Abstracts

DATA BASE OF LAMINAR-FLAME PROPERTIES IN HOMOGENEOUS AIR MIXTURES OF METHANE AND HYDROGEN IN PRESENCE OF STEAM

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Based on the solution of the problem on the planar laminar flame structure, the authors have developed the data base of laminar-flame properties in homogeneous methane–hydrogen–steam–air mixtures in wide ranges of initial temperature (up to 800 K), pressure (up to 40 atm), fuel-air ratios (from 0.7 to 1.5), initial steam content (up to 0.2), and hydrogen content in the fuel (up to 0.2). Fragments of data-base tables for the laminar flame velocity, as well as for prompt NO concentration and for the maximum concentration of CO in the reaction zone are presented.

COMPARISON OF KINETIC CALCULATIONS USING GRI AND KONNOV'S MECHANISMS FOR METHANE–AIR MIXTURES WITH EXPERIMENTAL DATA OBTAINED IN SHOCK TUBES AND RAPID COMPRESSION MACHINES

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The experimentally measured ignition delay times of methane–air mixtures have been compared with the values calculated using detailed GRI-Mech and Konnov's Chemkin mechanisms for the temperature range 900–1740 K. The experimental data used for this comparison were obtained in shock tubes and rapid compression machines. Calculations were performed for ideal conditions without regard for heat loss and fluid dynamic effects. The GRI-Mech mechanism was shown to provide more accurate predictions for high temperatures (1400–1740 K), whereas at lower temperatures (900–1300 K), the Konnov's mechanism shows better performance.

MEASUREMENTS OF IGNITION DELAYS IN METHANE–AIR AND HYDROGEN–AIR MIXTURES AT INTERMEDIATE TEMPERATURES

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Presented are the results of ignition delay measurements in undiluted methane–air and hydrogen–air mixtures in a rapid compression machine at temperatures 900–1200 K. The measurements revealed a large scatter in experimental data caused by authors' opinion by fluid dynamic and other phenomena.

THE EFFECT OF HYDROGEN ADDITIVES ON SELF-IGNITION OF HYDROCARBON FUEL–AIR MIXTURES

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For the first time, the numerical simulation of self-ignition and combustion of homogeneous and heterogeneous (drop suspensions) mixtures of heavy (n-heptane and n-decane) hydrocarbon fuels with air without and with hydrogen addition was performed using a detailed reaction mechanism of fuel oxidation. It has been shown that the reactivity of the composite hydrogen-containing fuels in air is not always higher than that of the pure hydrocarbon fuel. This fact has to be taken into account when considering practical applications of hydrocarbon–hydrogen fuel blends.

THE EFFECT OF HYDROGEN ADDITIVES ON THE LEAN FLAMMABILITY LIMIT OF METHANE

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The effect of hydrogen additives on combustion of methane–air mixtures has been studied experimentally. Mixtures with equivalence ratios ranging from 0.43 to 1 and with hydrogen additives to methane in amounts

of 10 and 20 %(vol.) were tested at initial pressures of 1, 5, and 10 atm and initial temperatures ranging from 20 to 300 °C. Hydrogen additives were shown to intensify combustion of mixtures with equivalence ratio (ER) exceeding 0.5 and inhibit it at ER = 0.43.

SELF-IGNITION OF MODEL MIXTURES OF ASSOCIATED PETROLEUM GAS WITH HYDROGEN ADDITIVES

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The effect of hydrogen additives on low-temperature autoignition of model mixtures of associated petroleum gas with oxygen has been studied in a static apparatus with rapid mixture injection. Experiments demonstrated that hydrogen additives increase the self-ignition temperature threshold by about 140 K, that is, they inhibit hydrocarbon ignition. A plausible kinetic mechanism has been suggested that accounts for the observed effect. The essence of the mechanism reduces to the fact that hydrogen additives introduce a chain terminating step $H_2 + R = RH + H$ followed by a fast H conversion into HO_2 (which is inactive at low temperature) in the branched hydrocarbon oxidation via its hydroperoxide.

MODELING OF BENZENE OXIDATION IN AIR BASED ON A DETAILED REACTION MECHANISM

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The detailed kinetic mechanism of benzene oxidation has been developed. The results of calculations with this mechanism have been compared with available experimental data on ignition delays behind reflected shock waves and laminar flame velocity, as well as on variation of species concentrations in flow reactors and in the flame of stabilized plane burners. The results of numerical simulations on the formation of polyaromatic hydrocarbons in fuel-rich benzene–oxygen mixtures have been also provided.

