select the most appropriate to fit the requirement on ignition time of the motor. In this phase different architectures are compared involving: different ignition chain (pyrotechnic igniter devoted to igniting a pyrogen igniter and then the SRM; pyrotechnic igniter devoted to ignite directly the motor), different basket geometry (cup like vs tube-like), pellets charge mass. Once defined the igniter design and demonstrated its capability in fulfilling the motor ignition requirement, the pyrotechnic igniter undergoes to production and performance dispersion is mostly ascribed to production dispersion related to pellets production lot dispersion, despite the requirement to comply with the same regulation (MIL-P-46994B). In the final paper, for the development phase, the performance dispersion is analyzed with the aim to discern the main parameters needed to define the performance envelope to be used in the design process. This study allows to optimize the safety margins in the design phase assuring the needed performance at motor level, reducing item inert mass. On the other hand, for the production phase, pellets acceptance characteristic dispersion within the same production lot (intra-lot) and between lots (inter-lot) are analyzed to retrieve a correlation between pyrotechnic pressure curve and the corresponding acceptance properties. Great impact has been found from crush strength, heat of reaction and burning rate. This analysis allows to identify the characteristic to be put under strict control in lot acceptance phase to limit performance dispersion.

Modelling complex ageing behavior of tensile modulus in CTPB-bonded propellant – parametric and kinetically based procedures

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Keywords: CTPB-MAPO binder; E-modulus; post-curing; splitting of binder; reaction kinetic descriptions.

Composite rocket propellants with CTPB-binder (carboxyl terminated polybutadiene) are in use besides the ones which are based on HTPB-binder (hydroxyl-terminated polybutadiene), which are cross-linked via polyisocyanates to a polyurethane network. CTPB binders are cross-linked with substances containing aziridine (aza-cyclopropane) groups or epoxide (oxirane, oxa-cyclopropane) groups. In each case polyaddition reactions occur. A system consisting of CTPB + MAPO is considered here. MAPO is called tris-[1-(2-methylaziridinyl)] phosphane oxide. Curing with MAPO works well, but problems can occur. One drawback is the splitting of the P-N-bond, because it is very susceptible to hydrolytic cleavage. The mechanical properties of samples of a CTPB-MAPO propellant with AP and plasticizer were aged at 45řC during nearly 3 years and investigated by uniaxial tensile measurements. The tensile modules (Young modulus, E modulus) showed a complex behavior: first increasing, then decreasing and further decreasing with lower rate. With rubber systems, the Young modulus is proportional to cross-link density. The cross-link density is a state property of the binder. Because of proportionality of the modulus with the chemical property cross-link density, it can be used directly in kinetic modelling. The task was with the available measurement data to develop a kinetically based description. The increase and following decrease of modulus are caused by post-curing and binder backbone splitting. The decrease can be distinguished in two parts, where the second one originates by diffusion-control of the water migration in the propellant. The kinetic modelling is performed in two ways: at first parametric descriptions are tried which are only formally based on kinetic concepts; secondly, kinetically based models are applied. With both types, complete data description can be achieved. But the character of these modellings are different. Post-curing and splitting of the binder could be modeled with combined reactions of second order.

Energetic polymers derived from oxetanes

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Keywords: energetic binder; polyoxetane; dinitrogen pentoxide.

Within energetic formulations, polymeric binders are frequently used to both disperse and homogenise the components into a polymer matrix, and to provide stability by improving structural and mechanical integrity. Energetic polymeric binders play a key role in enhancing the stability of these formulations, while also contributing to enhanced outputs. One of the most widely used energetic binders is nitrocellulose, but this poses several challenges, namely: it is derived from cellulose and therefore has natural variation in both structure and properties; it has a high glass transition temperature that means formulations must be plasticised to ensure acceptable mechanical properties; and stabilisers are required to prevent autocatalytic degradation. Because of this inherent variability and difficulty in sourcing reliable NC, attention has turned to the development of synthetic energetic polymer alternatives. For this study, polyoxetanes have been selected due to their tunability and relatively simple synthesis. The synthetic approach for the preparation of nitrate ester functionalised polyoxetanes can follow two pathways. The first involves the direct nitration of the oxetane-based heterocycle using a highly selective nitration method of dinitrogen pentoxide (N2O5). Utilising this nitrating agent removes the need for strong acids as the reaction medium, thereby allowing the ring to remain intact. Following this, the energetic monomer can be polymerised using cationic ring opening polymerisation (CROP). The second approach to achieving nitrate ester functionalised polyoxetanes involves polymerising the oxetane species before nitrating the inert polymer. The steps taken to date to prepare energetic binders by these two approaches are reported here, along with comparisons of their structure property relationships, and sensitivity to initiation.

Isocyanate-free energetic polymer binders

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Keywords: polymer bounded explosives; thermo-mechanical properties; silicone; epoxy; acrylic.

There are numerous classes of energetic materials, including them polymer-bonded explosives (PBX). They are used in the defense industry, generally in metal containers such as shells. These energetic composites have two main constituents, the energetic charge and an inert binder. Usually, the binder is a polymer matrix, the purpose of which is to give the material mechanical strength and to phlegmatise it. As they do not comply with REACH regulations and are incompatible with recently developed energetic charges, the isocyanate functions limit the use of polybutadiene-based polymer matrices which is are commonly used in PBX systems. There is therefore a desire to find substituents polymers that does not contain isocyanates. The latter must meet certain criteria, such as not having a phase transition over its range of use [-47 to 70°C]. Two types of matrices are therefore distinguished, so-called "low Tg" matrices, which have a glass transition below -47°C, and "high Tg" matrices, which have a glass transition above 70°C.Thermomechanical tests were carried out on matrices synthesized on a laboratory scale, with and without mimetics fillers of the energetic charges. A "Low Tg" polymers exhibit elastomeric behaviors at the temperature of use, characterized by a low elastic modulus and high elongations at break, with a high capacity to absorb stresses such as shocks. Silicones and certain acrylic polymers are promising "low Tg" matrices. Composites based on silicones and acrylics with non-reactive mimetic fillers have been successfully synthesized and thermo-mechanically tested. The "high Tg" materials obtained have very different mechanical properties to those of elastomers, they have a much higher elastic modulus but a much lower elongations at break. This class of material could meet other needs in the polymer-bonded explosives domain. Epoxy polymers and certain other acrylic polymers are potentially interesting "high Tg" matrices for this application.

Energy output of HMX-based aluminized explosives with varying aluminum (Al) and polytetrafluoroethylene (PTFE) ratios

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Keywords: aluminized explosive; PTFE; heat of explosion; afterburning; air blast.

Fluorinated oxidizers are attracting oxidizers for aluminized explosives, mostly due to the combination of high heats of formation of AlF_3, comparable to that of metal oxides, with the relatively high vapor pressure of metal fluorides, which volatilize more readily than refractory oxides for most of the energetically interesting metals. In our previous work, polytetrafluoroethylene (PTFE, C_2F_4) has been used as the fluorine carrier and typical oxidizer for Al, with a high content of fluorine (76%), exhibiting high heat of explosion for aluminized explosives. In this work, several formulations of HMX-based polymer bonded explosives (PBXs) containing varying contents of Al and PTFE were manufactured by acoustic resonance and rotary cutting methods. First, the theoretical energy performance was calculated by the VLW thermodynamics code. Then, the heat of explosion, detonation velocity, detonation pressure, air blast and underwater explosion of those explosives were tested and compared. Results show that PTFE as an oxidizer can increase the heat of explosion, and exhibits significant post-detonation reaction potential with metal fuels. And the optimal contents of Al and PTFE were suggested. Further analysis on the reaction between PTFE and Al was conducted based on the theoretical calculation and experimental results.

Aluminized highly energetic materials simulation under partial chemical equilibrium assumption with HEMSim

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Keywords: emulsion explosives; cylinder test; JWL; aluminized.

We are pleased to introduce the first version of EUDETCODE, an advanced computational code for ideal detonation analysis, capable of handling the presence of aluminum in high-energy reactants. The hard coded model incorporates the variable percentage of aluminum reaction completion during detonation, reflecting its influence on the detonation process. Key outputs include the Chapman-Jouguet (CJ) point and the fitting of the Jones-Wilkins-Lee (JWL) equation of state, both of which are validated against experimental results. The validation demonstrates the code's accuracy and reliability in predicting detonation behavior for energetics containing reactive metals.

Thermal isolation modeling of aluminized energetic materials for low-cost computational code

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Keywords: aluminium; thermal isolation; detonation; isentropic expansion; JWL.

