Abstracts

EFFECT OF VARIOUS FACTORS ON THE LAMINAR BURNING VELOCITY OF METHANE–HYDROGEN–AIR MIXTURES

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The effect of initial temperature, pressure, and hydrogen concentration in methane on the laminar burning velocity of fuel–air mixtures is studied experimentally. Appreciable improvement of burning characteristics of methane–air mixtures can be achieved when no less than 20 %(vol.) of hydrogen is added to methane. Some limitations imposed on the range of measured laminar burning velocities are ascertained.

LOW-TEMPERATURE SELF IGNITION OF H_2–CO–CO_2–AIR MIXTURE IN A SHOCK TUBE UNDER MULTISTAGE COMPRESSION

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The measurements of self-ignition delay time of 7% H_2–10% CO–2% CO_2 + 81% air mixture were performed in a shock tube with the total length of 6.6 m equipped by the pressure transducers and a photodiode. The overtailored operation mode was used for the extension of observation time behind reflected shock waves. The temperature dependence on time was calculated according to adiabatic isentropic compression model on the base of the recorded pressure history. Experimental data were compared with the results of calculations by Konnov detailed kinetic mechanism. At temperatures 700–750 K and pressures 1–2.5 MPa, the measured delay times were about 2 to 3 orders of magnitude shorter than the calculated values.

IGNITION OF METHANE–AIR MIXTURES BY COMPRESSION UNDER THERMAL ACTIVATION

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Ignition of fuel ultralean and fuel-rich methane–air mixtures in conditions of free-piston compression with heat recirculation (thermal activation) has been studied

computationally. The use of thermal activation was shown to significantly extend the limits of self-ignition of such mixtures. The ignition limits were determined as a function of the thermal-activator temperature and air content.

EQUATIONS OF STATE OF METHANE, OXYGEN, AND THEIR MIXTURES: CALCULATION OF TEMPERATURE AND PRESSURE OF THE MIXTURE IN THE COMBUSTION CHAMBER OF LIQUID-PROPELLANT ROCKET ENGINE BEFORE IGNITION

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The calculation method of thermodynamic parameters of methane–oxygen mixture in the combustion chamber of liquid-propellant rocket engine before ignition has been developed. The method has been applied for calculating the temperature and pressure of the equilibrium state of the fuel-rich and stoichiometric methane–oxygen mixtures near the injector head of the rocket engine, as well as for calculating the density of such mixtures at specified values of the common pressure and individual temperatures of mixture components, and at specified common pressure and equilibrium temperature of the mixture.

THE KINETIC MECHANISM OF CHEMICAL TRANSFORMATIONS IN THE GAS MIXTURES OF ACETYLENE WITH AMMONIA

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The detailed reaction mechanism of ignition and combustion of binary gas mixtures of acetylene and ammonia and their components both in the absence and presence of oxygen has been developed. The mechanism was comprehensively tested against available experimental data on self-ignition, combustion, and thermal decomposition of acetylene, as well as self-ignition and combustion of ammonia mixtures with oxygen. The mechanism was also used for systematic calculations of reactivity of binary gas acetylene–ammonia mixtures of various compositions in a wide range of initial temperatures and pressures. Pure acetylene was shown to be the most reactive compound among all binary acetylene–ammonia mixtures. Therefore, when working with the binary mixtures of acetylene with ammonia, safety precautions established for pure acetylene should be applied.

LOW FLAMMABILITY LIMIT FOR SURFACE COMBUSTION IN A SLOT CAVITY

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The surface combustion limit for lean methane–air mixtures in a slot cavity was determined both theoretically and experimentally. Essential widening of the lower flammability limit of surface combustion was demonstrated at transition from a flat opened permeable matrix to volumetric configuration of two matrices separated by a slot. The pressure rise and heat recuperation was shown to provide the steady-state surface combustion at the air–fuel ratio of up to 2.6.