OXIDATION AND COMBUSTION MECHANISMS OF NORMAL PARAFFIN HYDROCARBONS $C_{11}H_{24}$–$C_{16}H_{34}$

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New nonempirical detailed reaction mechanisms of oxidation and combustion of alkane hydrocarbons — from $C_{11}H_{24}$ to $C_{16}H_{34}$ have been developed. The salient feature of the mechanisms is their capability of predicting a multistage low-temperature self-ignition with cool and blue flames and hot explosion. Satisfactory agreement between predicted and measured data on ignition delays and flame propagation velocities was obtained.

SIGNIFICANCE OF CHAIN REACTIONS FOR CRITICAL CONDITIONS OF FLAME PROPAGATION IN GASES

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A set of experimental data demonstrating the dominant role of chain branching and termination processes in the establishment of critical conditions of flame propagation in gaseous reactive systems at both low and elevated initial temperatures have been analyzed.

STUDIES OF BIOFUEL COMBUSTION CHEMISTRY, EFFECTS OF FLAME RETARDANTS, AND FORMATION OF NANOPARTICLES IN FLAMES BY MOLECULAR BEAM MASS SPECTROMETRY

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Presented are the recent developments in application of molecular beam mass spectrometry to studies of biofuel combustion chemistry, effects

of retardants on flame propagation, and formation of nanoparticles in flames. The data obtained are valuable for elaborating new technologies in power engineering and material science.

TOWARDS COMPRESSION-INDUCED IGNITION OF BIOGAS–AIR MIXTURES

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The possibility of compression-induced ignition of biogas–air mixtures with different CO_2/CH_4 ratios in the free-piston ballistic machine with two-stage compression has been demonstrated experimentally. The maximum compression pressure required for ignition was 20 atm.

DIAGNOSTICS OF AVERAGE PARAMETERS IN REACTING AND NONREACTING TURBULENT METHANE JETS BY THE METHOD BASED ON TALBOT EFFECT

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High-resolution spatial distributions of average admixture concentrations in turbulent reacting and nonreacting methane jets have been obtained experimentally by measuring the local light refraction index of long-exposed Talbot images of the jets.

EFFECT OF IRON PENTACARBONYL ADDITIVES ON SOOT FORMATION IN SHOCK WAVES

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A strong effect of iron pentacarbonyl additives on soot formation during the pyrolysis of C_3H_8/Ar mixtures behind shock waves was revealed. A novel kinetic mechanism of the thermal decomposition of $Fe(CO)_5$ and the formation of free iron atoms and iron nanoparticles was tested. This mechanism correctly describes the available experimental data. A qualitative explanation of the experimentally observed

effects of $Fe(CO)_5$ additives on soot formation was proposed. In authors' opinion, the nascent iron nanoparticles serve as soot precursors for further surface growth with the formation of soot particles. The influence of small $Fe_n(CO)_m$ fragments and small Fe_n clusters on soot formation process is less probable because of a rather short life time of these species.

DATA BASE FOR CALCULATING SOOT PARTICLE SIZE DISTRIBUTIONS IN INTERNAL COMBUSTION ENGINES

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A unique data base for calculating soot particle size distribution functions in the course of soot formation in internal combustion engines (ICE) has been developed and tested. The data base was arranged in the form of lookup tables and can be used in multidimensional computer simulations of the ICE operation process. The paper provides a brief description of the data base and a three-dimensional (3D) test case of its implementation for the diesel engine.

COAGULATION OF SMOKE PARTICLES IN THE EXHAUST SYSTEM OF PISTON ENGINE

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The model of coagulation of smoke particles in the exhaust system of piston engine has been suggested and implemented into a 3D gasdynamic code. The model includes Brownian, turbulent-diffusion, and turbulent-kinetic coagulation mechanisms. Calculations revealed that the coagulation process exerts a strong effect on the ensemble-mean size of smoke particles at the exit of the exhaust pipe (the mean particle diameter can increase by nearly an order of magnitude), and the Brownian mechanism plays a dominant role in the coagulation process.

