ON MATERIALS' CAPABILITY TO DETONATE

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Abstract:
The idea of how to determine the composition of mixtures of liquid explosives with inert diluents and solutions of solid explosives in inert solvents which are still capable to detonate has been introduced. It has been demonstrated experimentally with nitromethane/acetone mixtures and diethanolnitramindinitrat/acetonitril solutions that the most weak composition still capable to detonate is that which detonation's CJ pressure is still larger than the minimum shock pressure necessary to initiate the detonation. Considerations have been proposed on conditions at which so called gasless detonation could be realized theoretically.

NEW HIGH EXPLOSIVES AND PROPELLANTS BASED ON BIURET AND TETRAZOLE COMPOUNDS

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Abstract:
The synthesis of energetic, non-nuclear materials for possible military application has been a long term goal in our research group. Modern high-energy-density materials (HEDM) derive most of their energy either (i) from oxidation of the carbon backbone, as with traditional energetic materials or (ii) from their very high positive heat of formation. Examples for the first class are traditional explosives such as TNT, RDX and HMX. Modern nitro compounds such as CL-20, TEX or the recently reported hepta-and octanitrocubanes possess very high densities and have enhanced energies due to substantial cage strain. The most recent and most exciting members of the second class of compounds are 3,3'-azobis(6-amino-1,2,4,5-tetrazine) and various salts which are based on the 5,5'-azotetrazolate dianion, which derive most of their energy from their very high positive heats of formation. The heavy metal salts of 5,5'-azotetrazolate, particularly lead 5,5'-azotetrazolate dihydroxide, have been investigated for use as initiators. The ammonium, guanidinium and trimetazoguanidinium salts of 5,5'-azotetrazolate were found to be powerful, yet smokeless gas generators. Since in general, tetrazole derivatives are very useful building blocks in the chemistry of highly nitrogen-rich compounds, in this contribution we report on the synthesis and characterization of several tetrazole based energetic materials with up to and over 90% nitrogen.

The synthesis, NMR spectroscopic characterization and structure determination of highly explosive tetrazole azide, a very nitrogren-rich material (88.3% N) is reported. The computed electrostatic potential suggests a pronounced shock and friction sensitivity which was confirmed experimentally. Quantitative valence bond (VB) calculations were performed for the most important 21 VB structures in order to obtain the structural weights and to obtain an assessment for the importance of the various individual VB structures considered.

The synthesis, reactivity and physical properties of new nitrogen-rich, highly energetic materials is presented.

Examples of nitrogen-rich compounds with up to 95% nitrogen content by weight include hydrazinium azide hydrazinate, $\text{N}_2\text{H}_5^+\text{N}_3^-$-$\text{N}_2\text{H}_4$ (91.5 % N) and trinitrotetrazidobenzene, $\text{C}_6(\text{N}_3)_3(\text{NO}_2)_3$. Also presented are new, highly energetic tetrazole derivatives and derivatives of tetrazene.

The heats of combustion ($\Delta H_{\text{comb}}$) of dinitrobiuret (DNB) and dianimotetrazole nitrate (HDAT-NO$_3$) were determined experimentally using oxygen bomb calorimetry: $\Delta H_{\text{comb}}$(DNB) = 5195 ± 200 kJ kg$^{-1}$, $\Delta H_{\text{comb}}$(DAT-NO$_3$) = 7900 ± 300 kJ kg$^{-1}$. The standard heats of formation ($\Delta H_f^\circ$) of DNB and HDAT-NO$_3$ were obtained on the basis of quantum chemical computations: $\Delta H_f^\circ$(DNB) = - 353 kJ mol$^{-1}$, - 1829 kJ kg$^{-1}$; $\Delta H_f^\circ$(HDAT-NO$_3$) = + 254 kJ mol$^{-1}$, + 1558 kJ kg$^{-1}$. The detonation velocities (D) and detonation pressures (P) of DNB and HDAT-NO$_3$ were calculated semiempirically: D(DNB) = 8.66 mm µs$^{-1}$, P(DNB) = 33.9 Gpa; D(DAT-NO$_3$) = 8.77 mm µs$^{-1}$, P(DAT-NO$_3$) = 33.3 Gpa.

Integral to this research are investigations concerning the explosive nature and safe-handling of...
such compounds. The sensitivity of the compounds towards heat, friction and electrostatic shock have been both experimentally (drop hammer, steel sleeve and firing tests) and theoretically investigated (calculation of electrostatic potential surfaces). Possible applications for these energetic materials will be highlighted, in particular with respect to new detonators and rocket propulsion systems.

NEW SAFETY THINKING APPLICABLE TO EM SYNTHESIS AND MANUFACTURE

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Abstract:
The occurrence of major accidents in the chemical process industry has over the years stimulated world wide safety thinking. This resulted also rather recently in interesting new concepts in the approach to design and the control of operation of processes with hazardous materials. A practical concept applicable in many situations is the layer of protection analysis. This kind of top down barrier thinking encompasses both technical and organisational measures and is very suited for risk control both in the laboratory and in the case of industrial installations. It involves the user and his management and can optimise cost-benefit. It can be used in new design, but also for installations that have been operated already for years. Thinking starts of course with the question what are the risks and can these be prevented. The inherent safer approach offers a number of check list items which can be checked off. Improvements can semi-quantitatively be measured by indexing. Of course with energetic materials inherent safer working has its limitations, but sometimes by selecting different solvents, other installation lay-out etc. considerable improvements can be made. Subsequently independent layers of protection are defined. Independence is not easy to realise, but is a crucial condition. In a second part specific hazards of energetic materials are highlighted. This is covering the initiation and explosion severity of energetic materials themselves, the process runaway risk when manufacturing them and the health hazards solvents may present.

INFLUENCE OF TAMPING ON PERFORMANCE OF LINEAR SHAPED CHARGES

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Abstract:
Nowadays we are often confronted with limitation of quantity of explosives in terms of protection of surroundings, hygienic standards etc. Linear shaped charges (LSC) as such represent significant reduction in quantity of explosives (when compared with open charges) at blasting work, especially at demolitions of metal structures. Further decrease in quantity of explosives is achieved by tamping. This report deals with finding of relationship (represented by cavity depth produced by jet of LSC in steel plate with 30 mm thickness) between tamped and open LSC of the same performance.

LIQUID PHASE AND SOLID PHASE NITRATION OF AROMATIC COMPOUNDS: GREEN SYNTHETIC ROUTES

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Abstract
Selective mono- and di-nitration of aromatic hydrocarbons with various nitrating agents are discussed. Nitration of hindered diamines with potassium nitrate in conc. sulfuric acid yielded 80-95% di-nitro derivatives. Nitration using 40% nitric acid with montmorillonite K10 and ferric nitrate supported on montmorillonite K10 showed high p-selectivity for mono-substituted substrates and also avoids the use of sulfuric acid. The total omission of sulfuric acid and the reduction of nitric acid concentration to 40% considerably reduce the emission of environmental pollutants. The montmorillonite K10 used as the solid support and catalyst is reusable by removing the water formed in the reaction followed by washing with acetone and subsequent drying in an air oven at 110°C.

DEVELOPMENT OF ENERGETIC SALTS FOR PROPELLANTS

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Abstract:
The development of new energetic salt compounds composed by an ammonium cation fixed on an energetic nitrogen heterocycle and a nitrate anion are presented here. On one hand, these materials are more stable than their counterpart with nitro groups because of ionic charges which increase the cohesive energy. Despite the latter reduces the solid state heat of formation, the presence of ammonium and nitro groups on the energetic backbone decreases this effect. On the other hand, the nitrate group provides the oxygen necessary to generate stable reaction products. Moreover, the synthesis of these compounds requires methods to estimate their performances which depend on the density and the heat of formation. This provides information to lead chemists to promising components. A contribution groups method to estimate the density and semi-empirical methods to evaluate the heat of formation of salts have been developed because of the lack of suitable methods for ionic species.

STUDIES ON THE NITRATION OF NEW POTENTIAL PRECURSORS FOR FOX-7

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** Swedish Defence Research Agency (FOI), SE-147 25 Tumba, Sweden

Abstract:
The initial microstructure of hot pressed polymer bonded explosives and its evolution under thermal and mechanical aggressions were studied. The thermal aggressions include low temperature freezing and frozen combustion. Mechanical aggressions include tension, compression, ultrasonic wave insult and long-pulse low-velocity impact. The mechanical properties under tension and compression were studied and compared. Brazilian test was used to study the tensile properties. The failure mechanisms of polymer bonded explosives under different loading conditions were analyzed.