Aluminum is one of the main additives used to improve energetic materials' performance. Furthermore, the presence of aluminum in detonating substances increases the non-idealities of the material, creating a mixture that is not in thermodynamic equilibrium once ignited. The non-idealities of aluminum can be described using theories such as the Wood-Kirkwood (WK) theory or Detonation Shock Dynamics (DSD). However, such approaches require algorithms with high computational costs. The purpose of this work is to provide a less computationally expensive alternative that adequately describes the thermodynamic behavior of aluminized explosives both during the reaction and the subsequent expansion. Less computationally expensive models, such as the Chapman-Jouguet (CJ) model and the isentropic expansion model, are based on assumptions of thermal and mechanical equilibrium among the various phases of the product mixture. Mechanical equilibrium operates over very short timescales, shorter than those of chemical kinetics, and remains a valid assumption even for aluminized explosives. However, the assumption of thermal equilibrium among the phases, in the presence of aluminum, is uncertain due to the rapid nature of the phenomenon. Two different hypotheses can be made in this regard: thermal equilibrium and thermal isolation. The latter hypothesis has been introduced into the CJ and isentropic expansion models, and a code capable of implementing the new model has been developed. Finally, the obtained results are compared with those available in the literature, and the isentropic expansion curve is fitted with the Jones-Wilkins-Lee (JWL) equation of state.

Construction of a composite surface coating layer with high efficiency on desensitization of HMX

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Keywords: HMX particle; composite desensitizing agent; mechanical sensitivity; surface coating; synergistic effect.

Matching and optimizing the characteristics of desensitizing agent and constructing uniform, complete surface layer were key factor to achieve efficient desensitization of energetic materials. Combined the advantages of wax and MoS2, a composite desensitizer surface layer was constructed, which exhibited improved performance to decrease mechanical sensitivity of HMX crystals. In addition, a surfactant was designed and prepared to improve the wettability between solid (HMX and MoS2) and liquid (melted wax), obtaining an evenly dispersion of MoS2 in melted wax, as well as a complete surface layer. With 0.95 % weight percentage of desensitizing agent, the impact sensitivity and friction sensitivity of HMX-Composite particles were 0% and 0%, respectively, which showed high efficiency to desensitize the HMX particles, satisfying the application demands of insensitive munitions.

Synthesis and characterisation of the energetic plasticiser Bu-AENA

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Keywords: synthesis; characterisation; energetic plasticiser; compatibility.

FOI has been in the research field of energetic plasticisers for decades. The efforts have been focused on substances that can plasticise the polymer GAP (polyglycidylazide). Many have been investigated and all discarded.

This paper contains a comparison of the plasticising properties on GAP of the hitherto little described energetic plasticiser Bu-AENA (N-butyl-N-(2-azidoethyl)-nitramine) with other energetic plasticisers.

Initial studies in smaller scale, allowed the evaluation of its thermal stability with heat flow calorimetry (HFC). The same technique was then used to investigate its excellent compatibility to binders and fillers, which took place after a scale-up to kilogram batches.

Then Differential scanning calorimetry (DSC) showed its good plasticising capability on the low thermal properties of GAP, both uncured and uncured in a binder as well as in a GAP/ADN/FOX-7/BuAENA propellant.

An overview of vibration effects on energetic materials

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Keywords: vibrational loading; energetic material; hot spot; cook-off.

This work presents an overview of the most significant literature exploring the vibration effects of energetic materials, emphasizing the thermal energy derived from friction and viscoelastic behavior from stress concentrations in localized regions that can trigger ignition or material structure degradation. The mechanical and thermal actions on energetic materials can induce structural damage, cracks, and even decomposition or explosion. These phenomena are preceded by changes in the structural and physicochemical characteristics of the material, which can affect the mechanism and kinetics of decomposition reactions. Therefore, they are of significant scientific and technological interest because of the necessity to predict safe regimes during production, processes, transport, and operation. Notable findings include the transition from thermal decomposition to explosion of RDX crystals subjected to vibrational loading at 110 Hz and compression of 200 MPa, as well as changes in RDX crystal structures observed via X-Ray and IR spectroscopy. Two ignition mechanisms, hot spot and cook-off, are discussed: the former occurs when cooling relaxation time exceeds one stress cycle, while the latter involves an overall material temperature increase due to friction and viscoelastic effects. The existing literature suggests that, despite high temperatures, hot spots contribute only marginally to bulk heating, except under plastic deformation or high-frequency loading conditions. Recent studies on HMX crystals indicate that binder adhesion significantly influences localized temperature rise, with dynamic loading resulting in substantial thermal responses. This concise review underscores the necessity of comprehending localized heating phenomena in energetic materials to mitigate the risk of ignition, emphasizing the crucial role of incorporating vibration tests in safety validations.

A synthetic route to 3,5-dinitropyridine analogs and evaluation of their thermal properties

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Keywords: DSC; kinetics.

The search for new energetic materials that balance overall performance with stability has been at an increased demand over the past decade. Synthetic efforts towards this pursuit are often tedious and slow, resulting in hindered progress in this area of exploration. Thermal analysis studies such as differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) are fundamental experiments that can be used to gain preliminary kinetic information to provide insights into the long-term stability of these materials, along with their stability toward harsh environments. This work describes a synthetic route to new 3,5-dinitropyridine-based materials, including initial DSC and TGA analysis on the compounds' energetic properties that we anticipate will be useful in constructing a more developed understanding of how molecular structure affects both energetic performance and overall stability.

New green solvents for high dissolution and the mechanism of strongly hydrogen-bonded explosives

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Keywords: green solvents; dissolution; TATB; strongly hydrogen-bonded explosives.

Hydrogen bonds play an important role on improving the safety of energetic materials. Nowadays, there is a tendency to develop strongly hydrogen-bonded explosives including 1,3,5- triamino-2,4,6-trinitrobenzene (TATB), 2,6-diamino-3,5-dinitropyrazine-1-oxide (LLM-105), and 2,4,6-triamino-5-nitro-pyrimidine-1,3-dioxide (ICM-102). However, the solubilities of these explosives are severely inhibited by strong hydrogen bonds. For example, the solubility of TATB is 70 ppm in dimethyl sulfoxide (DMSO). Low solubility poses a huge obstacle for the recrystallization, purification and recycling of these explosives. Deep eutectic solvents (DESs) are regarded to be new generation of green solvents because of unique advantages including low cost, simple preparation, and easy biodegradation. The exchange of hydrogen bonds can occur between liquid DESs and other hydrogen-bonded materials to break and rearrange their hydrogen bonds, so DESs show potential dissolution toward most of poorly soluble materials. In this study, a series of new DESs based on tetra- nalkylammonium have been prepared and characterized for the dissolution of strongly hydrogen- bonded explosives. The DESs are liquid at room temperature, which is beneficial to dissolve solid explosives. Meanwhile, these solvents display high dissolution toward TATB with maximum solubility of 13 wt%, which is almost 2000 times higher than DMSO. The dissolution of TATB in DESs is fast, and solid TATB is completely dissolved within 2 min. The DES solvents also have good dissolution toward LLM-105 and ICM-102. The dissolution mechanism has been investigated by experimental characterizations and theoretical calculations. Hydrogen bonds of these explosives are disrupted through forming Zundel-type complexes between TATB and the anions in DESs, and then the complexes are surrounded by the cations in DESs through self-assembly of electrostatic interaction to avoid the disrupted TATB reconnecting with coriginal networks. Therefore, this work provides a valuable strategy for designing new solvents to dissolve strongly hydrogen-bonded explosives and performing various applications such as the purification, recycling and recrystallization.

An improved statistical analysis of 72 sensitivity datasets

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Keywords: sensitivity testing; statistics; impact sensitivity; friction sensitivity.

This paper addresses the statistical estimation of sensitivities of energetic materials to friction and impact. The NATO Standardisation Agreements (STANAGs) for sensitivity testing still rely on a pen-and-paper approximation of maximum likelihood estimation from 1948. Although useful for its time, this approximation is today unnecessary as maximum likelihood estimation is easily implemented in virtually any general-purpose programming language and spreadsheet software. In this paper we show how the use of the approximation manifests itself in practice by analysing 72 datasets for impact and friction sensitivity of multiple energetic materials. For a substantial minority of the datasets, the use of the approximation is not valid, as a certain simplification of the likelihood function cannot be applied. Despite the STANAGs'Ź requirement to discard such datasets, we find that the maximum likelihood estimates exist and provide perfectly valid results for all of them. For the remaining datasets, where the use of the approximation is valid, we find that it performs poorly when constructing confidence intervals. For extreme quantiles, we obtain a relative error as high as 20%. In conclusion, our paper serves as further evidence that the 1948 approximation should be abolished and replaced with direct maximum likelihood estimation.

Optimization of fiber optic probe for measuring detonation velocity

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Keywords: FOP; fiber optic probe; detonation velocity.

Detonation velocity is one of the basic parameters for the characterization of explosives. One of the possible methods of obtaining the velocity is the use of a fiber optic probe. In principle it is an optical fiber which has perforated insulation and core to such an extent that it can absorb light perpendicular to the fiber but, still retains the capability of transporting light without a significant loss of intensity. Such fiber placed parallel to the explosive's axis inside or at its surface will send light signals in defined intervals as the detonation front passes along the perforations. This study investigates how different diameters, depths and number of the perforations affect the signal quality. Applicability of this technique to different types of explosives is discussed. With the right combination of diameter and depth, measurements with 50 perforations on a single fiber are possible, allowing this technique to track changes in detonation velocity along the charge.

Triazol polymer, first step for a self-healing PBX

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Keywords: self-healing; triazol; azide; Huisgen reaction.