HOMOGENEOUS PYROLYSIS OF ISOBUTANE UNDER PULSED ADIABATIC COMPRESSION

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Thermal decomposition of isobutane has been studied under pulsed adiabatic compression in a temperature range 830–1010 °C. The main and minor products of the reaction have been identified. It is shown that at low conversions, the isobutane pyrolysis may be described by the transformations: i-$C_4H_{10} \rightarrow H_2 + i$-$C_4H_8$ and i-$C_4H_{10} \rightarrow CH_4 + C_3H_6$. Soot was not found in the products. Both increase in the pyrolysis temperature and decrease in the residence time did not result in the growth of the isobutene formation selectivity.

ON THE ROLE OF BUTANE ISOMERS ADDITIVES IN SINGLE-STAGE CONVERSION OF ASSOCIATED PETROLEUM GAS IN A COMBUSTION REGIME

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Ignition delays of fuel-rich oxygen mixtures of n-butane and isobutane are measured in a static apparatus with rapid mixture injection in the reactor at low temperatures and atmospheric pressure. The negative temperature coefficient regions in mixtures with both butane additives are virtually identical. Soot yields are measured in flame burning regimes of rich methane–oxygen mixtures with n-butane and isobutane mixtures in a closed reactor at an initial pressure of 15 atm. Isobutane is found to increase the soot yield to a lesser extent than does n-butane.

ACCELERATION OF MULTIDIMENSIONAL GASDYNAMIC CALCULATIONS WITH DETAILED REACTION MECHANISMS OF OXIDATION AND COMBUSTION OF MOTOR FUELS

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The efficiency of existing procedures of accelerating detailed kinetic calculations when solving multidimensional gasdynamic problems has been analyzed. Three-dimensional computer simulation of the operation process in an n-heptane-fueled homogeneous-charge compression-ignition engine without and with the combined use of the In-Situ Adaptive Tabulation (ISAT) and Dynamic Adaptive Chemistry (DAC) approaches has been performed. The efficiency of the ISAT-DAC approach was shown to increase with the increase in the volume of the detailed reaction mechanism.

ON THE REACTIVITY OF EXHAUST GASES IN INERNAL COMBUSTION ENGINES

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An overview of the methods of fuel ignition activation in piston engines through recirculation of residual gases in relation to homogeneous-charge compression-ignition engine is presented.

THE EFFECT OF OPERATION PROCESS ARRANGEMENTS IN GAS-TURBINE ENGINES AND POWER PLANTS ON CARBON MONOXIDE FORMATION AT COMBUSTION OF HOMOGENEOUS MIXTURE

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The response of CO emissions to instantaneous changes in the external conditions of methane–air mixture combustion has been studied computationally using the model of staged combustion with a detailed reaction mechanism. It is shown that when the temperature and pressure of the combustion products decrease due to convective cooling of combustion chamber walls in the gas-turbine power plant or due to diluting the mixture with secondary air, the resultant CO concentration varies nonlinearly and can either decrease or increase.

NEW TYPE OF LOW-EMISSION COMBUSTION CHAMBERS FOR GAS TURBINES BASED ON PERMEABLE VOLUMETRIC MATRICES

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A new type of combustion chamber for gas turbine engines and power plants based on permeable volumetric matrices which provides ultralow emissions of ecologically hazardous matter and meet current and future ecological demands has been proposed. This type of combustion chamber was shown to emit less than 3 ppm NOx and less than 40 ppm CO even at high specific thermal loads on the matrix surface of up to 30 W/cm^2. Additional advantage of such combustion chambers is their capability of burning low-quality fuels, e. g., biogas with CO_2 content above 50%.

NUMERICAL STUDY OF NOx FORMATION IN MODEL H_2-FUELED SCRAMJET COMBUSTOR

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The analysis of NOx formation in model H_2-fueled scramjet combustor is carried out on the basis of numerical simulation. The formalism of two-dimesional Reynolds averaged parabolized Navier–Stokes equations for reacting gas is used. Kinetic model includes detailed reaction mechanism of H_2 oxidation in air and all known mechanisms of NO formation. It is shown that the flow regions of intense NO formation correlate with the regions of high temperature exceeding 3000 K. Computations demonstrate that for flight Mach numbers of 8–12, the NO emission index is as large as 28–43 g/(kg H_2) and the main mechanism of NO formation in scramjet combustor is the thermal mechanism.