A 1:1 HNS-DIOXAN COMPLEX

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Abstract:
HNS IV is commonly produced by crash precipitation of a DMF or NMP solution into water. The product usually contains 0.5-1.5 wt% of solvent trapped inside the HNS crystals. This residual solvent may be removed by washing with methanol containing dioxan. However, this also causes a dramatic change in particle shape and size, and, unless further washed with pure methanol, the product will contain a considerable amount of dioxan. We have found that this dioxan-containing HNS is in fact a 1:1 complex with a different crystal structure to that of pure HNS. The dioxan may be removed from the complex by either heating above the boiling point of dioxan or washing with methanol. This does not significantly change the outward appearance of the crystals, but it does change the inner structure to that of normal HNS.

**DETERMINATION OF RESIDUE OF EXPLOSIVES IN ENVIRONMENTAL SAMPLES**

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Abstract:
Modern TLC equipment was used for determination of 1,3,5-trinitro-1,3,5-triazacyclohexane (RDX, hexogen) post-detonation residues in environmental samples. Chromatographic system suitable for the analyte separation from matrix components and method of densitometric determination of RDX was proposed. A linear dependence of densitometric peak areas A on the analyte mass c [ng] in the chromatographic band was received (A = 26.302 - c - 484). A limit detection (150 ng) and maximal range of linear measurements (1800 ng) were determined. Methods of extraction were specified and recoveries of RDX were estimated (they were about 70%).

**CHARACTERIZATION OF THE CARBONACEOUS PRODUCTS OF HALOGENOCARBONS REDUCTION IN COMBUSTION WAVE**

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Abstract:
In the paper a method of synthesis of carbonaceous materials in self-propagating heat waves is described and results of some physical and chemical investigations of the materials are presented. The chemical (ultimate analysis) and phase (XRD) composition as well as the microstructure (SEM) of the solid reaction products were determined. Next, the relation between reactant composition and heats of reaction as well as the amount, type and structure of the reaction products was established. It was shown that some of the obtained materials are characterized by unique structural and surface properties.

**STUDY ON COMBUSTION OF LIQUID AND GELATINIZED GLYCIDYL AZIDE OLIGOMERS**

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Abstract
Effect of the molecular weight of glycidyl azide oligomers on the burning rate and effect of gelatinization have been examined. It has been shown that combustion of uncured GAP obeys usual rules of monopropellant burning of liquid energetic materials with all resulting consequences (turbulization, unusual burn rate-pressure dependence, etc.). Small additives of PMMA, used as a
gelatinizing agent to GAP oligomers appeared to influence drastically their burning behavior through alteration of the viscosity. Data on combustion of uncured neat azide oligomers and their compositions with the polymer as well as data of temperature measurements in the combustion wave have been used to propose the combustion mechanism of azide energetic materials.

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INVESTIGATION OF DIAMINODINITROETHYLENE (DADNE)

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Abstract:
DADNE (FOX-7 or 1,1-diamine-2,2-dinitroethylene) is investigated by methods of differential-thermal (DTA) and thermo-gravimetric (TGA) analyses. Two exothermal peaks that, presumably, correspond to transitions between polymorphic modifications of this HE, are registered on DTA curve. Heat of low-temperature polymorphic transition (~±13°C) is estimated as ~25 J/g. Heat of high-temperature transition (~+158°C) is ~20J/g. Presence of two exothermic peaks (+207°C and +277°C under the heating rate of 2°C/min) on DTA of DADNE is confirmed. It is shown, that DADNE decomposes in two stages at heating over +210°C. The product of the first stage of decomposition of DADNE is new explosive (DADNE-T). The DTA, TGA, FTIR of DADNE-T are carried. The endothermic processes in DADNE-T in the temperature range +20°C - 400°C are not founded. The beginning of exothermic decomposition of DADNE-T is recorded. By results of FTIR it is supposed that DADNE-T is the product of chemical transformation of two molecules of DADNE with participation of the part of amino and nitro groups. The crystals of three types (tetrahedral prisms, crystals of the trimetric form and hexahedral prisms) are received at crystallization of DADNE from acetone, water and water-acetone mixes. Received crystals are investigated by methods of FTIR, DTA and TGA.

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ESTIMATION OF THE THERMODYNAMIC PROPERTIES OF SOLID PROPELLANTS

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Abstract:
The paper presents a theoretical method, based on Corner’s method, for the estimation of the thermodynamic properties of solid propellants. The mathematical model contains the truncated virial equation of state, the equilibrium constant equation for each chemical reaction, the mass and energy conservation equations. The virial coefficients were calculated from the intermolecular forces using the Lennard-Jones 6,12 potential function. Based on this model, a computer program, called REAL, has been written. At the end, one presents some results obtained with this program for three gun propellants.

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APPLICATION OF NOVEL ENERGETIC MATERIALS FOR INITIATORS AND EXPLOSIVE TRAINS

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Abstract:
As well as improving the survivability of weapons and platforms, Insensitive Munitions (IM) reduce both casualty rates and mission losses. Their use also leads to improved safety during storage and transportation. For a munition to completely fulfil IM criteria each of its energetic sub-systems must be IM compliant.
The initiator and explosive train are the most critical of these sub-systems; their safety and reliability are paramount if the weapon is to be suitable for service use. They are generally the most difficult part of a weapon system to protect from inadvertent initiation since their primary function is initiation of the main charge explosive. In the last decade, a number of new high temperature compounds with improved power outputs and potential for both exploding foil initiator (EFI) and explosive train applications have been reported. Several of the more promising materials based on pyrazine, pyridine and polynitro-aromatic systems have been successfully synthesised and characterised.

MICROSTRUCTURE, MECHANICAL PROPERTIES AND MECHANICAL FAILURE OF POLYMER BONDED EXPLOSIVES

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** Institute of Mechanics, Chinese Academy of Sciences, Beijing 100080, China

Abstract:
The initial microstructure of hot pressed polymer bonded explosives and its evolution under thermal and mechanical aggressions were studied. The thermal aggressions include low temperature freezing and frozen combustion. Mechanical aggressions include tension, compression, ultrasonic wave insult and long-pulse low-velocity impact. The mechanical properties under tension and compression were studied and compared. Brazilian test was used to study the tensile properties. The failure mechanisms of polymer bonded explosives under different loading conditions were analyzed.

SYNTHESIS AND CHARACTERISATION OF NITROGUANIDINE BASED NITRATE AND PERCHLORATE SALTS OF-5-NITRO-2-NITROIMINOHEXAHYDRO-1,3,5-TRIAZINE

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Abstract:
The condensation of nitroguanidine, formaldehyde and amine followed by nitration afforded 5-nitro-2-nitroiminohexahydro-1,3,5-triazine (2). Compound 2 on nitric acid and perchloric acid treatment afforded the nitrate and perchlorate salts of 2.

DETERMINATION OF LOW CONCENTRATION TRINITROTOLUENE CONTENT IN WATER SAMPLES

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Abstract
Polynitroaromatic organic explosives (2,4,6-trinitrotoluene) are typical labile and environmental
that can transform with soil indigenous microorganisms, photodegrade by sunlight and migrate through subsurface soil to cause groundwater contamination. To be able to determine the type and concentration of explosives and their (bio)transformation products in different soil environments, a comprehensive analytical methodology of sample preparation, separation and detection in thus required. This present paper describes the use of solid-phase microextraction (SPME) and solid-phase extraction (SPE) for the extraction of nitroaromatic explosives for subsequent analysis by either GC/MS or HPLC/UV. The two techniques are examined in terms of procedure, chromatographic analysis and method performance. The adsorption temperature and adsorption times were examined by the using SPME fiber. SPE extraction was done by variable columns and microcolumns and was examined the columns with high efficiency and with short sorption time.

NTREM, PARDUBICE, 2004 page 157-163
FLUID PROPERTIES: NEW MODELS FOR THE DENSITY AND THERMAL STABILITY OF ENERGETIC COMPOUNDS
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Abstract:
Many properties of molecular fluids may only be estimated using group contribution methods. Some of them lend themselves naturally to such an additive scheme (e.g. the density) while this is not the case for others (e.g. the thermal stability). Alternative models are presented to calculate the density and decomposition temperature of molecular liquids. For the density, the accuracy of the new scheme is similar to that of the most reliable available methods, despite a drastic reduction of the number of empirical parameters. For thermal stability, a simple kinetic model is shown to be a better basis to develop predictive tools than any group contribution schemes.

