

CEPA 14 - A MECHANISM FOR EUROPEAN COLLABORATION ON ENERGETIC MATERIALS AND THEIR APPLICATIONS

A. S. Cumming
Chairman CEPA 14

Defence Science and Technology Laboratory (Dstl), Sevenoaks, UK

Abstract:

In a world where science and technology develops rapidly, and where there is need to maintain credible defence capability, there is a real need for collaborative mechanisms to enable allies to work together on Research and Technology. Only in this way can limited budgets be used most effectively, while maintaining an awareness and involvement in the state-of-the-art. CEPA 14, one of the Western European Armament Group CEP As, covers Energetic Materials and their Applications and provides a means for such collaboration. Its history and purpose are outlined together with a description of the programmes both under way and planned. Future strategy is also described.

NTREM, PARDUBICE, 2002 page 11-17

PRE-EXPLOSIVE PROCESSES IN HEAVY METAL AZIDES

B.P. Aduiev, E.D. Aluker and A.G. Krechetov

Kemerovo State University, Krasnaya 6, Kemerovo, 650043, Russia

Abstract

The results of the investigations of the processes of slow and explosive decomposition of heavy metal azides are summarized. A new class of chemical reactions - solid-phase chain reactions involving quasi-particles has been discovered on the basis of numerous experimental data.

NTREM, PARDUBICE, 2002 page 18-28

1,2-DINITROGUANIDINES: STRUCTURE - PROPERTY RELATIONSHIPS

Alexander M. Astachov *, Alexander D. Vasiliev **, Maxim S. Molokeev **, Ludmila A. Kruglyakova * and Rudolf S. Stepanov *

* Siberian State Technological University Krasnoyarsk, Russia, 660049

** Institute of Physics RAS (Sib. branch) Krasnoyarsk, Russia, 660036

Abstract:

Structure and some properties of two 1,2-dinitroguanidines, 1-nitro-2-nitrimino-imidazolidine and 1-methyl-1,2-dinitroguanidine, have been investigated. Their crystal and molecular structures were found by X-ray analysis. The structure data have been compared with thermal stability and impact sensitivity. Detonation parameters of the compounds were calculated by thermodynamic and correlation methods.

NTREM, PARDUBICE, 2002 page 29-41

STUDY ON THE DESENSITIZATION OF PLASTIC BONDED BIS(β,β,β -TRINITROETHYL-N-NITRO)ETHYLENEDIAMINE

Li Bing-ren and Li Xianming

Institute of Chemical Materials, China Academy of Engineering Physics, Mianyang,
621900, Sichuan, China

Abstract:

The crystal form and granularity of Bis(fi,fi,fi-trinitroethyl-N-nitro)ethylenediamine (BTENED), and the type and content of desensitizer have different effects on sensitivity of plastic bonded BTENED (PB-BTENED). TATB-graphite-wax (TATB-G-W) was discovered to be the best desensitizer. Mixing BTENED with HMX, added little TATB-G-W, The sensitivity of PB-BTENED could reach an expectantly low level.

NTREM, PARDUBICE, 2002 page 42-47

THERMOCHEMICAL ANALYSIS OF COMBUSTION PROCESS OF GAS GENERANTS CONTAINING SODIUM AZIDE

Stanislaw Cudzito and Waldemar Andrzej Trzcinski

Military University of Technology Kaliskiego 2, 00-908 Warsaw 49, POLAND

Abstract:

Thermochemical calculations and calorimetric experiments were performed for gas generating mixtures containing sodium azide and various oxidisers (KNO₃, CuO, MoS₂, S, C₆Cl₆, polytetrafluoroethylene and chlorinated polyvinyl chloride). An influence of the kind of an oxidiser and its contents in the mixture on the heat of reactions, the adiabatic combustion temperature and the composition of combustion products was determined. Mixtures producing low combustion temperatures as well as effective ways of the temperature minimisation were chosen.

NTREM, PARDUBICE, 2002 page 48-55

IRON OXIDE/ALUMINUM FAST THERMITE REACTION DRIVEN PROPAGATION

Luisa Duraes*, Jose Campos and Antonio Portugal***

Laboratory of Energetics and Detonics

*Chem. and **Mech. Eng. Departments - Fac. of Sciences and Technology University of Coimbra -
Polo II - 3030-290 Coimbra - PORTUGAL

Abstract:

Reaction between iron oxide (Fe₂O₃) and aluminum (Al) is the reference of the classic thermite compositions. Ignition of those thermite compositions is recognized to be problematic and the regression rates of its self-sustained reactions are commonly low. Also the efficiency of the reaction, for a given initial composition of Fe₂O₃ and Al, is evaluated by the final temperature and by the mass ratio of Al₂O₃/AlO in products of combustion (in condensed phase).

In order to increase pressure of the products of thermite reaction, the original composition based on Fe₂O₃/Al mixture is mixed, with an original twin screw extruder, with a small percent (< 3%) of propellant binder composed of ammonium or potassium nitrates, mixed with a polyurethane solution. The products of combustion and pyrolysis of this binder, reacting with thermite products, generating high temperature conditions, allow an easier but relatively slow propagation. These experimental thermodynamic conditions are also predicted using THOR thermochemical code. The study also presents DSC and TGA results of components and mixtures, and correlates them to the ignition phenomena and reaction properties. The experimental regression rate of combustion and its final attained temperature, as a function of the pressed thermite composition, are presented and discussed.

In order to generate a fast driven propagation in thermite material, an original configuration is used, driving the reaction with a continuous spark discharge, between an central electrode and the external

confinement, from a capacitor discharge. The driven reaction can then be correlated to the original self-sustained reaction, as a function of the composition and of capacitor discharge level. Results show an existing different reaction process, where the energy release, from the capacitor discharge, accelerates and enhances the thermite reaction propagation. Results are presented and the evaluation of additives contribution in this particular case is discussed.