Self-healing is a technique used to fix physical defects in polymers caused by various aggressions (mechanical, chemical). In the field of energetic materials, cracks induced by stress on a polymer-bonded explosive (PBX) can represent a risk, making it essential to mitigate this hazard. The self-healing solution appears to be an ideal approach due to its ease of implementation. The solution is based on the introduction of capsules which enable self-healing phenomenon through a chemical reaction with the polymer matrix when a crack appears. This innovation will help to reduce the reject rate due to nonconformity related to crack and will decrease the risk of accidents in operation.

Encapsulation The technique of encapsulation consists of encapsulating a reactive healing function of the polymer. The capsule is then added in the composition, during the process. After a crack, the capsule breaks and releases the healing matrix which will be able to react with the cast PBX formulation to fix the crack. For this purpose, the healing matrix is made up of chemical functions that complement and can react with the reactive functions of the cast PBX formulation. The mechanism selected here is based on the Huisgen reaction, leading to the formation of a triazole, resulting from the reaction between an azid group and an alkyne function.

Self healing principle demonstration As self healing phenomenon thanks to Huisgen reaction is based on the reactivity of the azide group with alkyne functions, alkyne multifunctional platforms have been developed. To react with alkyne groups of the multifunctional platform, Azide polymers has been synthetized. The demonstration of the feasibility of the Huisgen reaction between the azide polymer and an alkyne functionalised platform has been successfully completed and characterised. Lastly, the encapsulation of the alkyne platform has been studied and performed thanks to a microencapsulation process under solvent. With the realization of the azide functionalized cast PBX with encapsulated alkyne platform, the full concept could be validated after a voluntary stress has been applied to release the alkyne functions and thus enable the self healing of the polymer.

Research on material model and parameters of metal thin plate under close-in explosion load

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Keywords: explosion mechanics; Johnson Cook material model; Cowper Symonds material model; genetic algorithm.

The Johnson Cook material model and Cowper Symonds material model are commonly used models to describe the dynamic response of metal materials. To obtained the parameters of brass sheet materials under close-in explosion loading, close-in explosion loading on brass sheets experiments with different equivalent explosives were carried out, and then the displacement-time curve of center point of the sheet was measured. Besides, a joint simulation of genetic algorithm and finite element simulation program was developed to automatically calibrate the parameters of Johnson Cook material model and Cowper Symonds materials model. In addition, simulation of close-in explosion loading experiments on brass sheets were carried out. Meanwhile, the theoretical calculation was taken. The results show that the theoretical values, simulation values, and experimental values have good consistency. Under different conditions of explosion loading, the maximum deflection errors from JC model simulation and CS model simulation are 4.46% and 4.84%, respectively. Compared to the JC model, the strain rate sensitivity of the CS model is more significant. As the load increases, the maximum deflection value calculated by the CS model is larger than that of the JC model. The material model parameters obtained from the research have a high accuracy. The research provides a new method for calibrating the material model parameters of metal sheets, which has certain reference value for damage assessment and designation of protective structure.

Exploring complex potential energy landscapes of computationally modelled ballistic modifiers

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Keywords: ballistic modifiers; double-base propellants; computational.

Lead-based ballistic modifiers are the industry standard for double-base propellants (DBPs), though this is highly problematic due to their toxic nature. Incoming legislation will see a restriction in their use and hence, there is a required effort to find alternatives. To this end, a computational model has recently been created to help explore the combustion chemistry of propellants in the presence of ballistic modifiers in the form of metal oxides. A key takeaway from the model is how the metal oxides interact with carbon (soot) that is known to form during combustion. Given the highly non-equilibrium conditions of the combustion flame, the model draws on random structure generation, to explore the ensemble of states that could arise when different metal oxide clusters interact with growing amounts of amorphous carbon, and looks to draw trends based on competing metal-oxygen and metal-carbon bond strengths. Given the random nature of structure generation, at present a lot of computational time is wasted due to failure to focus in on the lower energy structures on the potential energy surface. Thus, this work seeks to streamline and improve the pre-existing computational model, in order to improve both computational efficiency and the reliability of trends that are emerging from the computed data set.

PETN under pressure

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Keywords: pentaerythritol tetranitrate; PETN; high pressure; impact sensitivity.

The performance of energetic materials is commonly linked to their crystal structure, which is well known to be affected by changing pressure and temperature. An energetic whose changing properties under pressure have not been widely studied is pentaerythritol tetranitrate (PETN). PETN is an impact sensitive explosive, commonly used as a part of plastic bonded explosives, including SEMTEX. As part of our study, experimental high-pressure neutron powder diffraction experiments were undertaken and showed changes in the behaviour of PETN around 4GPa. However, these are difficult to explain experimentally, so computational modelling can be used to help understand any structural changes and their effects. The computational work presented here will investigate changes in structure and vibrational spectra of PETN with up to 11GPa of applied pressure and evaluate how these changes can explain variations in properties, including sensitivity, under applied pressure.

Some issues of hydroxyl derivatives of ferrocene as modifiers of the combustion rate of composite propellants

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Keywords: ferrocene; hydroxyl derivatives; applications; synthesis.

For many decades, a significant number of scientific papers and patents have been published every year, indicating that a new derivative of ferrocene is emerging, which can be successfully used as a burning rate modifier for a solid composite rocket propellant (CP). Usually, authors of such works present only research results confirming their thesis about the usefulness of a given derivative. It cannot be ruled out that the authors of these works actually obtained a useful derivative, but - if comprehensive research results are lacking - this cannot be said with certainty. In this work, in the form of a discussion of case studies, the main aspects that - according to the authors - are worth paying attention to when analyzing literature reports on new ferrocene derivatives, useful as modifiers of the burning rate of CPs, has been characterized. Special attention was paid to ferrocene derivatives containing hydroxyl group, because on the one hand they have been known for a long time, and on the other hand they have been studied relatively rarely.

Long term decomposition and crystallisation kinetics of ADN under some crystallographic aspects

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Keywords: ADN; stability; XRD.

Ammonium dinitramide [NH4]+[N3O4]- (ADN) is a very promising replacement for the chlorine bearing oxidizer ammonium perchlorate, avoiding large scale hydrochloric acid release as well as a strong spectroscopic signature. Understanding the responsible mechanisms for the long- and short term decomposition processes requires the investigation of the crystal structure, the crystal growth and its resulting habitus as well as the thermal decomposition processes. Ammonium dinitramide obtained from aqueous solutions was investigated. Applied methods include in-situ PXRD, long term PXRD investigations, DSC, SEM, spectroscopy and in perspective in-situ single crystal diffraction experiments. The investigations suggest that decomposition reactions result in crystal cleaving along (020) planes, which are energetically unfavorable faces of slow growth. The proposed mechanism in question combines aspects of acidity, thermal stress and vacuum stability. A significant factor is the presence or absence of ammonia and acids to inhibit decomposition reactions NH4+ -> NH3 ↑+ H+ triggering H+ + N3O4- -> HNO3 + N2O ↑ and HNO3 + NH4N3O4 -> NH4NO3 + H+ + N3O4-. Understanding the mechanism of decompositions helps to improve the fabrication of ADN-based fuels, avoiding potentially harmful treatment. Avoiding perchlorate caused environmental and detectability issues is of great concern for rocket applications.

Towards purifying polyvinyl nitrate

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Keywords: polyvinyl nitrate; thermal; mechanochemical; polymers.

Energetic polymers such as nitrocellulose and glycidyl azide polymer (GAP) are of great interest for applications in solid propellants as these increase energetic output and performance. Previously, polyvinyl nitrate (PVN) was considered as a potential energetic binder, but it has been reported to suffer from poor thermal stability and chemical stability, combined with variable levels of chemical purity. In the current work, we have developed an improved methodology for the preparation of PVN in order to produce a material of greater purity and chemical stability than previously reported. For this reason, we are exploring structure-property relationships of PVN including sensitivity to initiation, polymer chain length, extent of nitration and compatibilities with selected solid oxidisers, stabilisers and plasticisers. In addition, we are also exploring the effects of crosslinking as a technique for modifying the properties of PVN using a range of analytical techniques including GPC, NMR spectroscopy, and DSC/TGA. This presentation will outline recent steps towards demonstrating high purity PVN with comparison to the thermal and mechanochemical properties of nitrocellulose.

Novel explosive method for the synthesis of silver nanoparticles

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Keywords: nanoparticles; silver azide; silver fulminate; BANG.

The detonation of explosive materials creates unique and extreme conditions, which typically require expensive, specialized equipment to replicate and are far more time-consuming than simple detonation processes. These extreme conditions, however, can be harnessed for the synthesis of functional inorganic materials. Recent investigations into silver-based explosives have demonstrated the generation of silver nanoparticles during detonation, marking a significant advancement in the BANG (Bristol Accelerated Nanoparticle Generation) method, previously limited to gold. This solvent-free synthesis enables the creation of uncapped, heterogeneous nanoparticles, offering enhanced versatility for subsequent functionalization or application. Nanoparticle formation was verified using transmission electron microscopy (TEM), while their composition was confirmed through electron/X-ray diffraction techniques.

Comparing thermal and chemical analysis of aged and unaged NC-based propellants

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Keywords: stabilizer; nitrocellulose based propellants; ultra high performance liquid chromatography.