MULTIDIMENSIONAL CALCULATION OF THE OPERATION PROCESS IN A SPARK-IGNITION PISTON ENGINE

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The new model of turbulent combustion recently developed in Semenov Institute of Chemical Physics has been applied to massively parallel calculations of the operation process in a spark-ignition piston engine. Contrary to other available models of turbulent combustion, the new model accounts for the most important features of chemical transformations in flame and preflame zones: the reactions in flame proceed with the strong effect of heat and diffusion fluxes whereas the preflame volumetric reactions are governed by chain origination processes.

FLAMMABILITY LIMIT FOR A FUEL-RICH GAS MIXTURE IN A PERMEABLE MATRIX BURNER

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The flammability limit of fuel-rich methane–air mixtures on flat and volumetric permeable surfaces has been determined theoretically and experimentally. Considerable expansion of the lower flammability limit (in terms of the air-to-fuel ratio) was demonstrated due to transition from flat to volumetric permeable surface. Heat recirculation in the volumetric permeable matrix burner was shown to provide steady surface burning of natural gas – air mixtures at the air-to-fuel ratio as low as 0.35.

CONVERSION OF BIOGAS INTO SYNGAS IN VOLUMETRIC PERMEABLE-MATRIX BURNERS

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Experimental study of biogas oxidative conversion under conditions of cavity-captured infrared radiation due to combustion in a 3D

permeable-matrix burner is reported. The possibility of biogas to syngas conversion in a wide range of biogas composition (from 5% to 50% CO_2 in the mixture with CH_4) has been successfully demonstrated.

SELECTIVE OXYCRACKING OF HEAVY INGREDIENTS OF ASSOCIATED PETROLEUM GAS

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The novel technology of oxidative cracking of heavy ingredients of associated petroleum gas into lighter compounds with higher Octane number rating has been developed. The technology does not require the use of catalysts, absorbers, or other consumable materials, and does not require auxiliary energy for gas compression or cooling.

THERMAL EQUATION OF STATE FOR AMMONIA

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The new thermal equation of state for ammonia — one of the most important products of chemical industry widely used for production of explosives, rocket fuels, etc., as well as for the catalytic conversion of nitrogen oxides — has been developed. The equation of state provides good accuracy of p–V–T data (better than 1.5%) at pressures up to 500 atm and temperatures from 500 to 750 K.

INITIATION OF HYDROGEN–AIR DETONATION AT THE SEMISPHERICAL SHOCK WAVES COLLISIONS

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Numerical simulation of detonation initiation due to collisions of semispherical shock waves was performed using a commercial 3D code for a model gas with thermochemical parameters corresponding to the stoichiometric hydrogen–air mixture at normal conditions. The multiple semispherical shock waves were generated by planar shock reflection from a perforated plate. The critical conditions of detonation initiation

downstream from the perforated plate were shown to be defined by the incident shock intensity and plate permeability. The analysis of computational results demonstrated that detonation occurred via localized self-ignition due to collisions of multiple shock waves.

ANALYSIS OF BURNING AND DETONATION MODES OF GASEOUS MIXTURES INSIDE POROUS BEDS

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Numerical modeling of fast modes of burning and detonation of hydrogen–air mixtures with 35% and 15% H_2 inside the porous inert media has been conducted using a one-dimensional version of EFAE computer code developed earlier in the frame of mechanics of two-phase reactive media. The results of calculations were compared to available experimental data with varying the initial pressure and grain size of porous beds. Besides, the steady solution has been analyzed to better understand the structure of the reaction zone and the rule to select the supersonic burning mode and velocity.

THRUST PERFORMANCE OF AIR-BREATHING PULSED DETONATION ENGINE IN SUPERSONIC FLIGHT AT DIFFERENT ALTITUDES

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Multidimensional numerical simulations of transient gasdynamic flow inside and outside the duct of pulsed detonation engine (PDE) operating on gaseous propane at supersonic flight with the Mach number of 3.0 at altitudes 8, 9.3, 12, 16, and 20 km have been performed and analyzed. The possibility of high-frequency (50 Hz) cyclic operation process with mixture ignition by a weak energy source (0.1 J) and deflagration-to-detonation transition (DDT) has been demonstrated computationally. The fuel-based specific impulse was shown to attain 1600–1800 s and to monotonously decrease with the flight altitude.