NTREM, PARDUBICE, 2002 page 56

DETERMINATION OF ADDITIVES FROM EXPLOSIVE MATERIALS WITH GC/MS (EI,NCI)

Eisner A.*, Ventura K. * and Varga R.**

* Univerzity of Pardubice, Faculty of Chemical - Technology, Department of Analytical Chemistry, Nam. Cs. Legii 565, Pardubice 532 10, CZ

** Univerzity of Pardubice, Faculty of Chemical - Technology, Department of Theory and Technology of Explosives, Nam. Cs. Legii 565, Pardubice 532 10, CZ

Abstract:

Actual problem of these days is terrorist activities. The identification of explosive materials after terrorist attacks is necessary. The concentration of post-blast residues is very low, therefore is necessary to use very sensitive detection techniques. In this paper a comparison of two ionisation techniques for GC/MS is described. This is a electron impact ionisation and negative chemical ionisation.

NTREM, PARDUBICE, 2002 page 57-59

DETERMINATION OF THE DETONATION VELOCITY EMULSIONS EXPLOSIVES IN THE DIFFERENT THERMAL CONDITION

L. Cacic*, Z. Ester and M. Dobrilovic****

*Ministry of Interior Zagreb, Republic of Croatia

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

Abstract:

Detonation velocity is the velocity at which the chemical reaction zone propagates through a given explosive. It is one of the most important detonation parameters. Bearing in mind the fact that detonation velocities of known high explosives may reach nearly 10 mm/microsecond, the experimental determination of the detonation velocity is not easily achieved. However, when compared to the other detonation parameters, its accomplishment represents the least complicated task. The determination of the detonation velocity is based upon the measurement of the time interval needed for the detonation wave to travel a known distance through the explosive being tested. The measuring equipment used for the determination of the detonation velocity should provide the detection of the arrival of the detonation wave using suitable velocity probes. The measuring of the very short time-intervals (on a microsecond scale) needed for the detonation wave to travel a known distance through the sample between two velocity probes. Velocity of detonation shall be determined at the minimum diameter placed on the market, or the minimum diameter recommended by the manufacturer.

NTREM, PARDUBICE, 2002 page 60-68

THERMOLYSIS OF A PLASTIC BONDED EXPLOSIVE

Gurdip Singh and Prem Felix S

Department of Chemistry, DDU Gorakhpur University, Gorakhpur - 273 009, India

Abstract:

The thermolysis of pure RDX and its plastic bonded explosive (PBX) with hydroxyl terminated polybutadiene (HTPB) has been undertaken using TG-DTG and DTA techniques. Isothermal TG has been done and the data therefrom has been used to evaluate kinetic parameters using a model free isoconversional method. Explosion delay studies have also been undertaken using tube furnace technique. The results of the work done are discussed briefly on a comparative basis by analysing the departure of the thermal behaviour of the PBX from that of RDX.

NTREM, PARDUBICE, 2002 page 69-77

NEW METHODOLOGIES FOR MILITARY EXPLOSIVE MATERIALS TESTING IN THE CZECH ARMY

Marcel Hanus

Military Institute for Weapon and Ammunition Technology (VTUVM) 763 21 Slavcin, CZ

Abstract:

This paper summarises results of a transformation of the Czech Army testing system on military explosive materials and presents new testing methodologies implemented into the Czech Army procedures. Qualification of new explosive materials for military service in NATO countries according to STANAG 4170 and Czech Defence Standard 137601 was the first main target in implementation of NATO standards in the armament area. Based on experience gained with implementation of qualification procedures, modernisation of Czech Army surveillance procedures on in-service explosive materials was later managed and standardised by Czech Defence Standard 137603.

NTREM, PARDUBICE, 2002 page 78-86

STABILITY INVESTIGATION OF PLASTIC EXPLOSIVES DURING THEIR AGEING PROCESS.

Martina Chovancova, Peter Ocko, Rastislav Sevcik, Eubos Cavojsky and Jozef Lopiich

Military Technical and Testing Institute Zahorie, Slovak Republic

Abstract:

This elaboration investigates the ageing process influence on the stability and the mechanical properties of plastic explosives.

NTREM, PARDUBICE, 2002 page 87-92

THE INFLUENCE OF REACTION CONDITIONS ON TEX SYNTHESIS

Zdenek Jalovy and Robert Matyas

University of Pardubice, Department of Theory and Technology of Explosives, 532 10 Pardubice, Czech Republic

Abstract:

4,10-Dinitro-2,6,8,12-tetraoxa-4,10-diazatetracyklo[5.5.0.0.0]dodecane (TEX) was prepared by the reaction of 1,4-diformyl-2,3,5,6-tetrahydropiperazine (DFTHP) and glyoxal trimer hydrate in nitric acid. The influence of reaction conditions on the yield of product was examined. The varied reaction conditions were as follows: DFTHP/nitric acid ratio, reaction temperature, reaction time, glyoxal/DFTHP ratio.

INITIATION STRENGT

The samples of pure DMDNB did not exhibit increase in thermal stability in consequence of storage at elevated temperatures. Start of decomposition process can be observed at lower temperatures due to a melting process of mixtures of DMDNB with PETN and RDX respectively.
NTREM, PARDUBICE, 2002 page 128-135

THERMODYNAMIC PROPERTIES OF BINARY SYSTEM NITROCELLULOSE+ 2,4,6 - TRINITROTOLUENE

A. Ksi[^]zczak* and T. Wolszakiewicz**

*Department of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00 - 664 Warsaw, Poland

**Institute of Organic Industrial Chemistry, Annopol 6 03-236 Warsaw, Poland

Abstract:

Enthalpy of melting and mixing of system 2,4,6 - trinitrotoluene and nitrocelulose was determined by DSC method. The enthalpy of mixing of components was calculated. Maximum of mixing enthalpy in melting point is $n_{max} = -3.29 \text{ kJmol}^{-1}$ for molar fraction $X_{W2,4,6-TNT} = 0.503$. The Flory-Huggins interaction parameter was determined using calculated enthalpy of mixing. Temperature of glass transition (T_g) was determined using the sequential cycle of measurements. It was predicted by Lu-Weiss model which takes into consideration the Flory-Huggins interaction parameter. The second measurement on the same sample was performed after the few day storage of samples in the room temperature. The interpretation of melting peaks leads to the conclusion that the melting process of 2,4,6-TNT undregoes in the limited space of microfibre and unlimited space, outside the fibre.
NTREM, PARDUBICE, 2002 page 136-145