Nitrocellulose (NC)-based propellants gradually decompose during ageing. Stabilizers are used to mitigate NC degradation, ensuring safer storage and performance. Traditionally thermal analysis techniques such as Differential Scanning Calorimetry (DSC), Thermogravimetric Analysis (TGA), and Pressure Vacuum Stability Testing (PVST), along with accelerated ageing studies using Heat Flow Calorimetry (HFC), have been used to evaluate the stability and predict the lifetime of propellants. While these methods provide valuable insights, they are often limited in their ability to detect localized variations in composition within propellant samples. This study investigated the stability of two double-base NC-based propellants subjected to ageing under two distinct temperature conditions: a hot environment and a cold environment. Samples were analyzed at different locations within the propellant: top edge, middle, bottom and inhibitor layers (top and bottom), to evaluate spatial variations within the sample. Analytical methods included HFC, DSC, PVST, and Ultra High Performance Liquid Chromatography (UPLC). While HFC and DSC results showed no significant differences between aged and unaged samples, PVST and UPLC analyses revealed local variations in nitroglycerin (NG) and stabilizer content. UPLC detected a decrease in NG levels, particularly from the middle to the bottom section of the propellant. Furthermore, stabilizer content measurements confirmed expected reductions with ageing. These findings highlight the complementarity of UPLC in detecting localized chemical changes due to ageing, which thermal analysis techniques may not reveal. This study highlights the importance of combining multiple analytical techniques to assess the ageing behavior of NC-based propellants. By using UPLC, the identification of localized variations in the composition of a gun propellant due to ageing, which might not be revealed with thermal analysis alone, might be crucial for improving the predictive accuracy of propellant stability and ensuring their safe and reliable use.

Reinvestigation of alkali and alkaline earth metal styphnate salts as components for priming compositions

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Keywords: nitroaromatics; priming mixture; primary explosive; styphnate.

A primary explosive is a crucial component in the initiation chain, forming a shockwave from external stimulus. Commonly used heavy metal based primary explosives, such as lead styphnate (LS) and lead azide (LA) are known to contaminate the environment and exhibit high toxicity. Therefore, use of lead-based explosives is planned to be prohibited by the European Union in the near future. Although, the trend of research is currently more focused on energetic coordination compounds (ECC), the rich history, application and the cost of nitrophenol-derivatives and their salts remains attractive for development of future primary explosives. Together with 2,4,6-trinitrotoluene (TNT) and 2,4,6-trinitrophenol (PA), 2,4,6-trinitrobenzene-1,3-diol (styphnic acid) has played a large role in the development of modern energetic materials. As noted earlier, lead styphnate has been successfully employed in current priming mixtures. With this in mind, taking a step back from synthesis of novel ECCs and following the more conventional route of creating non-toxic nitrophenol salts was the point of interest in the following research. Multiple literature known compounds such as potassium styphnate, as well as novel alkali metal and alkaline earth metal styphnates were synthesized for this purpose. Following those syntheses, the constitutions of different styphnate salts were confirmed using single crystal X-ray diffraction, and its purity was determined by elemental analysis (EA). To evaluate the applicability of these styphnate salts, standard analysis methods for energetic materials were employed. These methods included, differential thermal analysis (DTA), hot plate (HP)/hot needle (HN) test, initiation test, as well as the sensitivity measurements for impact (IS), friction (FS) and electrostatic discharge (ESD).

Measuring powder flow parameters of inert simulants for 3D printing explosives

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Keywords: FT4-rheometer; powder flow; rheology; particle.

It is important to study the powder behavior of energetic materials before using them in either conventional or novel manufacturing processes such as 3D printing to ensure the safe handling of the energetic materials. This project studies different powder materials as simulants for RDX powder. The focus is to familiarize with the Freeman Technology FT4 powder rheometer to gather data on the flowability and powder properties of the simulants powders and compare them to the powder properties of RDX powder, in particular with a focus on applications in additive manufacturing. The work focuses on data analysis of FT4 results in order to obtain measurements that provide an accurate and thorough understanding and can be used to evaluate if the selected powder simulants can mimic the powder behavior of RDX. The experiments are done in atmospheric conditions and the powder simulants used are inert with different particle size distributions. The conducted experiments are stability and variable flow rate test, aeration test, compressibility test, permeability test, shear cell test, and wall friction test. The stability and variable flow rate test and the aeration test showed that ammonium sulfate requires more energy to flow. The compressibility test showed that melamine is more compressible in comparison to ammonium sulfate. Moreover, the shear cell test showed that melamine is more cohesive, and the wall friction test showed that ammonium sulfate is less cohesive to walls compared to melamine.

The effect of graphene oxide (GO) on the bulk crystallization of ammonium nitrate

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Keywords: ammonium nitrate (AN); graphene oxide (GO); crystallization; phase transition; phase stabilization.

Ammonium nitrate (AN) is used extensively as a high nitrogen fertilizer and acts as an oxidiser in the energetic materials field. It is well known that its usage as part of a composite propellant is limited due to undesirable characteristics such as low burning rate, high hygroscopicity, low stability, and phase transformations. Even with these limitations, there is substantial interest nowadays in the development of AN based propellants as a replacement for Ammonium Perchlorate. This project studies the effect of Graphene Oxide (G/GO) on the polymorphic stability, phase transition behaviour and crystal structure of AN. G/GO exhibits a number of properties such as large surface area, energetic reactivity, good thermal conductivity and strong mechanical properties which may enhance the behaviour of AN. This study examines the crystallisation and behaviour of AN when doped with G/GO, using a range of crystallisation methods and considers the effect of growth conditions in addition to the role of G/GO as a nucleating agent. This workshows that the behaviour of AN when crystallised in the presence of G/GO differs from that where AN is crystallised onto G/GO surfaces.

Replacement of RDX by TKX-50 in a plastic bonded explosive based on Viton A

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Keywords: TKX-50; PBX; Viton-A; detonation; thermal.

In this study, Dihydroxylammonium 5,5ť-bistetrazole-1,1ť-diolate (TKX-50) has been prepared and purified. The morphology of the crystals has been investigated by scanning electron microscope. TKX-50 was studied in the form of plastic explosive bonded by Viton A polymer and the results were compared with the RDX bonded by the same polymer. Sensitivity to impact and friction were measured. The thermal behaviour was studied using differential scanning calorimetry (DSC). The detonation characteristics were calculated by means of EXPLO 5 code. Based on the mutual comparison of all the obtained results, it was concluded that replacement of RDX by TKX-50 in the PBXs compositions has decreased both the impact and friction sensitivities. Thermal behavior of both PBXs have close maximum decomposition peaks. The detonation parameters calculated by EXPLO 5 code showed that PBX based on TKX-50 are higher than that based on RDX.

Hazard evaluation of nitrocellulose synthesized from okara (soy bean-curd refuse) as a raw material

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Keywords: nitrocellulose; okara (soy bean-curd refuse); hazard evaluation.

Nitrocellulose (NC), used in gunpowder and paints, is synthesized by nitrating cellulose through a reaction with mixed acids (sulfuric acid and nitric acid). While cotton linter and wood chips are commonly used as cellulose-containing raw materials, recent studies have explored NC synthesis techniques using previously untapped materials such as nata de coco. In this study, nitrocellulose was successfully synthesized using 'Okara' (soybean-curd refuse), a waste byproduct containing 42% insoluble dietary fiber, generated during the production of 'Tofu,' a traditional Japanese food. The raw Okara was pretreated to remove impurities using an alkaline solution, and followed by a nitration reaction. Finally, the product was collected after repeated hot water washing. Structural analysis of the resulting pale yellow powder using Fourier-transform infrared spectroscopy (FTIR) revealed three peaks derived from nitrate groups, suggesting the formation of NC. Thermal analysis and friction sensitivity tests were conducted on the obtained NC, and the results were compared with those of conventional NC used as a propellant material. DSC results revealed that the exothermic onset temperature of Okara-derived NC was lower than that of conventional NC, but the peak shape mostly corresponded to that of conventional NC.

Enhancing the rheological and processing properties of PBX explosives containing boron through surface modifications and compatibilization with the binder

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Keywords: boron powder; pre-pasivated boron; thermobaric PBX; compatibility; rheology.

Besides commonly used aluminium or magnesium, boron is one of the attractive metal powders for thermobaric PBX explosive formulations, particularly due to its high gravimetric and volumetric heat of oxidation. However, there are some important challenges such as compatibility issues with the most often used hydroxy-terminated polybutadiene (HTPB) binders and high suspension viscosity of these formulations. Mitigation strategies like particle phlegmatization and the addition of compatibilizing agents may improve the processing characteristics of the PBX formulations. This study investigates the influence of boron powder particles on the rheological behavior of polymeric binders used in cast-cured PBX formulations and possible options to improve the castability of these explosive compositions. In the first part of the research, suspensions were prepared: boron powder in HTPB, boron powder in carboxyl-terminated polybutadiene (CTBN), boron pre-passivated with HTPB in HTPB, and boron with the addition of octadecylamine as a compatibilizer in HTPB. In the second part of the study, two HMX-based thermobaric explosive formulations were manufactured, with boron powder and HTPB-pre-passivated boron. Morphology of B powder and phlegmatized B particles was examined by scanning electron microscopy and particle size analyses, to observe particle size and shape. Differential thermal analyses were performed to estimate the extent of compatibility between boron and the binders. The rheological characteristics were determined of pre-polymer suspensions based on HTPB/CTBN containing boron powder, phlegmatized boron powder, or boron powder with octadecyl amine. These analyses included viscosity-shear rate dependencies, dynamic rheological properties, and deformation amplitude-frequency responses, tracked by a rheometer. The obtained results will contribute to a deeper understanding of the rheological behavior of boron-containing PBX formulations, offering insights into the potential optimization of their processing properties.