SEARCHING THE WAY TO IMPROVE CHARACTERISTICS OF WORKING PROCESS IN MODEL VALVELESS-SCHEME PULSED DETONATION ENGINE WITH TAKING INTO ACCOUNT VISCOSITY

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The influence of gas viscosity on thrust performances of a model valveless PDE operating on hydrogen–air mixture has been studied numerically. Viscous effects were shown to be capable of deteriorating the PDE performance essentially. Physical reasons of this deterioration were analyzed and various ways to improve the performance were considered.

THREE-DIMENSIONAL NUMERICAL SIMULATION OF CONTINUOUS DETONATION OF HYDROGEN–AIR MIXTURE IN AN ANNULAR COMBUSTOR

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The results of 3D numerical simulation of continuous detonation of hydrogen–air mixture in the annular flow-through combustor with external diameter of 306 mm, length of 665 mm, and width of 23 mm are reported. The mixture was fed to the combustor through the annular gap and through multiple radial nozzles in the external lateral wall. Calculations allowed the detonation existence domain to be identified which appeared to be close to available experimental findings.

APPLICATION OF X-RAY VISUALIZATION FOR MEASURING VELOCITY AND PHASE COMPOSITION OF MULTIPHASE FLOW

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The X-ray visualization technique for simultaneous online measuring of multiphase flow velocity and composition has been developed and tested for two- and three-phase compositions containing water, Diesel oil, and

air. The test experiments indicated that the novel measurement technique is capable of providing reliable and accurate online information on multiphase flow structure, velocity, and phase composition.

DISTRIBUTED PARCEL MODEL FOR SIMULATING TWO-PHASE SPRAY FLOWS IN INTERNAL COMBUSTION ENGINES

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The standard Parcel model widely used for multidimensional simulation of two-phase sprays was modified to reduce the grid dependence of computational results on mixture formation in internal combustion engines with direct fuel injection and diesel engines. A novel Distributed Parcel model providing considerably lower grid dependence of various spray characteristics (penetration, vaporization, etc.) has been developed and validated.

COMPUTATIONAL CODE FOR SIMULATING THE OPERATION PROCESS IN COMPRESSION IGNITION ENGINES

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A new computational code allowing simulation of the operation process in internal combustion engines with Diesel cycle as well as with the Gas Diesel and Homogeneous Charge Compression Ignition cycles has been developed and tested. The most important specific features of the code are (*i*) the possibility of applying both overall and detailed reaction mechanisms for modeling fuel oxidation and pollutant formation (NO, CO, soot, etc.) and (*ii*) the account for spray effects (screening effects of neighboring drops) on autoignition and combustion of dense drop suspensions under conditions of variable volume of a combustion chamber. Several test cases demonstrating code capabilities have been considered.

COMBUSTION OF LOOSE LAYERS OF IRON PARTICLES IN OXYGEN

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Presented are the results of experimental investigations on interaction of burning loose layers of iron particles 45 to 250 μm in diameter with stainless steel substrates in oxygen atmosphere at pressures up to 20 bar. The loose layers of different shape (narrow strips, strips on the inclined groove simulating an incline pipeline, and discs) were considered. The results obtained are important for evaluating the risks of explosion phenomena in dusty gas systems.

THE KINETICS OF COMBUSTION OF PREMIXED ALUMINUM IN STEAM

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Premixed combustion of Al vapors in steam with the formation of aerosol particles was studied computationally. Formation of condensed-phase nuclei was modeled in terms of homogeneous nucleation of Al_2O_3 molecules using the classical thermodynamic model. The time histories of various gas species concentrations and concentrations of aerosol particles during combustion were obtained and discussed.

LAWS OF ALUMINUM OXIDATION BY WATER SOLUTIONS FOR AL ACTIVATED BY In–Ga–Sn EUTECTIC

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The rates of oxidation of aluminum polycrystal blocks covered by In–Ga–Sn films in water solutions have been estimated quantitatively. The information obtained can be used for predicting the rates of hydrogen generation using aluminum blocks of various crystal structure.

IGNITION OF WEDGE-SHAPED BODIES AT CONSTANT SURFACE TEMPERATURE

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A problem of ignition of a wedge-shaped body with an arbitrary apex angle at constant surface temperature has been solved numerically within two-dimensional approximation. The conditions of ignition spot formation in a body of such geometry were shown to differ considerably from those obtained from one-dimensional considerations: the ignition spot was formed in the depth of the body and the ignition time was essentially shorter.