ANALYSIS OF POSSIBILITY OF WASTE ENERGETIC MATERIAL APPLICATION IN MINING BLASTING AGENTS

Andrzej Maranda*, Katarzyna Lipinska and Marek Lipinski**

*Military University of Technology, 2 Kaliskiego str. 00-908 Warsaw, Poland **Institute of Industrial Organic Chemistry 6 Annopol str. 03-236 Warsaw Poland

Abstract:

Some problems connected with the application of waste energetic materials (smokeless powder propellants, composite propellants, high explosives) as raw materials for the production of various products useful in civilian applications was presented. The mining industry is a basic consumer of commercial explosives and one of the ways of waste energetic material recycling is to use them as ingredients of mining blasting agents. Some examples of commercial products were showed.
NTREM, PARDUBICE, 2002 page 146-150

MECHANICAL DESTRUCTION OF ENERGETIC POLYMERIC COMPOSITES (EPC)

V.A. Malchevsky, N.A. Zarytovskaya and T.A. Mikhailikova

D.I. Mendeleev Russian Chemical Technological University, Miusskaya pi. 9, Moscow, 125047

Abstract:

The research relates to the area that deals with one of the most important issues of the physical-chemical mechanics of polymeric materials - the problem of "kinetic" and "critical" alternatives for the evaluation of mechanical destruction of polymeric composites. It sets a practical goal of developing a method for the calculation of kinetic parameters of the mechanical destruction process

on the grounds of tests with the use of standard tearing machines at constant straining velocities ($s = \text{const.}$), i.e. trials based on the understandings about mechanical destruction as a critical phenomenon. The research resulted in a number of interrelated dependences that facilitated calculations of the EPC destruction kinetics on the basis the strength- temperature function $\sigma = f(T)$ and the strength-loading velocity (V or strength-tension (s) dependence. The results of the analysis of EPC strength characteristics attained on the basis of tests at uniaxial stretching and $a = \text{const}$ or $e = \text{const}$ show that they do not contradict and are complementary.

NTREM, PARDUBICE, 2002 page 151-158

DETONATION AND APPLICATION CHARACTERISTICS OF THE LATEST GENERATION OF EMULSION EXPLOSIVES

Andrzej Maranda*, Barbara Golajbek and Johann Kasperski**

*Military University of Technology, Warsaw, POLAND **BLASTEXPOL, Duninow, POLAND

Abstract:

Emulsion explosives have been very important blasting agents since some years. That results from their unquestionable advantages and introduction of new emulsion explosive generations into the market. The range of application of individual emulsion explosives in Polish and western countries mining are presented. Compositions, detonation parameters and properties of some types of emulsion explosives offered by "Blastexpol" are also presented and their ecological advantages are showed.

NTREM, PARDUBICE, 2002 page 159-164

CAST TNAZ MIXTURES

Pavel MARECEK and Kamil DUDEK

ALIACHEM a.s., Division SYNTHESIA, Research Institute of Industrial Chemistry (VTJPC), 532
17 Pardubice - Semtin, Czech Republic

Abstract

Preliminary testing of TNAZ mixtures with active components (HMX, RDX) has been performed in laboratory scale. The parameters evaluated were compatibility, sensitivity to impact, sensitivity to friction, thermal stability, shock sensitivity and detonation velocity. The results especially with regard to utilization of TNAZ as a component of explosive charge, are discussed.

NTREM, PARDUBICE, 2002 page 165-169

DETERMINATION OF PHYSICAL CHARACTERISTICS OF DETONATION PRODUCTS

Frantisek Masaf, Pavel Vavra and Jif 1 Vagcnknccht

University of Pardubice, KTTV, 530 12 Pardubice, CZ

Abstract:

Physical characteristics of detonation products such as velocity, conductivity and length of conductive zone were measured. Influence of potassium nitrate addition into the explosive was consequently determined.

NTREM, PARDUBICE, 2002 page 170-174

SYNTHESIS OF NEW HETEROCYCLIC AZIDONITRAMINES

Alevtina S. Medvedeva*, Luybov P. Safronova, Maria M. Demina, Galina S. Lyashenko, Vladimir V. Novokshonov, Andrei V. Afonin and Galina I. Sarapulova
A. E. Favorsky Irkutsk Institute of Chemistry, Siberian Branch of the Russian Academy of Sciences,
664033 Irkutsk, Russian Federation

Abstract:

Syntheses of new six- and seven-membered heterocyclic azidonitramines are presented. These nitramines are: 3-azidoethyl-1,5-dinitro-1,3,5-triazacycloheptane, 5-azido-1,3-dinitro-1,3-diazacyclohexane and 5,5'-diazido-1,3,3'-tetranitro-1,1',3,3'-tetraaza-2,2'-dicyclohexane. The molecular structures of them are confirmed by IR and ¹³CNMR spectroscopies.

NTREM, PARDUBICE, 2002 page 175-177

DEVELOPMENT OF THE DIVERGENT DETONATION WAVE IN PBX BASED ON RDX

R. Mendes, J. Campos, I. Plaksin and J. Ribciro

LEDAP - Lab. of Energetics and Detonics, Mech. Eng. Dept., Fac. of Sciences and Technology, Polo II, University of Coimbra, 3030-201 Coimbra, Portugal

Abstract

To characterize the initial phase of the divergent detonation wave in PBX, a hemispheric explosive sample was initiated by a long cylindrical charge with the same explosive composition. The tested PBX is formed by 85 % (in mass) of RDX (bimodal particle distribution - 75 % of $d_{50} = 96\ \mu\text{m}$ and 25 % of $d_{50} = 22\ \mu\text{m}$) and 15 % of HTPB binder, presenting an effective density of $1.574\ \text{g/cm}^3$ (> 99 % TMD) and detonation velocity of $7.90\ \text{mm}/\mu\text{s}$. An optical method based on 64 optical fibers ribbon ($250\ \mu\text{m}$ of diameter each fiber) connected to a fast electronic streak camera, allows the measurement of the detonation velocity inside the PBX sample, as a function of the run distances, for several angles with the axis of initiation channel. The results, presented as a radius-time and velocity-radius diagrams, show the evolution of a divergent detonation wave in its run, up to the radius of 33 - 34 mm (6.6 - 6.8 times the diameter of the cylindrical initiation channel). The obtained real shape of the divergent detonation wave is significantly different from those predicted with an ideal propagation model. Measurements of the pressure in the induced shock wave in an inert standard barrier were performed, from the divergent detonation wave generated by the long cylindrical PBX charge. It presents an initial divergent detonation wave of positive constant curvature with relatively significant amplitudes in velocity and pressure values.