Effects of the explosion-generated plasma on the ammunition shell

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Keywords: explosion-generated plasma; EGP; explosive ordnance disposal; EOD; artillery shell.

Inspired by the work of our dear colleagues from the University of Pardubice and OZM Research, Jirman, Kucera, Selesovsky and Pachman, presented in the 26th NTREM, our goal was to test whether the explosion-generated plasma (EGP) can penetrate the artillery shell. If proven so, this can be practically implemented in the in situ explosive ordnance disposal. This paper presents the research of the EGP effect on 82 mm mortar shell and 100 mm shaped charge artillery shell. The tests were also conducted on thin steel plate and brass cartridge casing retrieved from the 76 mm artillery round. Used leading tube was made from plastic in cylindrical form and from metal in the conical shape.

Effect of 3D printed shaped charge liner on the effectiveness of shaped charges

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Keywords: shaped charge liner; 3D printing; Czech Army; Pl Np 10; engineer corps.

The possibilities of 3D printing have significantly expanded in recent years, driven by the continuous development of new materials, technologies, and methods of application. 3D printing is no longer limited to industrial use or hobbyists; it is increasingly finding applications in advanced fields such as military engineering. These innovations are also being integrated into the structures of the Czech Army and other armed forces, enabling new approaches to solving technical and operational challenges. This article focuses on the use of 3D-printed shaped charges in military demolition works and their effectiveness in destroying target. The charges were designed with varying stand-off distances from the target, allowing for thorough testing of their efficiency and impact. Advanced methods were employed to analyze the results, including precise machine measurement of the resulting entry holes and metallographic examination of the damaged materials and shaped charge liners. Particular attention was given to testing the 3D printing filament used, which contained copper. This significantly influenced the formation and effectiveness of the shaped charge, by using 3D printed liners. The results demonstrated that this technology enables both full penetrations and partial damage to target materials, depending on the configuration of the charges and the stand-off distance. This research confirms that 3D printing offers not only flexibility in the design and production of specialized explosive devices but also opens new opportunities for optimizing military equipment. The article concludes by discussing the achieved results and their potential practical applications, including further development and refinement of these innovative technologies within armed forces.

Research on TNT equivalence of different PBX with aluminium and magnesium

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Keywords: detonation; air shock wave; TNT equivalence; PBX.

Coefficient of TNT equivalence can be used in performance and safety considerations. It is effectively used for evaluation of the blast performance for different high-explosives. In this study, experimental data is used to assess TNT equivalent of polymer-bonded high explosive compositions with RDX or HMX, ammonium perchlorate, aluminium, magnesium and hydroxyl-terminated polybutadiene polymer binder. The detonation velocity was experimentally determined using fibre-optical probes connected to a photo detector and a time counter. The TNT equivalency of these compositions is determined using experimental measurements of peak overpressures and impulse of air shock wave at different distances using appropriate measuring system with pencil-type piezoelectric sensors. That results were compared with experimental data for explosive charges standard melt-cast TNT in order to determine coefficients of TNT equivalence.

Thermal characterization of CHNO-oxidizer TNEF

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Keywords: TNEF; thermal stability; microcalorimetry; mass loss; gas evolution.

The pure CHNO oxidizer TNEF (tris (2.2.2-trinitroethyl) orthoformate) has the potential to replace the oxidizer AP (ammonium perchlorate) and to improve the environmental aspect of composite rocket propellants. The oxygen balance with respect to CO formation from carbon content is 30.4% (AP: 34%, ADN: 25.8, HNF: 21.9%). Impact sensitivity and friction sensitivity are with 5 Nm and 95 N in well manageable ranges. Because of the three trinitroethyl groups in TNEF a bit of concern is allowed about the thermal-chemical stability of TNEF. In other molecules of this type the stability demands could not be reached. To leave no doubt about this important aspect thermal loads at several low and medium temperature condition where performed using mass loss, heat generation rate, gas evolution and adiabatic selfheating. DSC measurements in high pressure crucibles at several heat rates are used to determine the Arrhenius parameters along the decomposition conversion. The results are discussed and evaluated.

Numerical study regarding the functioning of solid rocket motor using 3d printed grain

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Keywords: additive manufacturing; numerical study.

Fast advance made in the additive manufacturing of solid propellant grains leads to new possibilities for obtaining a wide spectrum of thrust curves. Additive manufacturing, commonly known as 3D printing, represents an innovative approach in the production of rocket propellants, offering significant advantages over traditional manufacturing methods. This technology enables the creation of complex geometries for solid propellants, known as grains, which optimize combustion characteristics such as burn rate, pressure, and thrust performance. In this paper, we propose a numerical study conducted using ANSYS Fluent, a computational fluid dynamics (CFD) tool, to simulate the combustion dynamics of 3D-printed solid propellants and evaluate their performance in rocket motors.

Study on performance and safety characteristics of multilayer composite propellants

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Keywords: composite propellant; mutilayer propellant; performance characteristic; safety characteristic.

Solid propellants have become indispensable in propulsion systems, particularly in rocket engines, where they are used in over 90% of aerospace applications. Advances in propellant technology, especially the development of multilayer propellants, have addressed the need for more precise burn rate control. This study focuses on the formulation and experimental evaluation of multilayer composite propellants. Two propellant mixtures were developed and configured in parallel layers for testing. This research investigates the safety and performance characteristics of multilayer composite propellants through a series of rigorous tests. Key parameters, including density, burn rates, friction and impact sensitivity, heat of combustion, thermal stability, mechanical sensibility were studied, as well as closed vessel tests were performed in order to determine ballistic properties.

Synthesis and evaluation of HEDOs in propellant formulations

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Keywords: HEDOs; propellant; SMX; TNEF; oxidisers.

The feasibility of high-energy formulations, able to sustain high performances while using significant amounts of burning rate modifiers was investigated for spherical propellants. The latter are traditionally used for small-calibre applications, and this work investigates the use of HEDOs (high-energy dense oxidisers) to provide enough oxygen to maximise the combustion potential of the nitrocellulose matrix and achieve higher performances. This may be a potential route to broaden the applicability of spherical propellants to mediumcalibre applications.

Tris(2,2,2-trinitroethoxy)methane, also known as TNEF or trinitroethyl formate[1], and SMX (1,4-dinitrato-2,3-dinitro-2,3-bis(nitratomethylene) butane[2]) were chosen for the study, synthesised and characterised, on a hundred-gram scale.

The processability of formulations containing SMX and TNEF was studied. Spherical and extruded propellants were prepared, containing increasing amounts of TNEF or SMX using green stabilisers [3, 4]. The results obtained for the synthesis of the additive, the formulation and production of the propellants are presented in this poster. The next steps will consist in the evaluation of the propellants in closed-vessel and ballistic tests.

Synthesis and characterization of 1-hydroxy-5-methyltetrazole and its energetic salts

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Keywords: tetrazole; high energetics; cycloaddition; oxidation.

The main goal of this work was the synthesis and characterization of novel insensitive high explosives based on 1-hydroxy-5-methyltetrazole, which served as scaffold/anion from which several nitrogen rich energetic salts were prepared. The compounds were extensively characterized by ^{1}H, ^{13}C NMR and IR spectroscopy, high resolution mass spectrometry, elemental analysis as well as low temperature single crystal X-ray diffraction. The thermal stabilities were elucidated by differential thermal analysis and thermo gravimetric analysis. The sensitivities towards impact were measured with a BAM drop hammer, the sensitivities towards friction were measured with a BAM friction apparatus applying one out of six procedure. The energetic performances were calculated with the EXPLO5 code, using the room temperature converted X-ray densities and solid state heats of formation, which were calculated using the Gaussian G09 program and the method CBS-4M.

Numerical and experimental analysis of Semtex 1A blast wave parameters

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Keywords: blast wave; Semtex 1A; BlastFOAM; overpressure; near-field; far-field; simulation; experiment.

The propagation of blast waves in both near and far fields was studied using a numerical approach with the open-source software blastFOAM, validated by experimental data. The experiments involved 250 g and 500 g hemispherical charges of Semtex 1A placed on the ground. Pressure probes were deployed at distances ranging from 2 to 9 meters, while high-speed cameras were positioned at 13.64 m and 40 m from the charge to observe the blast wave velocity. The numerical simulations were done for hemispherical charge of 500 g of TNT, as well as for 250 g and 500 g charges of Semtex 1A, all placed on the ground. These simulations aimed to assess the effects of changing various simulation parameters on the pressure profiles, which were then optimized to match the experimental values. The optimized parameters were subsequently applied to near-field simulations. Experimental measurements and numerical predictions of incident over-pressures and arrival times were then compared.