IDENTIFICATION OF SOLID PROPELLANT COMBUSTION DYNAMIC CHARACTERISTICS FROM THE RESULTS OF EXPERIMENTS WITH REGISTRATION OF THE CURRENT BURNING FRONT POSITION

IDENTIFICATION OF SOLID PROPELLANT COMBUSTION DYNAMIC CHARACTERISTICS FROM THE RESULTS OF EXPERIMENTS WITH REGISTRATION OF THE CURRENT BURNING FRONT POSITION

Y.M. Milyokhin*, A.N. Klyuchnikov*, A. V. Fedorychev*, S.V. Gunin*, V.V. Serushkin**, V.P. Sinditskii ** and S.A. Filatov **

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** Mendeleev University of Chemical Technology, 9 Miusskaya Square, 125047 Moscow, Russia

Abstract:
A stable algorithm of structural and parametric identification of combustion dynamic characteristics from the results of experiments with registration of the current burning front position has been developed, which allows prediction of current values of burning rate \( U(T) \) and its frequency response with accuracy acceptable to practice. The proposed approach has been tested by simulation calculations with harmonic input signals, including superimposed noise of different intensity, to determine the accuracy of identification of the amplitude and phase frequency characteristics of burning. The approach has been used to study dynamic combustion characteristics of a model propellant under oscillating pressure. The transfer and response functions have been determined for a low frequency area. It has been shown that the approach is favorably distinguished from other procedures by higher accuracy and authenticity of estimations.

DEVELOPMENT OF COMPUTER CODE FOR QUALITATIVE PREDICTION OF HEAT OF FORMATION OF HIGH ENERGETIC MATERIALS

PART I

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Abstract
A computer code has been developed to predict heat of formation based on two methodologies. In first methodology, the logic of Stine and Kramer method of predicting heat of formation has been used and extended to terminal functional groups such as -OH, -NH, -NH₂, -NO₂, -H and C=O. In the second methodology, a new equation for heat of formation has been derived by merging the equations of Stine et al and Rothsetien et al, which are being used for the theoretical prediction of velocity of detonation. The linear regression coefficient \( R^2 = 0.9387 \) and 0.8358 are obtained for
heat of formation predicted by this code and compared with those reported in literature, using
methodology I and II respectively. This new technique of predicting heat of formation from elemental
composition of HEM's has been successfully appended in a windows based user-friendly software
code named LOTUSES (Linear Output Thermodynamic User-friendly Software for Energetic
Systems) developed by our team. The LOTUSES code also simultaneously predicts properties
such as molecular weight, oxygen balance, velocity of detonation, C-J pressure, density, heat of
explosion, relative strength of an explosive in comparison to 2,4,6-trinitro toluene (TNT) as well as
the possible explosive decomposition products after explosion, volume of explosion products and air
blast effects has been reported recently by authors. The predicted heat of formation by LOTUSES
can be stored in various formats such as .txt, .html, .doc, .pdf and can be saved either in hard disk or
even in floppy diskettes/compact diskette. The predicted output can also be copied into RAM, which
can be pasted in other softwares such as microsoft word/powerpoint etc.. Also output of the
predicted heat of formation can be heard/listen from speakers attached to the PC through
multimedia sound card.

STUDY OF TNT METABOLISM IN PLANTS AND ITS
PRACTICAL APPLICATION FOR ENVIRONMENT
DECONTAMINATION
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Abstract:
Although a contamination of sites by TNT is an environmental problem all over the world, the
fate of its degradation products claims attention as well. A study of metabolism of TNT in plants
was focused on degradation of 4-amino-2,6-dinitrotoluene (4-ADNT), a stable degradation product.
Two plant species Senecio jacobea and Buphthalmum salicifolium cultivated under in vitro
conditions in the presence of different concentration of 4-ADNT for 3 weeks. The highest
concentration 50 mg/l of 4-ADNT was degraded by plants within two weeks but any major
degradation product was not detected in the medium. The IC$_{50}$ was not determined in the range of
used concentration therefore a linear regression was used for prediction of the IC$_{50}$ and 61,8 mg/l
and 70,2 mg/l were calculated for S. jacobea and B. salicifolium, respectively.

TEMCELV-EX. ADAPTATION OF TEMCELV SYSTEM TO
FIRE AND EXPLOSION HAZARD ASSESSMENT IN
MANUFACTURING OF EXPLOSIVES
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Instytut Przemysłu Organicznego, Annopol 6, 03-236 Warszawa, Poland

Abstract:
The main assumptions of a new research-technical project have been presented, which aim is to
adapt the system of evaluation and classification the process hazards in chemical industry, called
shortly Temclev, to the specificity of manufacturing of explosives. A brief description of the
original Temclev system has been given as well as a direction of its transformation into a new
version - Temclev-Ex.
EXPERIMENTAL INVESTIGATION OF IGNITION MECHANISMS IN CONFINED ENERGETICS

H. J. Prentice and W. G. Proud
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Abstract:
Detailed understanding of the response of confined energetic materials to different stimuli is critical to their design. This paper presents an experimental investigation of ignition mechanisms in Detasheet (a polymer-bonded explosive) when confined between copper plates and impacted at normal incidence with copper plates at velocities up to 600 m/s. High-speed photography and optical fibres are used to detect points of ignition and consequent reaction history. PVDF stress gauges are used to relate velocity of impact with pressure generated in the explosive. A Hugoniot curve for Detasheet has been plotted.

THE ETHICS OF ANALYSIS AND MEASUREMENT IS YOUR ANSWER THE CORRECT ANSWER?

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Abstract:
In spite of careful analysis and measurement, results are often incorrectly calculated and reported. This may have serious effects on the outcomes of the investigation -products, ammunition and associated systems may not meet the specifications and miss the target, time and materials are wasted and revenue eventually lost. This paper deals with the necessity for and principles of correct scientific numerical communication. The basic measuring units are initially reviewed followed by a discussion of the proper use of figures and correct handling of measurements. In conclusion the nature of measuring errors is studied and guidelines for its prevention provided. A number of exercises are provided in the text, the answers to be found at the end of the paper. The ultimate aim will be to improve the reliability of the reader as an analyst/researcher.

THERMAL AND THERMO-MECHANICAL INVESTIGATIONS OF LONG TIME STORED PROPELLANTS

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Abstract:
Samples of single based propellant (SBP) and double based propellants (DBP) stored a long time in non-heated military store houses were investigated up to 393 K. The dependences temperature / deformation were made by the heating rate 2oC/min. and the values of glass transition temperature (Tg) were determined. With the Flory-Fox-Biky equation the values of Tg(x) and K were calculated. After measuring the dimensions of the samples in several temperatures were calculated the coefficient of thermal expansion of the propellants. The influence of the time of storage of the propellants on their properties was determined.
** Explosia a.s., Research Institute for Industrial Chemistry, CZ-532 17, Pardubice - Semtín, Czech Republic

Abstract:
This paper includes the solution of testing Solid Propellant Rocket Motor with erosive burning part of burning process when gas generator is used for the purpose mentioned. Students of doctor’s study programs of Military Academy in Brno and members of Explosia a.s. provided the realisation of these tests.

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HIGH RESOLUTION OPTICAL ANALYSIS OF DYNAMIC EXPERIMENTS ON PBXs


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Abstract:
Previous research has provided information on the high strain rate behaviour of energetic systems. This paper outlines developments in the measurement of strain fields and strain localisation. In particular, the conditions for strain localisation in materials are discussed. The application of a photographic technique, digital speckle metrology, allows deformation fields to be measured. Although this does not provide sufficient resolution for strain localisations to be observed in detail, this aspect is being actively pursued.