NTREM, PARDUBICE, 2002 page 178-184

EFFECT OF DISCONTINUOUS PHASE OF EMULSION ON THE STABILITY OF EMULSION SLURRY EXPLOSIVES

Milka Matejic Grguric

Tehnicki opitni centar, Vojvode Stepe br. 445, 11000 Belgrade, Serbia, Yugoslavia

Abstract:

Emulsion slurry explosives (ESE) are modern blasting agents. It investigated the effect of the discontinuous phase of emulsion on the stability high emulsion type water-in-oil. Discontinuous phase of emulsion is saturated water solution some inorganic salts of nitric acid (ammonia nitrate, sodium nitrate, calcium nitrate). Stability of emulsion is changed by composite and pH value of discontinuous of emulsion in course of time. Changes of stability of emulsion were measured by changes of detonation velocity and waterproof of emulsion after 1, 2, 3, 6, 12 and 18 months. It was

considered that discontinuous phase had influence on stability of emulsion. With increased content of ammonium nitrate, water and pH solution salts was increased stability of emulsion.
NTREM, PARDUBICE, 2002 page 185-189

A CONTACT COMPATIBILITY INVESTIGATIONS BETWEEN SMOKELESS POWDERS AND EPOXIDE PAINT BY MEANS OF TGA, DSC THERMAL ANALYSIS AND ISOTHERMAL HEATING AT 75 °C

Maciej MISZCZAK, Eugeniusz MILEWSKI, Jan SZYMANOWSKI, Jacek BORKOWSKI, Andrzej MARCZUK and Beata SMIGIELSKA

Research Department of Combat Means, Military Institute of Armament Technology, Wyszynskiego 7, Str., 05-220 Zielonka, POLAND

Abstract:

In this paper there are presented investigations on contact compatibility between three types of nitrocellulose propellants and epoxide paint. Tested on contact compatibility material set up - smokeless powder / paint exists in packages used during transportation and storage of throwing materials. The tests on compatibility were done by means of differential thermogravimetry analysis (TGA) and differential scanning microcalorimetry (DSC) - both in dynamic option according to STANAG 4147 [1] and by isothermal heating at 75°C for 48 hrs due to UN method [2].

NTREM, PARDUBICE, 2002 page 190-199

CONTACT COMPATIBILITY INVESTIGATIONS OF HIGH-ENERGETIC MATERIALS USED IN MORTAR AUGMENTING PROPELLING CHARGES

Maciej MISZCZAK, Jacek BORKOWSKI, Eugeniusz MILEWSKI, Jan SZYMANOWSKI, Andrzej MARCZUK and Beata SMIGIELSKA

Research Department of Combat Means, Military Institute of Armament Technology, Wyszynskiego 7, Str., 05-220 Zielonka, POLAND

Abstract:

In this paper, investigations on contact compatibility between burning containers (made on the basis of nitrocellulose (NC)) and extruded - impregnated propellants (Elpropellants) manufactured on the basis of NC and nitroglycerine (NG) forming high-energetic materials set-up in mortar augmenting charges are presented. The investigations were done for these high-energetic materials unaged and aged at 75° C for 30 days (RHca.=50%). Compatibility measurements were done by means of Thermogravimetry Analysis (TGA), Differential Scanning Calorimetry according to STANAG 4147 and by thermostating at 75°C for 48 hrs due to UN test.

NTREM, PARDUBICE, 2002 page 200-207

IRON OXIDE/ALUMINUM FAST THERMITE REACTION USING

NITRATE ADITIVES

Joel Morgado*, Luisa Duraes**, Jose Campos* and Antonio Portugal

*Laboratory of Energetics and Detonics

Mech. and Chem. Eng. Departments - Fac. of Sciences and Technology University of Coimbra -
Polo II - 3030 Coimbra - PORTUGAL

Abstract

Reaction between iron oxide (Fe₂O₃) and aluminum (Al) is the reference of the classic thermite compositions. Ignition of those thermite compositions is recognized to be problematic and the regression rates are commonly low. The selection of an additive binder, based in ammonium or potassium nitrates, in small concentrations, generate a different global ignition phase, because the reaction between these additives and part of the existing aluminium generates enough energy that helps ignition and further reaction propagation between iron oxide and aluminium.

These experimental thermodynamic conditions are also predicted using THOR thermochemical code. THOR code assumes the thermodynamic equilibria of all possible products, for the minimum Gibbs free energy, using HL EoS. The code allows the possibility of estimating pyrolysis decomposition of additives, as a function of absorbed energy or as a function of final temperature in adiabatic conditions. The global reaction, predicted for isobar adiabatic conditions can then be correlated to the preceding decomposition results. The presented predictions prove not only the contribution of additives in global reaction but also the significant influence of transition phase from gas to solid of formed Al₂O₃.

The experimental study was performed mixing the original composition, based on Fe₂O₃/Al mixture, with a small percent (< 10 %) of propellant binder composed of ammonium and sodium nitrates (AN/SN), mixed with Paraffin. The reaction velocity is evaluated by the adimensional regression rate as a function of the adimensional time. When the ignition of AN/SN additives occurs, T_b decreases significantly - this effect with the expansion of combustion products gases show 5% to be the best AN/SN additives concentration with the most stable tested combustion.

NTREM, PARDUBICE, 2002 page 208-222

INFLUENCE OF TESTING CONDITIONS ON RESULTS OF DYNAMIC MECHANICAL ANALYSIS OF DOUBLE BASE ROCKET PROPELLANTS

Sanja Matecic Musanic, Muhamed Suceska and Bakija Sanko

Brodarski institut - Marine Research & Special Technologies Av. V. Holjevca 20, 10020 Zagreb,
Croatia

Abstract:

Dynamic mechanical analysis (DMA) is a powerful technique for determination of mechanical properties of rocket propellants. This technique enables determination of the storage and loss modulus of a propellant against time, temperature or frequency of an oscillation load, while the temperature of the sample in a specified atmosphere is programmed.