Rocket motor insulation – different fillers and their effect on rheological behavior and internal structure

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Keywords: rocket motor insulation; rheology; internal structure; filler.

The use of polymer composite materials in aerospace as heat protection systems has been a common practice for many years. Protecting structures against extreme temperatures are crucial here. These materials, also called insulations, must withstand temperatures of up to 3000 řC including abrasion effects. They are often consist of complex polymer mixtures filled with fibers and particles.

In cooperation with Ludwig Maximilian University Munich (LMU), Bayern-Chemie (BC) has conducted extensive research on rheological behavior of such complex polymer mixtures.

A special focus was on the influence of the fillers (fibers and/ or particles) on the internal structure. In order to examine these influences in more detail different simplified compositions were examined and compared by means of rheological oscillation measurements. Fiber mixtures have different internal structures compared to particle mixtures. These characteristics have different effects on the structure and influence the insulation according to the rheological behavior by variation of the amount of filler material.

Lead oxide(II, IV) replacement in gasless pyrotechnic time delay compositions

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Keywords: time delay compositions; detonators; solid state reactions; burn rate.

This research delves into the comparison of combustion kinetics of Al/Bi2O3, Si/Bi2O3 and Si/Pb3O4 time delay compositions. The study aims to explore compositions that exhibit combustion rates independent of pressure inside the detonator. The combustion rates of silicon (Si/Bi2O3, Si/Pb3O4) and aluminium-based composition (Al/Bi2O3) were systematically studied, revealing distinct ranges for each composition. Al/Bi2O3 exhibited rates of 30 to 130 mm/s while Si/Bi2O3 exhibited rates of 15 to 110 mm/s. Notably, the Si/Pb3O4 composition showcased the highest combustion rates, ranging from 35 to 175 mm/s. The variations in combustion rates were attributed to the unique quantitative compositions and densities of each mixture. Additionally, temperature profiles for each composition were obtained using a thin thermocouple Pt-PtRh. These profiles offer valuable insights into the thermal dynamics of the combustion process, enhancing our understanding of the energetic properties of the silicon-based mixtures. Furthermore, the investigation involved measuring the heat of combustion across a broad range of quantitative compositions. The gasless combustion of each composition was verified through Differential Thermal Analysis (DTA) and X-ray Diffraction (XRD) techniques. The determination of qualitative combustion product compositions facilitated the calculation of adiabatic temperatures. To complement the quantitative findings, Scanning Electron Microscopy (SEM) images of the combustion products were obtained, providing visual insights into the morphological characteristics of the resulting structures. The use of silicon as a common fuel in these compositions contributes to the diversification of available pyrotechnic options for time-delay detonators. This study not only expands our understanding of combustion kinetics but also highlights the potential applicability of silicon-based mixtures in the field of energetic materials.

Synthesis and characterization of novel transition metal coordination compounds of 5-(3,5-dinitro-1H-pyrazol-4-yl)-1H-tetrazole

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Keywords: DNPT; coordination complexes; crystal structure; thermal analysis.

Based on the energetic ligand 5-(3,5-dinitro-1H-pyrazol-4-yl)-1H-tetrazole (H_2DNPT) and the transition metals copper and nickel, two novel coordination compounds have been synthesised. The compounds were characterised by a combination of IR spectroscopy, microanalysis, as well as X-ray crystallographic and thermochemical methods. Crystals of the M(DNPT) compounds reveal coordination polymeric structures, involving Cu(II) or Ni(II) coordination centres, respectively, interlinked by DNPT(2-) ligands activating various coordination modes, as well as coordinated water. The crystallographic results indicate high crystal densities. The materials are thermally robust (T$^{on}_{dec}$ > 300 řC). According to the Kamlet and Jacobs' method for predicting energetic performance, intriguingly high detonation velocities and pressures were found in the range of secondary explosives and comparable to RDX (CuDNPT: Q = 5741 J g^{-1}, p$_{CJ}$ = 461 kbar, D$_{CJ}$ = 9.28 km s^{-1}). Considering that metal-based energetics usually display the behaviour of primary explosives, these results warrant further investigation into their initiation and sensitivity characteristics, in particular regarding their potential as lead-free initiators.

Strategies for treating explosives-contaminated wastewater: addressing the environmental and health challenges of yellow, pink and especially red water

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Keywords: wastewater treatment; yellow water; pink water; red water; literature review.

The production and handling of high explosives generates various types of wastewater such as yellow water, pink water and red water, each of which must be treated before discharge. Yellow water is produced during the manufacture of explosives and contains mainly nitroaromatic compounds and a high acid content, while pink water, which is produced during loading, assembly and packaging (LAP) processes and munition demilitarization, is contaminated predominantly with 2,4,6-trinitrotoluene (TNT), cyclotrimethylene trinitramine (RDX) and 1,3,5,7-tetranitro-1,3,5,7-tetrazocane (HMX). Red water originates from the sulfonation purification processes for TNT production, is highly toxic and contains DNT-sulfonates and other nitrobodies as recalcitrant pollutants. For decades, wastewater was traditionally disposed of by evaporation in large open air concrete basins and successive incineration. However, commonly occurring leaks during the evaporation process led to serious environmental pollution problems such as surface, groundwater and soil contamination. This form of wastewater disposal is therefore an outdated concept, and a new solution must be found. This work reviews methods for wastewater treatment strategies, particularly for yellow, pink and red water, with a focus on the need for adaptable approaches that ensure environmental sustainability while mitigating the risks associated with hazardous, explosives-containing effluents.

Surface structures of HMX crystals investigated by means of confocal and atomic force microscopy

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Keywords: topography; HMX; crystals; microscopy.

Three HMX grades - a standard, a high-purity and a reduced sensitivity grade - were investigated using 3D imaging with confocal and atomic force microscopy. The standard and high-purity grades showed euhedral particles, i.e. with well grown faces, edges and corners, but also, intergrown crystal domains, twinning, and surface steps. Besides local defects were characterized on the surface, such as outgrowths, ditches, grain boundaries or microcavities, and outgrowth concentrations were quantified at various high levels. The investigations revealed high concentrations on standard grade crystals compared to the high purity grade. The RS-HMX variant showed a different picture of crystal shapes still far from spherical but with rounded edges and corners and without surface outgrowths. Such particle surfaces without sharp structures may help reducing the sensitivity of explosive particles and the viscosity of particle binder mixtures, whereas a moderate roughness supports a proper binder particle adhesion.

LOVA propellants based on RDX and GAP energetic plasticizers - Part 2

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Keywords: gun propellants; RDX; LOVA; composite.

LOVA gun propellants are essential components for the development of insensitive munitions. A typical LOVA propellant consists in an energetic filler (very fine RDX or HMX crystals) and a binder matrix comprising CAB/CA inert polymer, NC energetic polymer and an inert plasticizer. The general aim of our study was to develop a NC free LOVA propellant, based on fine RDX, CAB/CA and an energetic GAP plasticizer, and a processing method that allows simultaneous generation and polymer coating of very fine RDX particles, without the use of complicated/dangerous milling procedures to be applied to RDX. In tis context a novel technique for the precipitation of RDX was developed allowing us to obtain micronic RDX crystals already embedded into a CA matrix, the composite being further processed by a typical solvent process for mixing and extrusion into propellant grains. Initial ballistic investigations using close vessel firings were also performed, in order to comparatively evaluate the ballistic parameters of the new propellant.

Comparative analysis of the ESD sensitivity of B/KNO_3 and B_4C/KNO_3 pyrotechnic compositions

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Keywords: electrostatic discharge sensitivity; pyrotechnic initiation; boron compositions; safety assessment.

This study evaluates the electrostatic discharge (ESD) sensitivity of boron and potassium nitrate (B/PN) and boron carbide with potassium nitrate (B_4C/PN) compositions. Previous investigations for the B/PN composition report limited ESD data, primarily in the undamped mode, showing insensitivity up to 5 J. However, prior work demonstrated a 50% initiation probability of 12 mJ in the damped mode, indicating higher sensitivity when measured under conditions more representative for pyrotechnic initiation by thermal decomposition. This study aims to compare the ESD sensitivity between B/PN and B_4C/PN compositions using different ratios of fuel and oxidizer to understand how different reactive components influence their sensitivity and safety profile.

Thermal decomposition behavior of nitrocellulose in the presence of nitric acid solution

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Keywords: nitric acid; nitrocellulose; thermal decomposition behavior; spontaneous ignition.

Nitrocellulose (NC) is extensively used as a raw material in explosives, paints, and various industrial applications. However, it is susceptible to spontaneous decomposition even at room temperature, potentially leading to spontaneous ignition due to the accumulation of decomposition heat. In our previous studies, we conducted thermal analyses under constant-rate heating conditions using a Calvet-type calorimeter to examine the thermal decomposition behavior of NC in the presence of reactive substances such as oxygen, nitrogen dioxide, and nitric acid, which are known to accelerate decomposition. Among these substances, nitric acid exhibited the most significant effect, greatly enhancing the decomposition rate. Notably, NC mixed with nitric acid decomposed at a relatively low temperature (approximately 100 řC) with rapid heat release. In this study, we visually observed 2 g of NC mixed with nitric acid under isothermal conditions at 95 řC using a custom-made glass apparatus. Simultaneously, we monitored temperature changes with a K-type thermocouple. The observations revealed that NC emitted a brownish gas, likely NO2, followed by a sudden temperature increase in the sample after approximately 10 hours. The induction time prior to the heat release and the observed temperature profile were consistent with the estimated thermal behavior derived from differential kinetic analysis based on the thermal analysis.