APPLICATION OF HETEROGENEOUS PHOTOSENSITIZERS BASED ON METAL OXIDES AND ORGANIC DYES FOR PHOTODYNAMIC EFFECT

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The method of photosensitization of compounds comprising highly dispersed ceramic materials and organic dyes has been optimized for obtaining the photodynamic effect. The heterogeneous photosensitizer produced by the authors (based on titanium dioxide and metal-free phthalocyans) allows efficient purification of water from organic contaminations at daylight conditions.

FIRE-PROTECTION SWELLING COVERS: THE MECHANISM OF THERMAL PROTECTION

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The functions of main ingredients of swelling fire-protection covers, the mechanisms of their interaction at fire-induced high-temperature pyrolysis, and the formation mechanism of a foamed on-surface layer required for reliable thermal protection have been identified and discussed.

DEFLAGRATION-TO-DETONATION TRANSITION IN HEPTANE–OXYGEN MIXTURES

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For the development of a liquid-fueled PDE, the detonation run-up distance and time in n-heptane–oxygen mixtures have been measured experimentally in a 22-millimeter diameter tube. The detonation run-up distance and time were shown to be 25–150 cm and 1–6 ms, respectively.

STEADY-STATE OPERATION MODES OF THE COUNTERFLOW DISPLACEMENT REACTOR: GAS–LIQUID SYSTEM

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Specific features of steady-state operation modes of the counterflow displacement reactor with two-phase gas–liquid reactants have been studied theoretically using one- and two-temperature models. The effect of phase velocities and interphase heat transfer on the steady-state operation modes with simple exothermic reaction in the continuous phase (liquid) was considered.

EFFECT OF AMMONIUM NITRATE ON BURNING OF HOMOGENEOUS PROPELLANTS

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The effect of ammonium nitrate on the burning rate of homogeneous propellants of different composition has been studied experimentally. The propellant compositions differed in terms of the reaction heat (by a factor of 2.7) and burning rate (by a factor of 4.3). Based on the results obtained, the heat balance in the condensed phase has been evaluated. The analysis shows that the major part of reaction heat required for propellant burning is released in the condensed phase.

BURNING WAVE PARAMETERS FOR PROPELLANTS BASED ON PLASTICIZERS WITH DIFFERENT BOILING TEMPERATURE

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The interrelation between the solid propellant surface temperature and the plasticizer boiling temperature has been studied experimentally. For this purpose, the samples of homogeneous propellants based on nitroglycerine, on the one hand, and nitroglycol, on the other hand, possessing similar energy potentials but different volatility have been tested.

DESIGN OF COMPOSITE PROPELLANT WITH STRONG PRESSURE DEPENDENCE OF THE BURNING RATE

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Discussed are possible approaches to control the burning rate of composite solid propellants by varying the oxidizer particle size distribution and binder properties and by using different substitutes of ammonium perchlorate.

THE BURNING MODEL OF DOUBLE-BASE PROPELLANT PARTICLE WITH THE OVERALL REACTION CHEMISTRY FOR THE ANALYSIS OF TRANSIENT BURNING PHENOMENA

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Discussed are the problems of modeling transient phenomena accompanying burning of a double-base solid propellant particle at constant and variable pressure conditions, using the overall reaction chemistry in both condensed and gas phase.

PROPELLANT GRAIN EXTINCTION IN A TRANSITION MODE OF MODEL ROCKET ENGINE OPERATION: PART II

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Experimental data for transition modes of model rocket engine operation due to fast variation of nozzle throat have been analyzed. The conditions of propellant extinction due to pressure drop in the engine were considered. An extinction criterion based, on the one hand, on the measured pressure history in the engine and, on the other hand, on the estimated relaxation time of the preheated layer in the propellant combustion zone has been suggested.

MODELING OF ANGULAR DISPLACEMENTS OF THE SOLID PROPELLANT GRAIN IN A SOLID ROCKET ENGINE WITH ELASTIC-PLASTIC LINER

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The asymptotic model of angular displacements of a propellant grain in a case-bonded solid rocket engine has been suggested. The influence of temperature distribution on the stress-strain state of the elastic-plastic liner was analyzed.