However, like many other thermal methods DMA gives results that may depend greatly on the conditions used during the experiment. Thus, it is very important to use such experimental parameters that will minimise the error caused by the dynamic nature of the experiment, sample dimensions, etc.

In this work we have studied influence of heating rate, frequency, and length to thickness ratio on results of dynamic mechanical analysis. The results obtained have shown that the experimental parameters may have significant influence on values of the viscoelastic function for double base propellant.

STUDY OF BIODEGRADATION OF SELECTED EXPLOSIVES BY PLANTS - ALTERNATIVE WAY OF SOIL AND WATER DECONTAMINATION

Ales Nepovim*, Radka Podlipna*, Hartmuth Thomas**, Andre Gerth**, Zdenek Jalovy***, Svatopluk Zeman*** and Tomas Vanek*

*Dept. of Plant Tissue Cultures, Institute of Organic Chemistry and Biochemistry, AS CR, Flemingovo nam. 2, 166 10 Praha 6, Czech Republic.

**Bioplanta GmbH, Delitzsch, Germany

*** Dept. of Theory and Technology of Explosives, University of Pardubice, 532 10 Pardubice, Czech Republic

Abstract:

Phytoremediation is a bioremediation technique used for cleaning contaminated sites by plants. The phytoremediation of trinitrotoluene (TNT), pentaerythritol tetranitrate (PETN), and glyceroltrinitrate (GTN) was studied. The plants were cultivated as a cell suspension culture and hydroponically cultivated plants under sterile conditions and thus were used as model system for description of metabolic processes. The metabolites of degradation were analysed by HPLC and identified by comparing retention times and UV spectra of standards of known or expected metabolites. Our results indicated that plants effectively degraded TNT, PETN, and GTN. All studied compounds were removed from the cultivation medium and transformed to the metabolites, which were partially excreted back into cultivation medium and rest bound to the cell structures.

NTREM, PARDUBICE, 2002 page 234-237

RESEARCH OF PHYSICOCHEMICAL PROPERTIES OF PLASTIC EXPLOSIVE

Andrzej Orzechowski*, Witold Pajjowski* and Andrzej Maranda**

institute of Industrial Organic Chemistry 2Military Academy of Technology

Abstract:

The users would like to receive plastic explosive of the appropriate plasticity, chemical and physical stability and appropriate explosive properties in range of temperatures -4(fC to +7(fC. Plasticity is one of the most important parameters and determine of the application. The influence of the polymer and its content, modifying agents and the content of explosive on plasticity was examined. Plastic explosive (PE) was produced in Poland, but this material did not have right chemical and physical stability. Liquid component exudation from plastic explosive results in the deterioration of its chemical and physical stability. The influence of the explosive and polymer content on the exudation of liquid component was investigated.

NTREM, PARDUBICE, 2002 page 238-246

SYNTHESIS AND CRYSTAL STRUCTURE OF TETRAACETYLDICHLOROACETYLHEXAAZASOWURTZIT ANE

TRIHYDRATE

Ou Yuxiang, Liu Lihua, Chen Boren and Lijin

School of Chemical Engineering & Material Science, Beijing Institute of Technology, Beijing 100
081, China

Abstract

A novel hexasubstituted hexaazaisowurtzitane - tetraacetyldichlorohexaaza isowurtzitane (TADCIW) was synthesized, and the colorless and transparent single crystal of TADCIW \cdot 3H $_2$ O was prepared by evaporating solvent slowly. The crystal belongs to monoclinic system and space group Cc with parameters $a = 1.0469(2)$ nm, $b = 1.5347(3)$ nm, $c = 1.5364(4)$ nm; $\beta = 95.00^\circ$; $Z = 4$; $V = 2.4591(9)$ nm 3 ; $D_c = 1.468$ g.cm $^{-3}$; $R = 0.0487$, $WR = 0.1168$.

NTREM, PARDUBICE, 2002 page 247-251

SOME ASPECTS OF SERVICE LIFE EVALUATION OF COMPOSITE

ROCKET PROPELLANTS

Jiff Pachman*, Marcel Hanus** and Jakub Selesovsky*

*University of Pardubice, Dept. Theory and Technology of Explosives, 532 10 Pardubice, CZ

**Military Institute for Weapon and Ammunition Technology (VTUVM), 763 21 Slavcin, CZ

Abstract:

This paper summarizes and comments experimental results of aging characterization of different in-service composite solid rocket propellants. The aim of this work was to determine and to evaluate changes in chemical composition (sol/gel content), thermal stability (TGA, DTA), mechanical properties (uniaxial tensile and compression tests, hardness), thermomechanical properties (DMA, TMA), sensitiveness to impact, friction and electric spark induced by aging.

NTREM, PARDUBICE, 2002 page 252-262

CHARACTERISATION OF EXPLOSIVE MATERIALS USING MOLECULAR DYNAMICS SIMULATIONS

Miroslav Pospisil*, Pavla Capkova*, Pavel Vavra** and Svatopluk Zeman**

* Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles
University Prague, Ke Karlovu 3, 12116 Prague 2, Czech Republic.

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

Abstract:

Classical molecular dynamics simulations of the unimolecular decomposition have been performed for selected molecules exhibiting different impact sensitivity and different detonation energy: (1) (CH $_2$ NNO $_2$) $_3$, more commonly known as RDX, (2) (CH $_2$ NNO $_2$) $_4$, known as HMX, (3) (NH $_2$) $_2$ CC(NO $_2$) $_2$, known as DADNE and (4) (NH $_2$) $_2$ CNNO $_2$, known as NQ (see figures 1-4a). A potential energy was described using empirical force field cvff_950. Molecular dynamics simulations were carried out in Cerius2 modelling environment. The analysis of dynamic trajectories enabled us to reveal step by step the mechanism of decomposition and to characterize the impact sensitivity and

explosives performance (detonation energy) of these energetic materials. The characteristic parameters determined from the dynamics trajectory simulations are in agreement with the experimentally measured sensitivity and detonation energy.

Keywords: energetic molecules, molecular decomposition, explosives, molecular dynamics simulations.