Investigation of reaction propagation in commercially available shock tubes

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Keywords: shock tube; DDT; high-speed camera; piezoelectric pin sensors; heterogeneous detonation.

Shocktube (also known as detonation transmission tubing, or by the trade name 'NONEL') is part of a non-electrical ignition system that is widely used in mining, construction, military and scientific applications. It is a thin, hollow polymer tube, with a small amount of explosive, usually HMX/Al based, on its inner side. Its purpose is to transmit an initiation signal, whether in the form of detonation or deflagration, to the fuse (detonator). However, the exact principle of reaction propagation is not yet fully satisfactorily explained in the available literature.

In this work, nine types of commercially available shocktubes were compared. The flame acceleration and the process of transition from deflagration to detonation were recorded at 1M FPS using a high-speed camera. The recordings were evaluated as x-t diagrams, from which it was possible to determine the rate of reaction propagation in different parts of the tube. The tubes were also fitted with piezosensors to detect the arrival of the shock wave, and by synchronising the recording of the high-speed camera and the piezosensors, the position of the shock wave relative to the radiant reaction region in the tube could be observed.

The results demonstrate that in the initial stages, at velocities lower than 1500 m/s, the shock wave precedes the radiant region and the reaction proceeds by deflagration. At higher velocities (greater than 1500 m/s), the arrival of the signal at the piezosensor coincides with the radiant region and the reaction proceeds by detonation.

Calorimetric bomb test as a method for the selection of optimal boron powder for pyrotechnic applications

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Keywords: calorimetric bomb test; energetic potential; boron powder; particle size; pyrotechnic mixture.

The performance of energetic formulations is highly influenced by their chemical composition and by the physical properties of the ingredients. The choice of metal powders as often used fuel components in propellants, pyrotechnics, and explosives, plays a crucial role in determining their decomposition performance, i.e., their combustion characteristics. This study investigates the application of calorimetry as an analytical method to select the optimal boron powder for pyrotechnic mixtures B/KNO3, focusing on the influence of particle size. Selected nano- to micron-sized boron powders were first analyzed using scanning electron microscopy and particle size analyses. They were incorporated in pyrotechnic mixtures containing potassium nitrate and phenol-formaldehyde resin. These pyrotechnic formulations with boron powders of different particle sizes were systematically tested for their heat release and combustion efficiency using a calorimetry bomb test to determine their energetic potential, and measurement of combustion velocity. The results reveal a significant correlation between particle size and the thermal behavior of the pyrotechnic mixture, with smaller particles exhibiting faster combustion rates and higher heat output. By analyzing the calorimetric data, the study identifies the ideal boron particle size for maximizing energy release and improving the overall performance of B/KNO3-based pyrotechnic formulations. These findings provide valuable insights into potential directions of design optimization of more efficient and controlled pyrotechnic compositions.

Effect of copper tube quality on the cylinder expansion test results

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Keywords: CYLEX; nitromethane; photonic Doppler velocimetry; Cu-OFE; Cu-DHP.

Cylinder expansion (CYLEX) test is a common technique for characterization of metal acceleration capability of energetic materials. Usually, the CYLEX tests are done in oxygen-free copper tubes (Cu-OFE). In this paper, the results obtained with Cu-OFE and the more common Cu-DHP tubes are compared. The CYLEX tests were performed with nitromethane sensitized by the addition of 1, 5, 10 and 15 % of 1,2-diamminoethane. The wall velocities were measured using photonic Doppler velocimetry. Two probes were used per each tube allowing the detonation velocities to be determined simultaneously. These two types of copper tubes provided quite similar results. The Gurney velocities obtained with Cu-DHP tubes were slightly higher compared to Cu-OFE tubes. Quantifying the difference between available copper tubes allows for optimizing future testing procedures. The results were also compared with predictions obtained using the EXPLO5 code.

OPTIMEX: Optimization of a simple plane wave generator

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Keywords: fiber optic probe; plane wave generator; 3D printed lens; plastic bonded explosive.

Plane wave generators (PWGs) are often used in detonation and shock physics to initiate explosive charges or to accelerate flyer plates. There are many different types of PWGs that are applicable in various test scales and provide different levels of shockwave flatness. Testing of the PWGs can be done by using various diagnostic methods including high speed cameras and interferometry. In this paper, the use of passive fiber optic probes to optimize the design of a 30 mm diameter PWG is presented. Three different test setups were developed to check the radial symmetry of the detonation wave, the output shockwave curvature and the available shock amplitude. The tested PWG was based on an ordinary moldable plastic explosive and a 3d-printed inert lens but the test procedures are applicable to any other PWGs or even ordinary boosters.

Microwave synthesis of triethylene glycol diazide (TEGDA): Advanced approaches and characterization

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Keywords: energetic plasticiser; energetic material; microwave; synthesis; TEGDA.

Plasticizers are essential components in composite energetic materials to improve the mechanical properties, lower the glass transition temperature and improve the processability of propellants and explosives. In this area, energetic plasticizers are specific compounds because they usually have positive heat of formations and therefore increase the energy content of the formulation. An example of such an energetic plasticizer is the azido-functionalized plasticizer TEGDA, which is also known as bisazido triethylene glycol (BATEG) or 1,2-bis(2-azidoethoxy)ethane (BAEE). It is commonly synthesized in batch reactions from its corresponding chloride through reaction with sodium azide with a phase transfer catalyst in water. To improve the efficiency of the reaction in terms of reaction time and yield and to avoid unwanted by-products, the TEGDA synthesis in this study was carried out in a microwave chamber. The differences between two different reaction routes were investigated and the thermal stability of the products was characterized.

Characterizing the decomposition and hydrate stability of sodium 5,5'-azotetrazolate

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Keywords: sodium 5,5′-azotetrazolate; hydrate; DVS; DTA; decomposition.

Hydrate changes of sodium 5,5ť-azotetrazolate were studied by dynamic vapor sorption (DVS). Conditions of sodium 5,5ť-azotetrazolate hydrates changes at various humidities and temperatures were studied by dynamic vapor sorption (DVS). Decomposion products of sodium 5,5ť-azotetrazolate dihydrate crystalized from dimethylsulfoxide and acetone were described by infrared and Raman spectroscopy, and mass spectroscopy.

Molecular simulation of reaction mechanisms and transition states

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Keywords: quantum chemistry; reaction pathways; transition states; molecular simulation.

Molecular simulations provide profound insight into the atomic and molecular mechanisms that determine the behavior of materials. A particular method for this purpose is DMol3. It a density functional theory (DFT) quantum mechanical program included in the Materials Studio software package. The methodological aspects of using DMol3 to study the decomposition of energetic materials or their components through the identification of transition states and the calculation of activation energies are presented. The initial step in utilizing DMol3 is the geometric optimization of the molecules involved in the reaction. The optimization process is followed by the search for transition states, which represent the molecular configurations on the reaction pathway. To achieve this, DMol3 employs a range of algorithms with the objective of identifying the energy barriers between the reactants and products. These barriers, also known as activation energies, are of great significance in the comprehension of reaction kinetics. An example of a complex reaction behavior is the curing of CTPB (carboxyl-terminated polybutadiene) with aziridine-type curing agents, such as MAPO (tris[1-(2-methylaziridinyl)] phosphine oxide). MAPO displays distinctive behavior, exhibiting not only the primary curing reaction but also the splitting of the binder network through the breaking of N-P bonds within its chemical framework. This bond breaking is investigated using DMol3.

Study on the influence of material properties and explosive quantities on the formation of Explosively Formed Projectiles (EFP)

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Keywords: numerical simulations; explosively formed projectiles (EFP); material properties; explosive charge optimization; LS-DYNA; armor penetration.

This paper analyzes the formation of explosively formed projectiles (EFP), a field of significant interest in technological and military research. These projectiles are employed in military and industrial applications, capable of penetrating armor due to their speed and shape. This paper presents a comparative analysis, using numerical simulation, of the formation mechanisms of explosively formed projectiles (EFP) and their effects on armor. The research focuses on varying the type of metal used for the liner, the quantity and type of explosive employed, and the geometry of the configuration, examining how these parameters influence EFP formation. By using different materials, we aim to identify correlations between their mechanical properties, physical dimensions, and the characteristics of the resulting projectile. The article addresses the topic of numerical simulation, with simulations conducted using the LS-Dyna software to validate calculations and hypotheses related to explosively formed projectiles. To reduce analysis time, given the multitude of configurations tested, an axisymmetric 2D model was formulated. Euler and Lagrange models were employed for the constituent elements of the developed model. The results were compared, leading to the establishment of an optimal EFP configuration model.