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INFLUENCE OF NC PROPELLANT SAMPLE SELF-HEATING ON ARRHENIUS KINETIC CONSTANTS DERIVED FROM NON-ISOTHERMAL DSC MEASUREMENTS

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Abstract:
Non-isothermal isoconversional kinetic methods described by Ozawa, and Flynn and Wall are widely used to study kinetics of energetic materials. However, to obtain valuable kinetic constants great care must be taken to ensure proper experimental conditions, as well as data treatment procedure.
In this paper we have discussed the influence of NC propellant sample mass and heating rate during non-isothermal DSC measurements, i.e. the influence of NC propellant sample self-heating on kinetic results derived in accordance with the Ozawa and Flynn and Wall methods.
It was calculated by the Ozawa method that the activation energy equals ~199 kJ/mol in the case when sample self-heating has been avoided, while in the case of sample self-heating existence the activation energy was calculated to be ~191 kJ/mol. Also, it was shown that the activation energy calculated by the Flynn and Wall method depend not only on sample self-heating existence but also on degree of conversion - it ranges between ~145 and 200 kJ/mol.

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MECHANICAL PROPERTIES OF GEL-PROPELLANTS WITH NANOPARTICLES

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Abstract:
Gel propellants provide rocket propulsion systems of high specific impulse, low sensitivity and low vulnerability in combination with the capability to control the thrust, i.e., variation of thrust and thrust cut off. The rheological characterization is essential for the development of adequate gel
propellant formulations and thus for the design of an applicable propulsion system. In this contribution, the rheological behavior of a gel propellant consisting of nitromethane as fuel and nanoparticles of silicon dioxide as gelling agent was examined. The experiments were conducted under steady state shear flow and oscillatory shear. The nitromethane/silicon dioxide gels exhibit non-Newtonian flow behavior over the whole concentration range examined. Additionally, a yield stress is determined for all the gels. The viscoelastic properties are typically gel-like in that the storage and the loss moduli are both independent of frequency.

**STUDY OF SUB-MICRON STRUCTURED PHOTOSENSITIVE PRIMARY EXPLOSIVES FOR LASER INITIATION SYSTEMS**


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**Abstract:**

Synthesis of nano-structures with predetermined characteristics and development of functional materials on their basis have become one of the priority problems in the materials science. Nanoparticles possessing the size in the range 1-100 nanometers often show in comparison with materials formed by particles of the micron size often possess unusual characteristics. Working out energetic condensed systems, especially photosensitive primary explosives for the systems of laser initiation is one of the primary branches of application of nano-structured materials. We have synthesized and investigated mercury (II) complex perchlorate with 5-hydrazinotetrazole as a ligand (compound (I)) as a potential photosensitive primary explosive. This complex having particles of 1.1 ±0.8 µm size demonstrated the highest sensitivity to laser irradiation combined with an extremely low initiation threshold. On the basis of compound (I) the photosensitive formulation EC-2 containing ~ 90 % of the complex mercury perchlorate and ~ 10 % of an optically transparent polymer as an inert matrix has been proposed. Formulation EC-2 has externally high sensitivity to Q-switch IR-laser irradiation. Formulation EC-2 with added ultra disperse diamonds (UDD) (<100 nm) has shown lower initiation thresholds in comparison with neat EC-2 or EC-2 with added sub-micron black carbon instead of UDD. To increase the safety, an optical detonator on the basis of EC-2 separated from the high explosive charge (HE) by a metal cup, has also been studied.

**STUDIES AND RESEARCHES REGARDING THE UTILIZING OF RESULTS OBTAINED AT THE BURNING OF POWDER IN CLOSE BOMB FOR SOLVING OF FUNDAMENTAL PROBLEM OF INTERIOR BALLISTICS**

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**Abstract:**

In this paper it is presented a mathematical model of firing phenomenon, using the results obtained during of the powder burning in close bomb. On the base of the mathematical model was elaborated an interior ballistic soft, which allows to study the variation of the powder gases pressure and the projectile velocity versus its displacement inside of grooved barrel and versus time. For an extant weapon, the theoretical results that was obtained with the aid of this soft and the experimental data are compared.

**NTREM, PARDUBICE, 2004 page 298-305**

**NTREM, PARDUBICE, 2004 page 306-316**

**NTREM, PARDUBICE, 2004 page 317-324**
EFFECTS OF THE COATING PROCESS OF HE MOULDING POWDERS ON SAFETY AND IM CHARACTERISTICS

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Abstract:
High performance warheads are very demanding on every component of the whole system. The HE "low cost" component has to fulfil performance and IM criteria. Two coating methods, slurry and paste process, promise better results and effectiveness for new moulding powders.

NTREM, PARDUBICE, 2004 page 325-332

BALLISTICAL AND CHEMICAL STABILITY OF ROLLED BALL PROPELLANTS

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Abstract
This paper presents in summary the work of a Belgian-French-German cooperation programme on the chemical and ballistical stability of a ball propellant for the 5.56 · 45 mm ammunition. The programme comprises thermoanalytical, analytical, ballistical and spectroscopical techniques applied on unaged and aged samples of the propellant K 5810.

The propellant K 5810 is chemically stable. This fact is proven by microcalorimetry; the maximum heat flow does not reach the limit values of STANAG 4582. Also the stabilizer content after ageing times which are comparable to a 10 years storage at 25°C is much higher than the limit values given in AOP-48, Ed. 2. The ageing mechanism is strongly dependent on the loading density of the ampoules and the atmosphere above the sample which underlines the big effect oxygen has on the ageing of nitrocellulose based propellants.

The slight energy loss during the ageing periods used here does not affect the ballistic behaviour significantly. In contrast to the 9 mm ammunition tested before there seems to be no incompatibility between the propellant and the Sintox primer because the propellant K 5810 does not contain isopropanol in contrast to the K 6210 propellant in the 9 mm ammunition.

The ballistic life time is limited by the migration of the deterrent. This migration leads to an increased burning rate and thus to an increased pressure in the early phase of the burning reaction. As not all samples are available at the moment a final value for the activation energy of the migration of the DBP can not be given. First estimations lead to a value slightly above the activation energy of the nitrate ester decomposition.

NTREM, PARDUBICE, 2004 page 333-347

DEFORMATION AND FRACTURE OF ENERGETIC MATERIALS AND THEIR SIMULANTS

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Abstract:
A detailed understanding of the deformation and fracture mechanisms of energetic materials is vital to ensure optimum performance and safety. A series of deformation and fracture experiments with optically derived results are being developed on a sugar based energetic simulant with the ultimate aim of transferring the proven experiments to energetic materials. The physical insight and quantitative data these experiments yield are crucial in developing accurate and predictive models of the response of energetic materials to mechanical stimuli. This paper outlines the results taken to
ON THE REACTIONS OF 2-(DINITROMETHYLENE) -4,5-
IMIDAZOLIDINE DIONE WITH ALKALINE AGENTS

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Abstract:
The new preparation methods of 1,1-diamino-2,2-dinitroethylene and 2-dinitromethylene-4,5-
imidazolidinedione from 2-methylimidazole were studied. The yield of 2-dinitromethylene-4,5-
imidazolidinedione was 20.3% by nitrating 2-methylimidazole in the sulfuric and nitric acid. Under
different alkaline conditions, 2-dinitromethylene-4,5-imidazolidinedione can process two different
reactions: in the alkalescent conditions, the main product is Fox-7; with alkali conditions, the
main product is potassium dinitromethanate. By optimizing reaction conditions, the yield of Fox-7
could be up to 95.3% and for potassium dinitromethanate, it could be 65%.

MECHANISTIC STUDIES OF DESTRUCTIVE NITRATION OF
2-ALKYL SUBSTITUTED 4,6-DIHYDROXY PYRIMIDINES

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Abstract:
The main stages of destructive nitration of 2-(4-oxo-6-hydroxy-2-pyrimidinylidene) acetic acid in
various nitrating mixtures have been identified. The effect of consecutive introduction of nitro groups
on the formation of the key intermediate responsible for the generation of 1,1-diamino- 2,2-
dinitroethylene (DADNE, FOX-7) has been demonstrated. A general scheme of chemical
transformations of 2- methyl-4, 6-dihydroxypyrimidine under the conditions of acidic nitration has
been suggested.