NTREM, PARDUBICE, 2002 page 263-271

THERMAL PROPERTIES OF A NITROCELLULOSE PROPELLANT UNDER ACCELERATED AGEING CONDITION

Masa Rajic and Muhamcd Sueska

Brodarski institut - Marine Research & Special Technology Av. V. Holjevca 20, 10000 Zagreb, Croatia

Abstract:

The stabiliser content, sample mass, thermal and kinetic properties of a nitrocellulose propellant were followed during the accelerated ageing at 100 °C.

The differential scanning calorimetry (DSC) and thermogravimetric analysis (TGA) were used for determination of the thermal and kinetic properties, while stabiliser content has been determined by UV-VIS spectrophotometer.

It was found out that, at selected ageing temperature, the stabiliser consumes almost completely after four-five days, while at the same time some thermal properties do not change so significantly (e.g. onset, endset, and peak maximum temperature on DSC thermogram). The kinetic and thermal parameters decrease with the ageing, however this decrease is not monotonous along the investigated ageing period.

NTREM, PARDUBICE, 2002 page 272-280

ENGINEERING CALCULATIONS OF GAS EXPLOSION PARAMETERS IN CLOSED AND VENTED VESSELS

Tadeusz J. Rychter and Andrzej Teodorczyk

Warsaw University of Technology, ITC, Nowowiejska 25, 00-665 Warszawa, Poland

Abstract

A simple mathematical model for the prediction of the pressure and temperature changes during a totally confined or vented gaseous explosion is presented. The model is based on solutions of conservation equations of mass, momentum and energy supplemented with equilibrium calculations of the physical and chemical properties of combustion products. The influence of turbulence on combustion is included by the use of empirical relations taken from literature. A computer program VEX, written to solve the mathematical model is presented in details for potential users. The program computes typical explosion problem in few seconds on PC computer. The program has graphical pre- and postprocessor enabling convenient input of data and output of results. A mixture of 6 fuels (H₂, CH₄, C₂H₂, C₂H₄, C₂H₆, C_sH_s) with air or oxygen can be used in calculations. Spherical, cylindrical and cuboidal geometry of the vessel with arbitrary axial ignition location and arbitrary location and size of the vent can be used. The predictions from the model have been validated against experimental results obtained from the literature and from author's studies. The program has also the separate option for calculations of equilibrium combustion products composition and temperature at constant pressure or constant volume.

NTREM, PARDUBICE, 2002 page 281-292

ACID-BASE CHARACTERISTICS OF FOX-7 AND ITS MONOHYDRAZO ANALOGUE

Camilla Sandberg*, Nikolaj Latypov*, Patrick Goede*, Rolf Tryman* and Anthony J. Bellamy**

* FOI, Swedish Defence Research Agency, Department of Energetic Materials, S-147 25 Tumba, Sweden.

** Department of Environmental and Ordnance Systems, Cranfield University, Royal Military College of Science, Shrivenham, Swindon, Wilts SN6 8LA, England.

Abstract:

l,l-diamino-2,2-dinitroethylene, FOX-7 (1) is a novel explosive with high performance and low sensitivity! >2. In addition l-amino-l-hydrazino-2,2-dinitroethene (Hydrazo FOX-7, HDF) (2) has recently been prepared by reaction of FOX-7 with hydrazine. Several studies of FOX-7 have been performed and complementary studies with acid-base characterization of both FOX-7 and HDF are presented in this paper. The effect of varying pH on both FOX-7 and HDF and the formation of their respective salts are discussed along with the basic hydrolysis of FOX-7 to dinitromethane. NTREM, PARDUBICE, 2002 page 293-300

KINETICS AND MECHANISM OF TRIAMINOGUANIDINE NITRATE THERMAL DECOMPOSITION

Sergey Smirnov and Boris Lurie

Mendeleev University of Chemical Technology, Miusskaya sq. 9, Moscow, 125047, Russia

Abstract:

Kinetics of Triaminoguanidine nitrate (TAGN) thermal decomposition have been studied in both solid and liquid (in solution of Ammonium nitrate and also of aromatic nitrocompounds)) states. Decomposition of the solid substance goes with strong acceleration. Its formal kinetic characteristics have been determined. The main cause of the acceleration is progressive melting of the solid substance during its chemical transformation. TAGN decomposition in solution goes with decreasing rate. This rate is in ten times higher than in the solid state. The main gaseous products of decomposition are N₂, N₂O and H₂O. Chemistry of the thermal decomposition process is discussed. NTREM, PARDUBICE, 2002 page 301-308

INFLUENCE OF THERMAL DECOMPOSITION KINETIC MODEL ON RESULTS OF PROPELLANTS SELF-IGNITION NUMERICAL MODELING

Muhamcd Succska

Brodarski institut - Marine Research & Special Technologies, Av. V. Holjevca 20, 10000 Zagreb, Croatia

Abstract

Thermal decomposition of nitrocellulose propellants is accompanied by generation of heat, and under certain conditions can lead to the well-known phenomenon of the self-ignition. Therefore, it is of great concern to predict whether or not a propellant specimen will ignite under given conditions (specimen mass and shape, surrounding temperature, etc.).

An own computer program, named THERMEX, based on the thermal explosion theory and the finite difference method, was developed in order to describe the reactive heat conduction phenomena in

infinite slab, cylindrical, and spherical geometry of an explosive material. Up to now the program is tested by the comparison of the calculated times to ignition with the times to ignition experimentally obtained or calculated by other authors. A good agreement was found under identical computational conditions.

However, it was noticed that, along with some input data (e.g. space and time increments), thermal decomposition kinetic model used in calculations have a large influence on the calculation results. The influence of three kinetic models, commonly used to describe thermal decomposition of propellants, on the results of calculation is analysed in this paper. It was found out that the power law kinetic model gives the best agreement between the experimentally obtained and the calculated values of times to ignition.