CRITICAL CONDITIONS FOR COMBUSTION-TO-EXPLOSION TRANSITION OF POWDERED EXPLOSIVES IN A SEMICONFINED VOLUME

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Presented are the results of experiments on combustion-to-explosion transition (CET) in powdered RDX at its ignition in steel tubes open from one end depending on tube dimensions (inner diameter and length), charge density, and particle size. The procedure of quantitative estimation of risks of CET and transition to detonation has been suggested.

THERMAL STABILITY AND MECHANISM OF THERMOLYSIS OF TRINITROPYRAZOLES

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Three new energetic compounds — trinitropyrazoles (TNP) have been synthesized and characterized by thermal analysis. In computer calculations, a comprehensive spectrum of transformations of intermediates on the way to the final products of thermolysis has been obtained. Based on the comparison of activation energies obtained by quantum chemical modeling and simultaneous thermal analysis, it is concluded that the most likely mechanism of TNP thermolysis is the intramolecular regrouping of nitro compound TNP with formation of aci-nitropyrazole with activation energy 112.65 kJ/mol.

SYNTHESIS, PROPERTIES AND BURNING RATES OF ACETATES, NITRATES, AND CHLORIDES OF METHYLOLNITRAMINES

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Presented is the overview of authors' works on synthesis, properties, and burning rates of acetates, nitrates, and chlorides of methylolnitramines.

DECOMPOSITION AND COMBUSTION OF POLYNITRIC ENERGETIC MATERIALS BASED ON NITROGUANYLTETRAZINE

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Thermal decomposition and combustion performance of nitroguanyl-1,2,4,5-tetrazine and its triaminguanidine salt have been investigated experimentally to reveal the mechanism of their combustion. The combustion mechanism was shown to be governed by condensed-phase reactions whereas the burning rate to be determined by decomposition reactions at burning surface temperature. Low oxygen content in polynitric

energetic materials based on nitroguanyltetrazine results in the formation of high-enthalpy compounds in combustion products and, thus, in incomplete energy release.

KINETICS OF POLYMORPHOUS TRANSFORMATIONS IN HMX AT MECHANICAL ACTIVATION

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The kinetics of polymorphous transformations in HMX samples of different modifications preliminary subjected to mechanical activation has been studied experimentally by the method of infrared spectroscopy. The kinetic modeling of polymorphous transformations using the scheme of successive reactions has been fulfilled and the kinetic parameters of the process have been determined.

STUDIES OF POLYMORPHISM IN SOLID ENERGETIC MATERIALS BY CRYSTAL STRUCTURE PREDICTION METHODS

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The polymorphism phenomena play essential role in the performance and behavior of energetic materials. Thus, pressure-induced transition into a higher-density polymorph is believed to take place in an energetic solid when its molecule starts decomposing in the tight crystal environment, for this is an obvious mechanism to explain the release of an extra space for the arrangement of product particles. While many actual polymorphic phases and their transitions are frequently hidden from direct observation by regular experimental techniques, the computational crystal structure prediction methods provide a powerful instrument capable of extending greatly our insight into the nature of solid state processes. The availability of experimental crystal structures allows further extending the scope of structure prediction methods towards new chemical classes of energetic compounds, in particular, the class of aromatic polynitrous heterocyclic compounds studied in this work.

THERMOCHEMISTRY OF ISOMERS PYRIDILAZOFURAZAN

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The combustion enthalpies in standard conditions of isomer pyridilazofurazans have been measured. The formation enthalpies of isomer pyridilazofurazans have been calculated and analyzed. The noticeable influence of donor–acceptor effects on energetic characteristics of isomers was revealed.

THERMOCHEMICAL PROPERTIES OF HETEROAZOLES

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The enthalpies of formation in standard conditions of some mononitroderivatives of heterocyclic compounds have been determined experimentally. The cleanness of the compounds was measured by the method of melting curve. To prevent explosions, the substances were burned in dimethylphthalate solutions. Also measured were the thermal effects of dissolution reactions of the tested substances in dimethylphthalate. The effect of nitrogroup introduction in the heterocycles was estimated. The variation of the formation enthalpy due to introduction of electronegative fragments to carbon and nitrogen atoms were analyzed.

THERMOPHYSICAL AND MECHANICAL PROPERTIES OF THE AL–AL_2O_3 COMPOSITE BASED ON THE MODEL OF ADDITIVE MIXING

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Based on the model of additive mixing, the equations of state (EOS) have been derived for a composite consisting of Al and Al_2O_3 as well as for the individual components of the composite. The EOS predicts

thermophysical, thermodynamic, and mechanical properties of the composite in a wide range of pressure and temperature. Also, the EOS predicts thermophysical and mechanical properties of the composite with nanocrystalline aluminum additive.