COMPARISON OF MODEL VALVELESS PULSE DETONATION ENGINE WITH AN EQUIVALENT RAMJET

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It is shown based on numerical simulation (URANS with finite-rate kinetics) that thrust characteristics of the model valveless Pulse Detonation Engine (PDE) with bypass shrouds are worse than those of the equivalent ramjet. There are several reasons: the first is the loss of mass flow-rate of air through the bypass shrouds and the second is the forced termination of fuel injection for about 1/3 of the cycle duration due to the danger of diffusive combustion. Comparison of thermodynamic cycles shows that the thermal efficiency of nonstationary and

highly nonuniform process in the PDE is also worse than that in the ramjet. The conclusion is made that PDE with the chosen operation process may have practical importance only as a way to create an engine without moving parts which would operate in a wide range of Mach numbers, beginning from M = 0.

THRUST PERFORMANCE OF AN AIR-BREATHING PULSE DETONATION ENGINE AT FLIGHT MACH NUMBER OF 0.8 TO 5.0

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It has been shown for the first time that hydrocarbon-fueled PDE with intermittent deflagration-to-detonation transition is a unique type of ramjet propulsion systems which can potentially be used in both subsonic and supersonic aircraft. Specific examples for flight Mach numbers 0.8, 3.0, and 5.0 indicate that such PDE thrust characteristics as specific impulse and specific thrust exceed those of ideal ramjets.

THREE-DIMENSIONAL NUMERICAL SIMULATION OF CONTINUOUSLY ROTATING DETONATION IN THE ANNULAR COMBUSTION CHAMBER WITH A WIDE GAP AND SEPARATE DELIVERY OF FUEL AND OXIDIZER

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The possibility of organizing cyclic operation of the combustion chamber with continuously rotating detonation in a wide annular gap comparable to the blade height of the last stage of the gas-turbine engine (GTE), and with separate delivery of fuel and oxidizer has been demonstrated by means of three-dimensional numerical simulation for the first time. A design of the inlet insulator providing almost complete damping of pressure oscillations downstream from the GTE compressor has been proposed. For the continuous detonation combustor with the inlet insulator, the 15 percent gain in total pressure has been obtained.

OPERATION PROCESS OF THE PULSE DETONATION BURNER

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Cyclic pulse-detonation (PD) operation of the natural-gas-fueled PD-burner prototype has been obtained in conditions of separate delivery of natural gas and air

at a speed of ~ 10 m/s. It is shown that in the PD-burner duct 150 mm in diameter equipped with flame-accelerating obstacles of special shape and placement, one can ensure reliable cyclic deflagration-to-detonation transition at a distance of 3–4 m from the ignition source for the time of about 20 ms. The maximum cycle frequency achieved in the experiments is 2 Hz. The results will be used in the development of industrial PD-burners of new type for rapid heating and fragmentation combining thermal and mechanical (shock-wave) impact on the target objects.

THERMAL TESTING OF PULSE DETONATION BURNER WITHOUT FORCED COOLING

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Steady-state temperatures of structural elements in the Pulse Detonation (PD) burner operating on the mixture of natural gas with air were measured during long-term testing in a PD mode with a frequency of up to 2 Hz without forced cooling. Knowledge of these temperatures is required for developing energy-efficient cooling system for the PD-burner. The experiments have shown that the maximum steady-state temperature (~ 500 °C) is reached after approximately 200-second operation for internal obstacles located in that part of the burner duct which is traversed by the detonation wave. The walls in this part of the burner duct are heated up to ~ 420 °C during the operation time of the order of 1000 s. In the part of the burner duct which is cyclically traversed by the deflagration wave, the duct walls and internal obstacles are heated to a steady-state temperature of no more than ~ 330 °C. The results show that the forced cooling is generally required only for those parts of the burner duct which are traversed by the detonation wave.

EXPERIMENTAL STUDY OF MAGNETOHYDRODYNAMIC EFFECTS OF PULSE HETEROGENEOUS DETONATION

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Magnetohydrodynamic (MHD) effect of pulsed heterogeneous (drop) detonation has been detected experimentally for the first time. In all experiments, stable generation of pulse electromotive force with a frequency settled by the operation of micro-PDE (pulse detonation engine) was observed on the partitioned electrodes of the MHD channel attached to the PDE outlet.