NTREM, PARDUBICE, 2002 page 309-323

AN ANALYSIS OF LARGE SCALE ETHYLENE RELEASE AND EXPLOSION

Andrzej Teodorczyk

Warsaw University of Technology, ITC, Nowowiejska 25,00-665 Warszawa, Poland

Abstract

In the paper an engineering analysis is presented of ethylene release from the ruptured reactor in the polyethylene installation of petrochemical plant in Poland. Gas release was also analysed by computer simulation using KIVA3 V CFD code. Approximately 100 kg of ethylene was released during pressure decrease in the reactor from 243 MPa to HOMPa. Time of release of 100 kg of ethylene calculated from the simple model was equal to about 3.1 s. This was is close to the time of pressure drop in the reactor from 243 MPa to 110 MPa, recorded by measuring equipment (about 4 s). In addition, simple analysis of the TNT equivalent of gas explosion was calculated, based on mass released and recorded damages.

NTREM, PARDUBICE, 2002 page 324-330

ANALYSIS OF THE MOTION OF METAL PLATES IN MODEL REACTIVE ARMOURS

Waldemar Andrzej Trzcinski, Radostaw Trębinski and Stanisław Cudzito

Military University of Technology, Kaliskiego 2, 00-908 Warsaw, POLAND

Abstract:

An analysis of the process of driving metal plates of model reactive armours by the gaseous products of the detonation was studied in experimental and theoretical ways. The detonation in confined layer of explosive was initiated by the fuse or by the jet at various incidence angles. The X-ray impulse photography was applied to record the motion of plates. The theoretical analysis was performed by the use of a simple model, in which the plate deformation and finite time of its acceleration were taken into account. The time-space characteristics of motion of model reactive armour elements obtained from experiments and numerical modelling can be applied for designing cumulative heads destined for destroying armours protected by reactive armour.

NTREM, PARDUBICE, 2002 page 331-338

FTIR SPECTROSCOPIC STUDY OF THE PROTONATION OF CONDUCTING POLYMER WITH ENERGETIC COMPOUND

Miroslava Trchova*, Irina Sapurina and Jaroslav Stcjskal*****

* Charles University Prague, Faculty of Mathematics and Physics, 180 00 Prague 8, CZ

** Institute of Macromolecular Compounds RAS, St. Petersburg 199004, RUS

*** Institute of Macromolecular Chemistry AS CR, 162 06 Prague 6, CZ

Abstract:

The preparation of materials combining the features of conducting polymers and energetic compounds is demonstrated. The FTIR spectra are used to discuss changes in the molecular structure of product of protonation reaction between two non-conducting compounds, poly aniline (PANI) base and 3-nitro-1,2,4-triazol-5-one (NTO). Three ways of preparation have been tested: the interaction of PANI base with NTO dissolved in water, the polymerization of aniline in the aqueous medium containing NTO, and solid-state blending of both components. The progress of protonation of PANI with NTO was assessed by the changes in conductivity.

NTREM, PARDUBICE, 2002 page 339-348

MEASUREMENT OF DETONATION VELOCITIES OF FORMED LINEAR CHARGES

Jifi Vagenknecht*, Zbynek Akstein and Pavel Vavra***

* University of Pardubice, Department of Theory and Technology of Explosives, 530 12 Pardubice, CZ

** Research Institute of Industrial Chemistry (RIICH), 532 17 Pardubice - Semtin, CZ

Abstract:

By measurement of detonation velocity in formed linear charge (FLC) of plastic explosive with parallel use of continuous and discontinuous method there was performed an experiment to study the influence of forming the charge on character of propagation of the detonation wave in profile of the charge.

NTREM, PARDUBICE, 2002 page 349-357

EFFECT OF INTERMOLECULAR FORCES ON SOME PROPERTIES OF EXPLOSIVES

Pavel Vavra*, Miroslav Pospisil and Jarmila Repakova****

* Department of Theory and Technology of Explosives Faculty of Chemical Technology, University of Pardubice 53210 Pardubice, Czech Republic

** Department of Chemical Physics and Optics, Faculty of Mathematics and Physics, Charles University 12116 Prague, Czech Republic

Abstract:

Values of total sublimation energy and its van der Waals, Coulomb, and hydrogen-bond energy contributions have been calculated for a selected set of explosives on the basis of their structural data, and their non-negligible effect on sensitivity parameters, densities and melting temperatures has been established. These parameters are significantly affected by hydrogen bonds and total magnitude of intermolecular forces. Also other factors affecting these parameters are discussed.

NTREM, PARDUBICE, 2002 page 358-369

ENERGETIC MATERIALS FOR INSENSITIVE MUNITIONS

Richard Wild *

Diehl Munitionssysteme GmbH & Co. KG, Werk Maasberg, MML, D-66620 Nonnweiler, Germany

Abstract:

Worldwide efforts are made to reduce the vulnerability of ammunitions and to bring Insensitive Munitions (IM) in use. In the past, cure cast PBX was considered to be the only solution for acceptable IM compliant ammunition, especially in strongly confined warheads. Some years ago we started to use special, pressed plastic bonded explosives for IM also in thick steel shells with IM results similar to cure cast filled warheads. Basis for our pressed IM are less sensitive Plastic Bonded Explosives with RDX and HMX. In this paper some of the parameters are discussed, we use to influence the sensitivity of ammunition by the high explosive, by the binder, by the preparation of the PBX and by the manufacturing process of the HE-charge.

The progress of the last 3 years in getting less sensitive moulding powders, can be demonstrated e.g. in the improvements of the impact sensitivity (BAM), in the better compacting behaviour of the granules and the higher initiation threshold of charges. The Bullet Impact test with a cure cast and a pressed PBX was chosen for an IM comparison of both production methods.

NTREM, PARDUBICE, 2002 page 370-383

PERFORMANCE PARAMETERS OF EXPLOSIVES: EQUILIBRIUM AND NONE-EQUILIBRIUM REACTIONS

F. Volk

Fraunhofer Institut Chemische Technologie (ICT) D-76327 Pfinztal-Berghausen

Abstract:

For the calculation of the performance parameters of combustion processes, equilibrium thermodynamic processes are being taken into account. On the other side, so-called none-equilibrium reactions occur, mostly connected with low pressure burning. In this paper, several explosives, explosive mixtures, solid and liquid propellants have been calculated. It was shown how energy-output and gas formation is dependent on the O₂-balance and the enthalpy of formation. It was found that the reason for the higher specific energy of liquid propellants was the increased formation of gases consisting of H₂, N₂ and H₂O, compared with conventional solid propellants based on nitrocellulose and nitroglycerine. None-equilibrium combustion of solid propellants was found at very low loading densities or pressures lower than 25 bar. In this case, the reaction products measured by mass spectrometry are metastable and highly toxic, producing a much lower heat of explosion compared with equilibrium burning measured and calculated.