MECHANOCHEMICAL ACTIVATION OF Si-BASED ENERGETIC MATERIALS: THE INFLUENCE OF NANOSIZE Si DEFECT STRUCTURE

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Two mechanochemical methods of preparation of Si nanosize particles (nSi) have been developed. The methods are based on the combination of activation of Si or Si/BN in high energy intensity mechanochemical devices followed by chemical etching in different acids. nSi with specific surface area of about 80 m^2/g and particle size of about 30 nm were prepared by these methods. The defect structure and reactivity under high-temperature oxidation were compared for 5 types of nSi prepared by different variants of mechanochemical methods and other methods. The presence of large concentration of "volume" defectiveness is one of the main advantages of the mechanochemical approach to prepare nanoparticles.

MECHANOACTIVATED COMPOSITES ON THE BASE OF MIXTURES OF SILICON AND ALUMINUM WITH PERCHLORATES

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The production technique of mechanoactivated energetic compositions (MAECs) based on ammonium and potassium perchlorates and solid fuels (Si and Al) has been developed. Both regimes, high-speed burning and detonation, were observed for the produced composites. The com-

posites were found to be highly sensitive to thermal stimuli and capable of exhibiting fast DDT. The results obtained allow considering these MAECs as promising components of new explosive compositions.

HEAT EVOLUTION IN DETONATION OF MECHANOACTIVATED NANOSILICON–AMMONIUM PERCHLORATE COMPOSITE

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The procedures for measuring heat release in the course of DDT in solid explosive compositions have been developed. The heat effect of detonation was studied for the mechanoactivated energetic nanosilicon/ammonium perchlorate (29/71) composite. This material was shown to possess a high heat effect of detonation. However, the measured heat release was only 83% of the stored energy. The degree of silicon oxidation appeared to be 67%–70%.

HEAT OF EXPLOSION OF MIXTURES OF HMX AND NANOSILICON

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Addition of aluminum to high explosives is known to result in the increase of the total work of explosion. Silicon can be considered as an energetic additive competitive to aluminum. With the aim of analyzing the influence of nanosilicon on the energy content of high explosives, the study of the heat of explosion was performed for the HMX-based compositions. Addition of nanosilicon, aluminum, and boron to HMX was shown to lead to an increase in the heat of explosion. However, nanosilicon-containing mixtures were shown to be inferior to the aluminum- and boron-containing compositions in terms of the heat of explosion.

DETONATION FRONT PARAMETERS IN DENSE CHARGES OF BENZOTRIFUROXAN

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Detonation front parameters for BTF (benzotrifuroxan) have been measured experimentally using the pyrometric method. At the charge density of 1.82 and 1.84 g/cc, the measured detonation pressures were 33.8 ± 1.0 and 34.5 ± 1.0 GPa, whereas the temperatures of detonation products were 3920 ± 150 and 4100 ± 150 K, respectively. The measured temperatures were found to be essentially lower than the temperatures predicted using various models.

NUMERICAL MODEL FOR ENGINEERING CALCULATIONS OF ALUMINIZED HIGH EXPLOSIVES

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The numerical model for aluminized explosives has been developed. The model consists of two main equations: the kinetic equation for aluminum burn process and the semiempirical JWS (Jones–Wilkins–Lee) equation of state for explosion products. The main features of the model are high accuracy and simplicity of the procedure for determining model parameters. The cylinder test experiment was used for model calibration. The model is rather simple and can be readily implemented into hydrocodes.

EXPRESS-METHOD FOR REVEALING STRONG SENSITIZATION

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To study sensitization effects of high explosives, the method of depositing additive spots (by means of powder deposition) on the surface of friction has been developed. If the sensitization effect appears more appreciable than the reduction of strength of the basic charge, the sensitization is considered strong. The results of about 40 tests were analyzed.

The preference was given to regular propellant components. The kinds of chemical interaction between the components are discussed.