SIMULATION STUDY ON ARMOUR-PIERCING EFFECT OF
ARMOUR-PIERCING BOMB

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Abstract:
Studying the armor-piercing effect of Armour-piercing bomb that attacks aluminum target is
essential because the target can be considered the simulation of the actual fight equipment. Based on
the hypothesis about building the fraction field, the armor-piercing effect of armor-piercing bomb is
analyzed, and the velocity and the intruding depth parameter model of armor-piercing effect are
established. Taking a certain armor-piercing bomb as example, the intruding processes of armor-
piercing effect are simulated by using the nonlinear finite element analysis program LS-DYNA,
while aluminum target simulates the wall of combat equipment in two different conditions. At last, the
finite element simulated results are given and analyzed that agree with the experiments.
EFFECT OF TNT CHARGES ORIENTATION ON GENERATED AIR BLAST WAVES NUMERICAL SIMULATION USING LS-DYNA

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*** Military University of Technology, Kaliskiego 2, 00 980 Warsaw, Poland

Abstract
The paper deals with numerical 3D simulation, through the code LS-DYNA, of the effects caused by air blast waves generated by cylindrical TNT charges (the mass of 25g and 50g) which are differently oriented respect to the pressure gauges placed relatively close to the charges (approximately 800 mm and 840 mm from the charges). As the first step for these simulations, the numerical study has been concentrated on the verification of the state equations for TNT and air continuum. It has been concluded that the JWL equation of state and ideal gas equation of state were proper representations for TNT and air respectively. Then, simple formulae for various oriented charges have been developed and verified. These formulae make possible to represent the original cylindrical charges like equivalent 3D ellipsoids (this approach is very important in order to obtain stable computational mesh). The final numerical simulations have been compared with the original experiments performed at Military University of Technology in Warsaw. On the basis of this comparison, it has been concluded that the 3D numerical simulations using LS-DYNA have been a very powerful and useful tools.

NTREM, PARDUBICE, 2004 page 380-389

DETERMINATION OF THE CONSEQUENCES OF POSSIBLE INDUSTRIAL ACCIDENTS

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*** Nuclear Power Plants Research Institute, Okružná 5, 918 64 Trnava, Slovak Republic

Abstract:
The paper is devoted to calculations of the consequences relating to accidental vapour cloud explosions. For this purpose, a general methodology has been developed and applied. The methodology consists of two steps: the first one deals with blast wave characterization - Multi-Energy method has been used, the second one deals with the propagation of the generated blast wave in surrounding air and wave-building interaction - the LS-DYNA code has been applied. The methodology has been applied to a case of unconfined non-obstructed hydrogen cloud explosion in site. An example of the application is presented in the paper. The methodology presented can be used both to determine the consequences of an accidental vapour cloud explosions for risk analysis purpose and at the same time also as an optimization design tool which enables to minimize consequences of possible explosions taking into account various plant layouts.

NTREM, PARDUBICE, 2004 page 390-400

TOPOGRAPHY OF REACTION ORIGINATION OF SILVER AZIDE EXPLOSION DECOMPOSITION UNDER INITIATION BY ELECTRON ACCELERATOR PULSE

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** Russian Federal Nuclear Center, All-Russia Research Institute of Technical Physics (RFNC-VNIITF) 456770, PO Box 245, Snezhinsk, Chelyabinsk region, Russia
Abstract:
The silver azide pre-explosive luminescence origination by electron pulse initiation in nidi and subsequent broadening of the luminescence ranges overlapping finally the whole sample. Hence, the origination nidi of the reaction are not caused by the local heating and they are not the hot spots in the true sense of the word.

NTREM, PARDUBICE, 2004 page 401-403

SPECTRAL-KINETIC CHARACTERISTIC OF PETN LUMINESCENCE UNDER INITIATION BY ELECTRON BEAM


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Abstract:
Spectral-kinetic characteristics of PETN single crystal explosive luminescence under initiation by a high-strength electron beam have been studied. It has been shown that spectra of radioluminescence arisen from the effect of an electron beam and spectrum of the following explosive luminescence coincide. The spectrum of pre-explosive glow has been found to be of luminescent nature. Linear spectrum of explosion products has been registered. It can be associated with molecular nitrogen luminescence.

NTREM, PARDUBICE, 2004 page 404-408

THE EXPLOSION PARAMETERS OF BENZOYL AND CYCLOHEXANONE PEROXIDES

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Abstract:
The ultimate objective of the work was to investigate the ability to heat explosion, burning and detonation of some organic peroxides. The main attention was paid in previous work to investigation of cumene hydroperoxide (CH). The properties of benzoyl peroxide (BP), and cyclohexanone peroxide (CHP) were collected and analyzed in this work. The explanation of the investigation results focused on identifying the most probable occurring chemical reactions at decomposition, heat explosion, burning and on reaction thermochemistry data. The data of investigation in couple with literature materials characterize net cyclohexanone peroxide, cumene hydroperoxide, and benzoyl peroxide as weak explosive, which are able to burning, low velocity detonation, and heat explosion. The results of investigation update the information concerning to explosion characteristics of CHP, CH, and BP and they could be used to achieve accident prevention goal on the plant facilities at its production, processing treatment, and transportation.

NTREM, PARDUBICE, 2004 page 409-418

AN EXPERIMENTAL CHECKING OF A DIVACANCY MODEL OF INICIATING HEAVY METAL AZIDES


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Abstract:
Main results are adduced of an experimental checking of a divacancy model of initiating heavy metal azides. The analysis result shows that a divacancy model of initiating heavy metal azides quantitatively do agree with available theoretical data.

NTREM, PARDUBICE, 2004 page 419-423

COMPARATIVE CHARACTERISTICS OF TWO ISOMERIC EXPLOSIVES: 4-NITRO-5-NITRIMINO-1H-1,2,4-TRIAZOLE AND 3-NITRO-5-NITRIMINO-1,4H-1,2,4-TRIAZOLE

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Abstract:
The comparative estimation of properties of two isomeric nitroderivatives of 1,2,4-triazole - 4-nitro-5-nitrimino-1H-1,2,4-triazole and 3-nitro-5-nitrimino-1,4H-1,2,4-triazole, is realized. In contrast to the C-nitrocompound, the N-nitrocompound has higher heat of formation, and as a consequence, the higher explosive characteristics. On the other hand, N-nitrocompound has lower thermal stability and higher impact sensitivity in comparison with C-nitrocompound.

NTREM, PARDUBICE, 2004 page 424-432

APPLICATION OF TLC FOR AN ANALYSIS OF INITIATING EXPLOSIVES

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Abstract:
Instrumental TLC was used for analyses of initiating explosives (IHE). A chromatographic system suitable for analyte separation and method of densitometric determination of some IHE complexes with ditizone were proposed. A linear dependence of densitometric peak areas A on the analyte mass c in the chromatographic band was obtained (Hg: A =33202c —1406 and Pb: A = 42643c - 83). A limit detection (Hg: 7.15 and Pb: 1.25 ng in the chromatographic band) and maximal range of linear measurements (Hg: 120 and Pb: 20 ng) was determined. The method developed was used to analyze chosen IHE in electrolytes.

NTREM, PARDUBICE, 2004 page 433-436

APPLICATION OF CARBONACEOUS PRODUCTS OF HALOGENOCARBONS REDUCTION FOR SOLID PHASE EXTRACTION

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Abstract:
The possibility of application of carbon materials sensitized in self-propagating heat waves for solid phase extraction (SPE) is presented. Extraction cartridges with the materials were prepared, and samples of water contaminated with pesticides (PDs) and polycyclic aromatic hydrocarbons (PAHs) were analyzed. Modern TLC equipment was used for analyses. Chromatographic systems and analytical parameters of PDs and PAHs were defined and these results were used to determine some retention and elution characteristics of the tested materials. Recovery and measuring errors were estimated (the recovery equaled ca. 50 % and the SD was below 6 %). It was shown that some of the examined materials can be applied as adsorbents for SPE. They are especially good for extraction of analytes with comparatively high polarity.