NTREM, PARDUBICE, 2002 page 384

HEAT CONDUCTIVITY MEASUREMENTS OF EXPLOSIVES

Stephan Wilker, Uldis Ticmanis and Gabriele Pantel

WIWEB AuBenstelle Heimerzheim, GroBes Cent, 53913 Swisttal, Germany

Abstract:

Chemical stability of explosives, especially nitrocellulose based propellants is of big interest, since from time to time propellant magazines blow off due to autocatalytical self-heating reactions. To avoid danger from exothermal reactions it is important to determine their temperature and time dependence. But as well the thermal transport properties of solid materials are a very important factor, since self-heating processes are only possible when the heat generation rate inside the material is faster than the heat transport to the surface.

In the past the determination of thermal transport properties of solid materials was a time-consuming and quite complicated job. Now, with a newly developed, so-called 'Hot Disk' method these difficulties are overcome. This apparatus delivers reliable and fast results of heat conductivity and thermal diffusivity and thus of the heat capacity. The measuring principle bases on heating up the sample by 0,2 to 10 K and recording the temperature/time curve by the same sensor that generated the heat. By mathematical treatment of the T/t data the thermal transport properties are available. The sample must not necessarily be a homogeneous block. Also bulk materials and even liquids can

be examined by this method. An independent check of the heat capacity by other method(s), e.g. DSC or microcalorimetry guarantees the correctness of the obtained data.

This paper describes the method, its advantages and limitations and gives an overview, how the data can be used for the prediction of the chemical stability of explosives and related items.

NTREM, PARDUBICE, 2002 page 385-399

EFFECT OF MOLDING POWDER PRODUCTION, CHARGE PRESSING AND AGING ON PARTICLE SIZE OF EXPLOSIVES

Shu Yuanjie, Dong Haishan, Liu Shijun, Liu Yonggang, Song Huajie, Hao Ying, Zhan Chunhong and Chen Jie

Institute of Chemical Materials CAEP, 621900, Mianyang, Sichuan, China

Abstract:

Influence of such processes as molding powder production pellets pressing and aging under different conditions on TATB HMX particle size was experimentally studied. The results obtained showed that particle size of these explosives was greatly changed before and after molding powder production but for different size grade of explosive this change was not the same; pressing process had great effect on explosive particle size also, but before and after ageing process explosive particle size did not change seriously.

NTREM, PARDUBICE, 2002 page 400-406

STUDY OF THE IMPACT REACTIVITY OF POLYNITRO COMPOUNDS

PART I.

IMPACT SENSITIVITY AS "THE FIRST REACTION" OF POLYNITRO ARENES.

Svatopluk Zeman and Miloslav Krupka

Department of Theory & Technology of Explosives, University of Pardubice, CZ-532 10 Pardubice, Czech Republic

Abstract:

The impact reactivity („ the first reaction") of 20 polynitro arenes was expressed as the drop energy E_d required for 50 percent initiation probability. Relationships have been found between the E_d values and heats of fusion, on the one hand, and UCNMR chemical shifts of carbon atoms in reaction centers, on the other. On the basis of the said relationships it was stated that the impact reactivity of polynitro arenes molecules depends on the electronic configuration within their reaction centers and intensity of their intermolecular interactions in the molecular crystals.

NTREM, PARDUBICE, 2002 page 407-415

STUDY OF THE IMPACT REACTIVITY OF POLYNITRO COMPOUNDS

PART II.

IMPACT SENSITIVITY AS A FUNCTION OF THE INTERMOLECULAR INTERACTIONS

Svatopluk Zeman and Miloslav Krupka

Department of Theory & Technology of Explosives, University of Pardubice, CZ-532 10 Pardubice, Czech Republic

Abstract:

Published data of impact sensitivity, detected for sound of 32 polynitro compounds were expressed as the drop energy, Edn required for 50 percent initiation probability. A logarithmic relationship has been found between the Edr values and heats of fusion of the said compounds. The relationship has been found to be in accordance with the idea of the role of plastic deformations of crystal played in the initiation of energetic materials by impact and shock. An analogous application of heats of sublimation has not given convincing results.

NTREM, PARDUBICE, 2002 page 416-426

STUDY OF THE IMPACT REACTIVITY OF POLYNITRO COMPOUNDS

PART III.

RELATIONSHIP BETWEEN ELECTRONIC CHARGES AT NITROGEN ATOMS OF PRIMARILY SPLIT OFF NITRO GROUPS AND IMPACT SENSITIVITY OF SOME POLYNITRO ARENES

Svatopluk Zeman*, Zdenek Friedl** and Radim Huczala*

* Department of Theory & Technology of Explosives, University of Pardubice, CZ-532 10 Pardubice, Czech Republic

** Faculty of Chemistry, Brno University of Technology, CZ-612 00 Brno, Czech Republic

Abstract:

*Electronic charges q at nitrogen atoms of eight polynitro arenes were calculated by means of ab initio DFT B3LYP/6-31G** and semi-empirical AMI methods. The relationships have been confirmed between impact sensitivities of the arenes and q -values for primarily split off nitro groups. These relationships directly specify the most reactive nitro groups of molecules with trinitrophenyl and trinitrophenylene building units in the initiation by impact.*

NTREM, PARDUBICE, 2002 page 427-434

STUDY OF THE IMPACT REACTIVITY OF POLYNITRO COMPOUNDS

PART IV.

ALLOCATION OF POLYNITRO COMPOUNDS ON THE BASIS OF THEIR IMPACT SENSITIVITIES

Svatopluk Zeman

Department of Theory & Technology of Explosives, University of Pardubice, CZ-532 10 Pardubice, Czech

Abstract:

A linear relationship has been found between the drop energies of impact sensitivity detected by sound and the drop energies of „ the first reaction" for 25 polynitro compounds. In the sense of this relationship, the compounds studied fall into three classes. The reason of the said diversification lies in the decomposition reaction rate at the temperature of beginning thermolysis.

NTREM, PARDUBICE, 2002 page 435-444