The danger related to the use of ammunition and explosives

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Keywords: ammunition; explosive; danger; safety engineering.

The basic requirements placed on explosives and ammunition by their users are production and operational safety and operational reliability. Therefore, their technical condition must be monitored continuously. It is important to withdraw from service those batches of ammunition in which inconsistencies have been found that reduce the safety of use and operation. The main component of ammunition that poses a danger is the explosive. It is usually placed in a metal or cellulose body and in the fuse. Most types of ammunition provide direct access to the explosive through a hole in the case for the fuse. The surface of the material is protected by a thin layer of varnish or a paper disc, which only protects it from mechanical damage. This protection does not prevent direct access to the explosive. This creates the possibility of obtaining the material illegally for terrorist purposes. The purpose of the article is to point out the problems associated with the use of ammunition and the explosives in it. The paper presents selected examples of inconsistencies found during diagnostic tests of ammunition.

Comparative analysis and charge modeling using additive manufacturing in explosive breaching

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Keywords: additive manufacturing; engineer support; explosive breaching; fused deposition modeling.

The paper deals with the issue of explosive forcible entry into objects (breaching) as a developing area in the operations of the Czech Armed Forces. This specific approach to overcoming obstacles is crucial in modern military and police operations, emphasizing efficiency and safety. The study focuses on innovative approaches to the creation of charges that use new technologies and materials, with the aim of increasing their effectiveness and reducing risks to intervening troops and the civilian population. The main contribution of the paper is the comparative analysis of new types of charges compared to traditional methods and the design of optimized models created through additive manufacturing techniques. In the context of this study, additive manufacturing refers to the use of plastic materials by Fused Deposition Modeling, which represents a limitation in terms of mechanical properties and thermal resistance of the resulting models. The conclusions provide a basis for further research and development in this area, and can be applied in practical operations of the Armed Forces.

New smoke formulations based on copper (II) phthalocyanine

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Keywords: smoke formulation; copper (II) phthalocyanine; colored smoke.

In this paper, we address various smoke formulations based on copper (II) phthalocyanine. Smoke formulations have a wide range of applications, with the primary focus being in the military sector. Since several components are suspected to be harmful to the environment and health, continuous research is necessary to find better alternatives. Research has already been conducted in this field, which we aim to continue in this paper by presenting new blue and violet smoke mixtures. These formulations will be analyzed according to various smoke analysis parameters.

Measurement of a single fragment's velocity by using a controlled fragmentation method

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Keywords: controlled fragmentation; fragment velocity; fragment trajectory.

The phenomenon of explosively driven fragmentation of metal cases was mainly studied with statistical approaches due to its randomness. The behavior of a single fragment have been outside of the research subject because of the size, shape, position and flying direction of explosively generated fragments are hardly predicted. We have been developing a novel method to control fragmentation by using the shaped charge effects with 3D-printed models. This method controls the fracture positions on the metal cylinder, which decides the size, shape and positions of fragments. The velocity and trajectory of a single fragment was analyzed using screen sensors up to 4.0 m from the explosives. The single fragment's velocity calculated from the time of arrival and the distance at each sensor was about 900 m/s, which was consistent with high-speed camera results.

IEM research labs at the start to safety 2.0

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Keywords: management of change; laboratory safety.

Published data from various countries around the world demonstrate that safety in research laboratories is a lively and insufficiently resolved problem. The number of events with significant consequences or even fatalities is relatively high. A description of the situation in the USA is readily available, where significant institutions have been systematically working on improving safety in university research laboratories for about 15 years. Our experience from IEM confirms the seriousness of this topic. At the institute, we have recorded a number of accidents in research laboratories in the last 15 years, at least two of which were serious. It cannot be said that this topic is not being paid attention. However, it seems that safety is not being effectively supported in the basic situation that every worker/student approaching a new research topic faces: How do the conditions that my new research brings differ from the conditions with which I already have experience? In other words, effective management of change is not being achieved in the conditions of a research laboratory. In industry, the management of change (MoC) task has been identified as one of the key tasks of safety management for decades. A number of procedures have been developed to support effective MoC. We believe that the experience from industrial MoC can also be used to improve safety management in research laboratories. We have initiated research aimed at developing and testing a recommended procedure for ensuring safety in research, which will use industrial experience with MoC as well as available experience from improving safety in foreign research laboratories. This procedure should be simple and convincing enough that our researchers can and want to use it consistently. The creation of such a procedure seems to be an ambitious but realistic milestone that can be described as safety 2.0.

Selective synthesis of energetic acrylates using microreaction technology

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Keywords: flow-chemistry; microreaction technology; energetic acrylates.

The additive manufacturing of eneregtic plasticizers is gaining more interest and importance in composite materials for rocket propellants. Especially acrylate based compounds are highly interesting due to their property of controlled UV-polymerization, which provides highly precise manufacturing of complex geometries with clean surface texture. Those characteristics can positively affect performance and burning rates of propellants. The use of acrylate-based plasticizers also allows the alignment of mechanical properties by using acrylates based monomers with selected functional groups. To obtain energetic acrylates having aspired functional groups the synthesis are carried out in a reaction system using microreactors. The target products are 2-Nitratoethylacrylate, also known as 2-NEA, and propyl-2-nitrate-1,3-di(propyl-2-nitrate)diacrylate. The microreaction technology enables the controlled synthesis and parameter studies of products difficult to obtain such as acrylates with their high tendencies to polymerize under the crude conditions of the synthesis.

Synthesis and characterisation of the novel energetic triazenide: PPN bis(1-methyl-3-nitro-1,2,4-triazol-5-yl)triazenide

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Keywords: triazenide; novel energetic materials; thermal analysis; crystal structure.

Conventional energetics rely primarily on the chemistry of C-, N- and O- nitrated compounds as well as azides. Progress in energetic materials chemistry now relies more heavily on the exploitation of hitherto underexplored explosophoric groups. One such group relates to the structural motif of the triazenyl (R-N=N-NR_2) or triazenido groups (R-N=N-$N^{(-)}$-R) to which only a narrow record is associated in the chemical literature. We report on an experimental investigation into the synthesis of novel triazenes and triazenides, followed by a brief assessment of their potential to function as both the basis for energetic materials, and as explosophoric ligands and proligands in the synthesis of novel energetic coordination compounds. The previously unreported bis(1-methyl-3-nitro-1,2,4-triazol-5-yl)triazene (H-B1M3NTT) was isolated as the hydrated 1 : 1 bis(triphenylphosphine) iminium salt, PPN (B1M3NTT) ů $3H_2O$. The crystal structure of PPN (B1M3NTT) ů $3H_2O$ was determined. No interactions between PPN cation and B1M3NTT anion are present. Hydrogen bonds were found involving B1M3NTT and H_2O. PPN (B1M3NTT) ů $3H_2O$ dehydrates between 80 to 100 ^{o}C, but is otherwise highly temperature stable, exceeding onset and peak decomposition temperatures of the analogous iminium bis(1-methyl-tetrazol-5-yl)triazenide salt PPN (B1MTT). Based on our estimates for crystal density and heat of formation, and methods used to approximate Q, D$_{CJ}$ and p$_{CJ}$ values, H-B1M3NTT is predicted to have higher density, greater heat of detonation, and higher detonation pressure than both H-B1MTT and the related bis(2-methyl-tetrazol-5-yl)triazene (H-B2MTT) - compounds previously investigated as nitrogen-rich candidate components of solid rocket propellants.

The desulfurization of high nitrogen heterocycles

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Keywords: desulfurization; nitrogen; heterocycles; tetrazoles.

High-nitrogen heterocycles, such as tetrazoles, play crucial roles in fields ranging from pharmaceuticals to energetic materials due to their high nitrogen content and tunable reactivity. Despite their utility, traditional synthesis methods for these compounds often involve inconvenient procedures or toxic precursors, limiting their accessibility and broad application. Addressing these limitations, we present an efficient, environmentally friendly synthesis of 1-substituted-5H-tetrazoles. Our method involves the desulfurization of 1-substituted-1H-tetrazole-5-thiones, easily synthesizable from commercially available precursors and comparatively easy to handle. Using zinc chloride as a desulfurizing agent, we demonstrate a reliable and safe pathway that yields high-purity 1-substituted-5H-tetrazoles with significantly improved yields compared to conventional desulfurization processes.

The synthesis and characterization of energetic materials containing both a tetrazole and a strained ring moiety

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Keywords: heterocycles; tetrazoles; strain; ring.

The reaction of cyanogen azide with primary and secondary amines containing strained rings led to the synthesis of novel energetic compounds, deriving their energy from both the strained ring systems and aminotetrazoles. Azo-coupling of the produced 5-amino materials resulted in high-nitrogen energetic materials at high yields. Comprehensive chemical characterization of the synthesized compounds was performed using infrared (IR) spectroscopy, nuclear magnetic resonance (NMR) spectroscopy, single-crystal X-ray diffraction, and high-resolution mass spectrometry. The sensitivity of these materials to impact and friction was experimentally assessed, and their energetic performance was evaluated through computational methods. The results demonstrate the potential of these compounds as high-performance, sensitive energetic materials with promising potential applications in various fields.

Keyword Index

Author Index