NTREM, PARDUBICE, 2004 page 437-442
THE EXAMINATION OF CHOSEN BALLISTIC PARAMETERS OF IGNITER CHARGE BKNO₃ FOR IGNITERS OF SOLID PROPELLANT ROCKET MOTORS

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Abstract
The preliminary results of pyrostatic investigations of ignition tablets BKNO₃ were presented. The investigations were performed in especially designed for this purpose rocket engine with established constant loading density. The time of burning and dynamics of process were estimated.
NTREM, PARDUBICE, 2004 page 443-450

SYNTHESIS AND SOME PROPERTIES OF BU-NENA

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Abstract:
Butyl-NENA was synthesized by two-step reaction in laboratory and pilot plant scale. The product was identified by means of H, ¹⁵NMR spectra, IR spectra and elementary analysis. Purity of the sample was determined by HPLC. Evaluated parameters were sensitivity to impact, DTA analysis and acidity of Bu-NENA. The results, especially with regard to utilization of Bu-NENA as a component of propellants and explosives, are discussed.
NTREM, PARDUBICE, 2004 page 451-458

ANALYSIS AFTER COMBUSTION OF PROPELLANTS

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Abstract:
The aim of this study is an identification of products after combustion of smokeless powders and solid propellants. In first a sample of smokeless powder was burnt on the clean sand. Then an isolation of compounds from this sand was tried. The accelerated solvent extraction and ultrasonication were used for the isolation of these compounds. Gas chromatography GC 17A with mass spectrometry detector QP505A was used for an identification of compounds.
NTREM, PARDUBICE, 2004 page 459-462

DINITROBIURET AND ITS SALTS

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Abstract:
The work summarizes knowledge about Dinitrobiuret (DNB) - about its important explosives characteristics and parameters. It is focused on preparation, determination of molecular structures and the results of IR-Raman and multinuclear NMR spectroscopic investigations.
NTREM, PARDUBICE, 2004 page 463-466
EFFECTS ON ENFRGETIC MATERIALS PROCESSED WITH POWER ULTRASOUND

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Abstract:
We present experimental results derived by the effect of a high power ultrasound on melts of explosives and solutions of propellants. An effect of increase of the speed of formation of crystallisation centers have been identified for 2,4,6-trinitrotoluene and mixtures on its base. We investigated the kinetics of destruction of nitrocellulose in ultrasound field in solution of gunpowders.

NTREM, PARDUBICE, 2004 page 467-471

STUDY ON RING CLEAVAGE AND ADDUCTIVE PROPERTY OF 2-(DINITROMETHYLENE)-4,5-IMIDAZOLIDINEDIONE

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Abstract:
Ring cleavage of 2-(dinitromethylene)-4,5-imidazolidinedione (1) was achieved by methanol for the first time and the product was 1,1-diamino-2,2-dinitroethylene (FOX-7). 2, the first adduct of 1, was synthesized by the reaction of 1 with methanol in certain conditions and its structure was characterized. Physical and chemical properties of the adduct were studied. Parabanic acid was synthesized by decomposition of 1 in methanol, losing nitrogen oxides and carbon oxides.

NTREM, PARDUBICE, 2004 page 472-478

AGEING INFLUENCE ON STABILITY AND SENSITIVITY OF PETN EXPLOSIVES

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Abstract:
In this paper the PETN explosives stability and sensitivity are investigated during their artificial ageing. It was observed their stability was not changed, but sensitivity was changed after ageing. The biggest change was recorded in sensitivity to electrostatic discharge of gelatinized PETN.

NTREM, PARDUBICE, 2004 page 479-486

EXPLOSIVE TYPE SELECTION WITH RESPECT TO THE VENTILATION CYCLE DURATION

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Abstract:
Extensive measurements of the ambient air quality have been conducted in the past years during excavation of road tunnels situated on the mountainous sections of the future Croatian highway Zagreb - Split. The objective of these measurements was to estimate the worker exposure to toxic gases. Since conventional mining methods have been used for excavation of the tunnels (drilling and blasting), as well as various types of explosives and initial systems, the impact on the workplace environment by toxic gases produced from blasting was also examined. In order to reduce the amount of toxicants in the workplace atmosphere, the field method for selection of the most appropriate types of explosives in the blast charge was developed.
DISSOLVER VER. 1.1 HELPS CENTRAL MINING RESCUE STATION

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Abstract:
This paper introduces new software package DisSolver v. 1.1, which was developed under the contract between Czech Mining Authority and University of Pardubice. The package consists of three individual codes - "Výbuchový trojúhelník", "Následky" and "Vodní zátky". Code "Výbuchový trojúhelník" solves the problems with explosibility of atmosphere inside the coal mines. Code "Následky" enables the user to calculate the consequences of accidental leaks of natural gas and crude oil during the drilling. Code "Vodní zátky" solves the mathematical model of the water column movement in the gallery as the method of the explosion-proof closing of the seat of fire in the coal mines.

EXPANSION OF METALLIC TUBES DRIVEN BY HEAD-ON GRAZING DETONATION

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Abstract:
Since the pressure gradient abruptly increase in the detonation products undergoing a head-on collision of two detonation waves propagating in the cylindrical charge embedded in a metallic tube, the movement of tube wall driven by which will be of particular pattern. The data of expansion, deformation and fracture of the tube are obtained in the experiments with diagnostics of pulsed x-ray shadowgraphy and highspeed photography. A 2-D elastic plastic hydrodynamic Lagrangian code TTD2C has been compiled during this work and succeeded in simulating the head-on collision of two detonation waves and the resulting products flow, also the expansion process of metallic tubes driven by it. The calculated and measured results agree well with each other. The result shows that the fracture time advanced because of the head-on collision.

NONAERATIONS SENSIBILIZATION OF EMULSIVE EXPLOSIVES

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Abstract:
The opportunity of reception bull water-tight (4100-4400 kJ/kg) emulsive explosives such as "water in oil" is shown on the basis of solution of nitrocalcites and ammonium at the expense of sensibilization by the solid high-energy additives. The sensibilization of emulsive explosives is carried out at the expense of the addition of powders of metals and alloys with high hardness, melting point and capacity to react with light-end products of detonating. The responsive efficient explosive is prepared out without padding aeration, introducing of microspheres and explosive reagents.
THE CONDENSED EXPLOSIVE SYSTEMS CAPABLE OF PROPAGATING DETONATION IN THE SPIN-PULSATATING REGIME

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Abstract:
Quite distinct inhomogeneity of the detonation front was found earlier at detonation of cast charges TNT/RDX and TNT/PETN. The ultimate objective of this work is to extend the number of explosive systems capable of propagating detonation in the spin-pulsating regime and to generalize the results. Cast TNT/DINA, TNT/TETRYL DNT/PETN and pressed HMX/paraffin charges were investigated. Systems, detonating with low (1~3 MHz) frequency spin pulsation at some content of sensitizer (Cs), have approximately the same calculated detonation parameters: DJ ≈ 7.3-7.4 km/s, $Q_V$ ≈ 5.4 MJ/kg. The compositions TNDINa with $C_s$ > 25%, which detonate without spin pulsation, have calculated values $Q_V$ and DJ higher than that named above. $Q_V$ and DJ of itself DINA sufficiently higher than 5.4 MJ/kg and 7.3~7.4 km/s, correspondingly, and spin pulsation at detonation of charges of liquid Dina were not observed.

DETONATION ABILITY OF SOLUTIONS OF AROMATIC NITROCOMPOUNDS IN NITRIC ACID

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Abstract:
The ultimate objective of our work was to measure the failure detonation diameters of solutions of nitro derivative of toluene: TNT, DNT and MNT, and of nitro derivative of benzene: TNB, DNB andMNB in strong nitric acid at oxygen balance $A$=0%. They were measured by means of technique of parallel-plate cells. The cells were glued from glass photo plates, each of them had the constant thickness (1.1-1.4 mm). The clearance of cells was made by means of placing teflone sheets between sides of glass plates Equivalent failure diameter of detonation of the solution of TNT and TNB was $d_f$=0.10 mm, of DNT and DNB - $d_f$=0.18 and 0.15 mm, and of MNT and MNB - $d_f$=0.6 and 0.2 mm, correspondingly. Simultaneously the detonation parameters of the solutions investigated were calculated by means ofSD computer code at experimentally measured densities of solutions. Distinction of $d_f$ values was explained by discrepancy of its calculated detonation parameters.

FAULT TREE ANALYSIS IN THE PROCESS SAFETY INCIDENT INVESTIGATION

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Abstract:
This contribution is focused on methods for incidents investigation and its application in chemical industry. It contains a literal retrieval focused on basic principles of incident investigation and in practice section using one of the basic investigation techniques -Fault Tree Analysis. System evaluation of gelatination of nitrocellulose oriented to fire in object is the result of this work. "Minimal cut sets" (MCS) was obtained from the basic events probability of the constructed fault tree. Probability of incidents was then determined from MCS causes and corrective actions were recommended. In final part of this contribution, benefits and deficiencies of this systematic incident investigation was compared with traditional investigation with commission.
INTERNAL BALLISTIC ANALYSIS OF THE 20 × 102 CARTRIDGE

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Abstract
Results obtained by two different methods of pressure measurement are discussed. Maximum pressures were measured simultaneously in the cartridge of medium calibre weapon 20 x 102 mm by copper crusher and piezo transducer. Results obtained by different methods were correlated and influence of testing temperature was discussed.