THE EFFECT OF IMPACT VELOCITY ON THE PARAMETERS OF MECHANICAL INITIATION OF LAYERED TEFLON–ALUMINUM COMPOSITIONS

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Presented are the experimental results on the initiation of samples composed of alternating layers of thin Teflon films and aluminum foil by drop-hammer impact loading. The effect of the impact velocity on parameters of the initiation of the multilayer samples was studied. The results obtained are indicative of the mechanochemical nature of the interaction between aluminum and Teflon layers under impact loading conditions.

THE SENSITIVITY TO IMPACT OF MIXES OF AMMONIUM PERCHLORATE WITH TEFLON

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The sensitivity of ammonium perchlorate – Teflon compositions to impact at various proportions between the components was determined by the method of critical energies. By extrapolating the obtained dependencies to a limit of pure Teflon, the maximum safe level of force action for Teflon in the course of mechanical handling has been evaluated.

BLAST WAVES GENERATED IN CYLINDRICAL DUCT BY NONIDEAL DETONATION OF HIGH-DENSITY ALUMINUM–TEFLON–RDX COMPOSITIONS

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The front overpressure and the pressure impulse of blast waves generated in a cylindrical duct in the course of expansion of nonideal detonation products of low-porosity charges prepared by pressing fine grained

aluminum–Teflon–RDX compositions have been measured experimentally. The recorded variables were related to the corresponding variables of blast waves produced by detonation of a TNT charge of the same mass (100 g). The relative variables were used to evaluate the TNT equivalency of the blast waves of tested compositions. The tested compositions differed in terms of particle shape (trade mark) of aluminum powder and Teflon/aluminum ratio with RDX content of 30%. The front overpressure was shown to exceed the value relevant to the TNT charge by 10%–30% in average almost regardless the distance travelled by the wave in the range from 0.8 to 3.8 m. The particle shape and content of aluminum in the mixture affected the front overpressure only slightly. In the same range of distances, the relative pressure impulse exhibited a strong increase from 0.5 to 2.1 and even more, mainly, due to increasing the wave compression phase duration.

PARAMETERS OF TNT EXPLOSIVE CHARGE CONTAINING BLOCKS OF HIGH-DENSITY METAL–PTFE COMPOSITES

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Promising areas of fundamental and applied research aimed at enhancing the damaging effect of ammunition by including various reactive materials in their composition have been analyzed. The main attention was paid to metal–PTFE composites (MFC). The specific and volumetric energy content of such systems has been estimated. To assess the potential contribution of MFC to explosions of charges in air and their impact on the near-field blast effect, comparative experiments with net TNT and composite charges were carried out. Two types of composite charges composed of a TNT block and high-density MFC were used, namely: MFC-1 (with W/Al/PTFE = 87.5/2.5/10.0 with a density of 8.04 g/cc) and MFC-2 (with W/Al/PTFE = 36/14.5/49.5 with a density of 2.81 g/cc). The replacement of TNT with the same amount (10%) of MFC-1 did not virtually change the parameters of TNT explosion in radial direction. The replacement of TNT with MFC-2 was found to increase the air blast wave parameters.

FRAGMENTATION SPECTRA OF STANDARD CYLINDERS FILLED WITH NEW ALUMINIZED EXPLOSIVES

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Presented are the results of experimental studies of brisant properties of novel aluminized explosive formulations (EF) developed in "Crystal" R&D Institute and designed for loading high-explosive ammunition. The new EF were evaluated using standard fragmentation cylinders (Russian Standard Fragmenting Cylinder — RSFS) of closed-end type No. 12 made of steel C-60 by the method of turning as well as by the method of stamping. Analysis of the fragmentation efficiency of new cold-pressed and injection-molded EF in comparison with data for standard explosives (TNT, A-IX-2, and Okfol-3,5) showed that new explosives based on RDX (HMX) containing 8%, 12%, and 15% aluminum provide an acceptable level of fragmentation of RSFS in terms of the basic fragmentation characteristics exceeding the level of A-IX-2.

PRESENTATION OF FRAGMENTATION SPECTRA OF STANDARD CYLINDERS FILLED WITH NOVEL ALUMINIZED EXPLOSIVES BASED ON STATISTICAL HYPEREXPONENTIAL MODEL

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The results of statistical analysis of fragment spectra of standard fragmentation cylinders have been reviewed. The possibility of representing the fragment spectra with the hyperexponential Odintsov–Grady distribution model is discussed. The adequacy of representing the fragmentation spectra by the Weibull model and the new hyperexponential statistical model has been assessed comparatively.