UNSATURATED POLYESTER INHIBITION SYSTEM FOR DOUBLE BASE PROPELLANTS

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Abstract:
Inhibitors are applied to those surfaces of the propellant grain where burning is to be prevented. We investigated inhibition system for double base propellants based on unsaturated polyesters resins. Measurements of the amount of nitroglycerine that migrates into the chosen inhibitors were done using a "sandwich" test. Double base propellant grains were inhibited by a casting technique and statically fired in rocket motor. The nature of P-t profiles suggested that it is potential inhibition system for double base propellants.

SYNTHESIS OF DI(1H-TETRAZOLE-5-YL)AMINE (BTA)

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Abstract:
New method of synthesis of di(1H-tetrazole-5-yl)amine is described in the paper. Di(1H-tetrazole-5-yl)amine was synthetized by reaction of sodium azide with sodium dicyanamide in water under presence of zinc chloride as catalyst. This new method eliminates disadvantages of other alternative methods, such as for example: work with expensive and toxic metals, work with excess of volatile and toxic azoimide or work with organic solvents. This synthesis is very simple, safe and provides a good yield.

CHANGES OF DYNAMIC MECHANIC PROPERTIES OF DOUBLE BASED ROCKET PROPELLANT DURING ARTIFICIAL AGEING

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Abstract:
Double based rocket propellants are subjected to a chemical ageing, as well as ageing due to physical and physical-chemical processes (migration of low molecular constituents: plasticizers, blasting oil, burning catalysts, degradation of molar mass, etc.). The ageing has significant influence on their relevant properties, including mechanical properties such as tensile strength, storage modulus, loss modulus, tan delta, and temperature of glass transition, etc. During use these changes can result in dangerous failures, such as rocket motor explosion. Therefore, it is necessary that after some time, temperature, and stress conditions, relevant properties of the propellants are still in the range of acceptable tolerance.

In this work we have studied changes of dynamic mechanic properties (loss modulus, storage modulus, tan delta, etc.) with the artificial ageing at higher temperature (90°C). The results obtained have shown that dynamic mechanical parameters change significantly after ~40 days of ageing.

It was found out that the most sensitive parameters on the ageing process are: storage modulus at the room temperature, glass transition temperature, width of peak on loss modulus curve in the glass transition region, and tan δ at the glass transition region.

APPLICATION OF SHEET EXPLOSIVE FOR METAL HARDENING

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Abstract:
This article contains a brief information on application of sheet charges for explosive hardening of metals. The paper defines basic requirements for the properties of the explosives used for explosive metal hardening, resulting from practical applications. At the same time the findings are given here obtained at application of the explosive at hardening of Hadfield steel.

INFLUENCE OF INSENSITIVE ADDITIVES ON DETONATION PARAMETERS OF PBX

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Abstract:
Plastic bonded explosives (PBX) are known as explosives which possess high energy, thermal stability, low insensitivity and good mechanical properties. We investigated plastic explosive based on hexogen. As an additive we used NTO. We researched influence of NTO additives on detonation parameters of plastic explosives. This additive generated the decrease of sensitivity without significant worsening detonation parameters.

AN UNDERWATER TEST FOR LWC EMULSION EXPLOSIVES

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Abstract:
In the paper results of some experimental investigations of underwater shock waves parameters generated by explosion of TNT and water-in-oil emulsion explosives are presented. In experiments, the overpressure history in transient shock wave generated by explosion of investigated explosive charges was measured. Moreover numerical evaluation of shock waves energy and bubble energy released during explosion is performed. These calculated parameters could be used as parameters of explosive performance. Comparison of the explosion energy of various kinds of explosives is
PREDICTION OF THERMODYNAMIC CONDITIONS FOR NITROESTER VAPOR CONDENSATION ON THE SURFACES OF PROCESS APPARATUS DURING THE PRODUCTION OF ENERGETIC MATERIALS

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Abstract:
A calculation procedure has been developed for finding thermodynamic conditions under which nitroglycerine, diethylene glycol dinitrate, and triethylene glycol dinitrate vapors are condensed on the surfaces of process apparatus during the production of energetic materials. Temperature − (plasticizer content in dry air) diagrams have been calculated and mapped. The diagrams allow one to estimate the condensation temperature of supersaturated nitroester vapor and to calculate the condensate weight. A procedure has been proposed for measuring the partial saturated vapor pressure of a plasticizer under the production conditions.

STUDY OF ELECTRON DENSITY OF MOLECULES, INTERMOLECULAR FORCES AND IMPACT SENSITIVITY OF EXPLOSIONS

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** University of Pardubice, Department of Theory and Technology of Explosives, Studentská 95, 53210 Pardubice, Czech Republic

Abstract:
The electron densities for the selective set of twenty explosives with composition C-H-N-O were calculated (i) for individual molecules and (ii) for molecules placed in crystal cell. Indirect linearity of absolute difference of charges for bonds C-NO₂, N-NO₂ and O-NO₂ versus the length of the bond was founded in both cases. The influence of non-covalent hydrogen bonds for distinctly decreasing of the impact sensitivity was confirmed. On the base of results from experimental methods such as the impact sensitivity and theoretical methods such as molecular mechanics and molecular density calculations for selected set of twenty explosives the possibilities of prediction for impact sensitivity of new energetic materials are discussed.

SPHERICAL NITROGUANIDINE AS COMPONENT OF HIGH EXPLOSIVES

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Abstract:
Researches on nitroguanidine (NGU) crystallization were conducted in order to obtain spherical crystals. We investigated plastic bonded explosive based on hexogen with NGU as an additive. Nitroguanidine, as a component of PBX generated the decrease of sensitivity to mechanical stress without worsening other parameters.
THE CHEMICAL KINETIC AT DETONATION OF AROMATIC NITROCOMPOUNDS - NITRIC ACID MIXTURES

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Abstract:
Detonation failure diameter $d_f$ of mixtures of six aromatic Nitrocompounds with nitric acid has been examined in the framework of A.Dremin theory. Shock and detonation parameters as well as characteristics ($P_3$, $T_3$ and $t_3$) of the reaction zone to determine reinitiation of detonation wave at low diameters of the charge were calculated by means of SGKR computer package. According to our calculations maximum of $T_3$ values was fixed at the concentrations of nitric acid corresponding to the minimum of $d_f$. Effective values of kinetic parameters of reaction between nitric acid and Nitrocompounds are defined.

NTREM, PARDUBICE, 2004 page 614-620

INITIAL STAGE DECOMPOSITION KINETICS OF NITROCELLULOSE PROPELLANT

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Abstract:
A thermal decomposition reaction in nitrocellulose, which is the basic component of homogeneous propellants, limits the safe use and safe storage time of propellants. Under certain conditions the decomposition may lead to the well-known phenomenon of self-ignition. In order to be able predict the shelf-life and thermal hazard potential of propellants it is of vital importance to know a true decomposition mechanism and true vales of kinetic constants. In this work we have studied decomposition kinetics of nitrocellulose propellant during the initial decomposition stage (up to 2% mass loss) at elevated temperatures ranging from 80 to 100 °C. The kinetic results were derived from sample mass loss-time/temperature. It was found out that the activation energy for this decomposition stage equals 123.4 kJ/mol, and pre-exponential factor $1.78-10^6$ 1/s. Also, it was found out, on the basis of the kinetic data obtained, that the reaction rate accelerating factor changes with temperature -from ~3 at 90-100 °C temperature range to about 5.5 at the room temperatures.

NTREM, PARDUBICE, 2004 page 621-629

DETERMINATION OF THE RELATIVE DENSITY OF MOLTEN EXPLOSIVES

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Abstract:
The Archimedes principle was used for the determination of the relative density of molten TNT. This method proves to be practical, easily conducted and quick, providing reliable results with high precision and sensitivity.

NTREM, PARDUBICE, 2004 page 630-635

COMBUSTION OF DINITRAMIDE SALTS

V.P. Sinditskii, A.I. Levshenkov, V.Yu. Egorshev and V.V. Serushkin
Abstract:
Burn rate studies have been carried out on dinitramide salts of common formula of $L \text{nHN(NO}_2\text{)}_2$, (where $n = 1 \text{ or } 2$; $L = \text{methylamine, trimethylamine, tret-butylamine, tetramethylammonium, urea, guanidine, aminoguanidine, triminoguanidine, ethanolamine, diethanolamine, ethylenediamine, hexamethylenediamine, aniline, 3-nitroaniline, 2-toluidine, benzylamine, phenylhydrazine, morpholine, piperaizne, pyridine, 3,5-dimethylpyridine, and 5-aminotetrazole) as well as lithium and barium salts of dinitramide. Most of the salts exhibit either combustion instability (like ADN) or a transition region on their $r_b(p)$ curves. The occurrence of this region depends upon the fuel reactivity and, largely, the surface temperature which is assumed to be dissociation one and dependent on the amine basicity. To disclose combustion mechanism, flame structure of hexamethylenediamine dinitramide (GMDADN) has been investigated with tungsten-rhenium microthermocouples. Besides, burn rate study of GMDADN within a wide initial temperature interval allowed the burning rate temperature sensitivity to be evaluated.

DETERMINATION OF CHEMICAL STABILITY OF GUNPOWDERs BY QUALITATIVE AND QUANTITATIVE METHODS
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Abstract:
This work presents the results from the analyses made on monobasic gunpowder, which consists of two types of stabilizers (diphenylamine and centralit I) with total mass of representation of about 1,3%.
The content of the residual stabilizer of gunpowder treated at different temperature and at different length of time was determined by using two quantitative methods. By processing and comparing the results gained at raised temperature an attempt was made to foresee the time of stability of the gunpowder in normal conditions of storing. As quantitative methods in this case the Hansen test and liquid chromatography (HPLC) were applied According to the first method the gunpowder was treated at 110 °C in the period from 0 to 72 h, and the results were validated by using pH - meter. The second method was used to determine the content of the residual stabilizer at the same gunpowder treated at 110°C as long as the content of the active stabilized does not go below 50% m/m from the starting one.

DETERMINATION OF EXPLOSIVE PROPERTIES
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Abstract:
This paper informs about testing of explosiveness of chemical substances according Ministry of Environment Decree which becomes valid to the date of entering the Treaty of Accession of Czech Republic to Europen Union into force.

GEMINAL DINITROCOMPOUNDS THERMAL DECOMPOSITION UNDER NON-ISOTHERMAL CONDITIONS
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**Siberian State Technological University 660049, Krasnoyarsk, prosp. Mira 82, Russia**

**Abstract:**
Depending on geminal trinitrocompounds structure, their thermal decomposition proceeds in one or two stages. It is a complex process that includes evaporation, destruction, secondary oxidation-reduction reactions, and autocatalysis. It is shown that thermal sensitivity is tied with temperature of initial decomposition. The steric effect of $\alpha$-substituent at geminal dinitrogroup significantly influences both decomposition rate constant and decomposition’s characteristic temperature. Corresponding quantitative correlations confirm it.

**NTREM, PARDUBICE, 2004 page 659-666**

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**DETONATION PERFORMANCES OF LOW-SENSITIVITY NTO/HMX EXPLOSIVES**

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Military University of Technology, Kaliskiego 2, 00 908 Warsaw, Poland

**Abstract:**
Detonating performances of new explosive compositions containing NTO and HMX are investigated in this work. Detonation velocity, pressure and energy of the mixtures tested and acceleration ability and equation of state of their detonation products are determined. Shock and impact sensitivity is evaluated in the gap test and heavy hammer test. The compositions investigated can be considered as a suitable insensitive explosive to replace TNT/RDX mixtures in munitions applications.

**NTREM, PARDUBICE, 2004 page 667-675**

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**TRACE ANALYSIS OF EXPLOSIVES BY LC-MSD TECHNIQUE**

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**Abstract:**
The aim of this work is the determination of LOD of explosive compounds using Agilent 1100 series LS-MSD system with the atmospheric pressure chemical ionization (APCI) source. At the analysis of explosive compounds LC-MSD with IONSCAN M 400 (Barringer Inc.), a detector of explosives and drugs, and with the gas chromatography with electron capture detector (agilent Technologies) were compared.

**NTREM, PARDUBICE, 2004 page 676-686**

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**LIFE-CYCLE-ANALYSIS AND "GREEN" ENERGETIC MATERIALS**

**J. Vávra* and P. Vávra **
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** Department of Theory and Technology of Explosives, Faculty of Chemical Technology, University of Pardubice, 53210 Pardubice, Czech Republic

**Abstract:**
This paper mentioned the main requirements on "green" energetic materials and the priorities in specific programs in R&D. In this connection with these new requirements are principles of Life-Cycle-Analysis (LCA) and Life-Cycle-Costs (LCC) applied. Possible use of these methods for costs reduction of new GEM during whole GEM’s lifetime is discussed.

**NTREM, PARDUBICE, 2004 page 687-693**
MODERN PROPELANTS FOR 30 MM AMMUNITION APPLICATIONS

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Abstract:
This short survey is to provide some important information about new trends in development of propellants for existing modern weapon systems, or, propellants for ammunition for elder weapon systems with improved performance.
NTREM, PARDUBICE, 2004 page 694-698

DIRECT MONTE-CARLO SIMULATION OF DETONATION PROCESS IN A GAS

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* Institute of Fundamental Technological Research, Polish Academy of Sciences Swietokrzyska 21, 00-049 Warszawa, Poland
** Institute of Heat Engineering, Warsaw University of Technology Nowowiejska 25, 00-665 Warszawa, Poland
*** Institute of Industrial Organic Chemistry Annopol 6, 03-236 Warszawa, Poland

Abstract:
The research on gaseous detonation has recently become a very important issue because of increasing importance of gaseous fuels. We propose to use the Direct Monte-Carlo Simulation technique, which is a very powerful tool for solving complex flow problems. We propose a very simple model of a molecular collision, which makes it possible to increase the thermal energy of a gas, which is similar to the processes in the flame. We show then, that this model can produce the wave, which has the features characteristic for a detonation wave.
NTREM, PARDUBICE, 2004 page 699-703

SYNTHESIS OF 4,6-DINITROBENZOFUROXAN

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Abstract:
Problems connected with nitration of benzofuroxan are of specific interest since potassium salt of dinitrobenzofuroxan is considered as promising ecologically pure initiating explosive. In this connection a study has been performed on nitration of benzofuruxan and its mononitroderivatives in nitric and sulfuric-nitric acid mediums. The main reaction products formed in the reaction have been identified.
NTREM, PARDUBICE, 2004 page 704-707

APPLICATION POSSIBILITIES OF POLAROGRAPHY IN STUDIES OF CHEMICAL MICRO-MECHANISM OF INITIATION OF POLYNITRO ARENES

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Abstract:
The half-wave potentials, E1/2, of twenty four polynitro arenes have been determined in aqueous
medium buffered at pH 7, the final concentrations of their solutions being $0.5 \times 10^{-4}$ M and $0.5 \times 10^{-5}$ M. The $^{13}$C NMR chemical shifts of carbon atoms carrying the most reactive nitro groups have been used for specification of the primarily reduced nitro group in the molecule. The found logical relationships between the $E1/2$ values and squares of detonation velocity are of the type of the modified Evans-Polanyi–Semenov equation for energetic materials. It has been stated that the strong dependence of $E1$ values on the conditions and way of realisation of the polarographic measurements considerably restrict the application of this method to studies of micro-mechanism of initiation of organic energetic materials.

IN SITU MEASUREMENT OF VELOCITY OF DETONATION AND COMPARISON OF HEAVY ANFO PRODUCED IN THE FIELD OF USAGE AND CARTRIDGE EXPLOSIVES

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** Faculty of Mining, Geology and Petroleum Engineering, University of Zagreb, Croatia

Abstract:
This paper describes methods of measuring the velocity of detonation in bore holes loaded with different types of bulk explosive, such as heavy ANFO and cartridge explosives. The explosives are produced at the point of use with mobile equipment. The measurements of the velocity of detonation (VOD) involved bore holes with different diameters. On this basis the interdependence of the VOD and the bore-hole diameter was determined. The VOD measurements, with different blasting parameters, can be used for the selection of the best explosives to be produced at the site, taking into account the geological characteristics of the blasting rock.

NTREM, PARDUBICE, 2004 page 708-716