NUMERICAL SIMULATION OF INTERNAL BALLISTICS PROCESSES AND GUN-MUZZLE FLOWS USING MULTIPROCESSOR COMPUTERS

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Multidimensional numerical simulation of the axisymmetric internal ballistic process in the gun channel equipped with a muzzle brake has been performed using a mathematical model of multiphase, multicomponent, two-velocity gas–solid propellant flow, taking into account burning of solid propellant and interphase interactions. Flow patterns of propellant gases in the muzzle brake as well as pressure histories at the gun shutter, temporal evolution of the projectile speed, and the level of pressure at different distances from the muzzle have been presented.

MATHEMATICAL MODELING OF GUN MUZZLE FLASH

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Efficient numerical algorithm based on the method of joint probability density function of velocity and scalars, which allows identification of location and time of gun muzzle flash caused by chemical reactions of gunpowder products (CO and H_2) with the surrounding air, has been developed and demonstrated. Demonstration calculations showed that the gun muzzle flash appears as a series of localized spontaneous ignitions in the hot spots, formed by mixing the powder gases with shock compressed air, as well as by the shock compression of the mixture in the areas of shock collisions.

BIFURCATION OF REFLECTED SHOCK WAVES IN ARGON AND AIR IN THE TUBE WITH DIFFERENT WALL ROUGHNESS

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The development of bifurcation structure behind the reflected shock wave depending on the incident shock wave Mach number and on the distance from the closed end of the shock tube with either smooth or rough walls has been investigated in the shock tube experiments in the air and in argon. The conclusions are drawn that the use of a rough surface stabilizes the flow near the wall and that the bifurcation structure near the flat and cylindrical surfaces is developed by different mechanisms.

EXPANSION OF TECHNOLOGICAL OPPORTUNITIES OF THE EQUIPMENT: THE FORMATION OF NANOCRYSTALLINE COATINGS

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The technology and equipment for deposition of nanocrystalline titanium coatings on the aluminum alloys samples were devepoled. The required gas mixture consumption (propane–oxygen–air) is less than 5 m^3 per 1 kg of powder. The dense layer from lamellas and deformed titanium particles is formed on the sample surface. Lamellas consist of the dislocation-free titanium nanocrystalline grains with the size of 30 nm. A mean of lamellas hardness is two–three times higher than the hardness of the deformed titanium particles. Skratch-test has shown that the coating is plastic and has the high adhesive and cohesive strength. The equipment also allows formation of nanocrystalline coatings on steel surfaces using nickel-based alloy powder.

THE INFLUENCE OF THE PARAMETERS OF A POWER-PLANT CHEMICAL REACTOR ON ITS CONTROLLABILITY

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The problems of operation control of a hybrid aviation power plant equipped with the solid oxide fuel cell (SOFC) battery and syngas generator (reformer) is discussed. The parametric region where SOFC battery operation can be effectively controled is shown to be independent of fuel cell parameters and its properties. The control range of SOFC battery is determined mainly by the reformer operation conditions and the value of heat leakage from the battery.

CORRECTNESS OF MIXED EVOLUTIONARY-BOUNDARY PROBLEM AND ITS DISCRETE ANALOG FOR MULTIPHASE FLOW

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It is shown based on simple examples of two-dimensional and one-dimensional two-phase flows that to ensure the correctness (well-posedness) of the mixed evolutionary and boundary problem and its discrete analog, it is necessary that the system of governing equations includes different pressures of phases and

the numerical solution algorithm provides simultaneous solution of at least two linearized equations of hydrodynamics.

EXPERIMENTAL STUDY OF NONISOTHERMAL EFFECTS IN SOOT FORMATION IN THE PYROLYSIS OF BENZENE AND ACETYLENE BEHIND SHOCK WAVES

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Time profiles of temperature, optical density of condensed phase, and sizes of growing carbon nanoparticles in pyrolysis of benzene and acetylene in initial temperature range of 1600–2500 K and pressure range of 3–8.5 bar were measured experimentally. The considerable temperature drop due to hydrocarbon decomposition at the reaction times of 50–100 μs and the subsequent temperature rise due to carbon condensation in pyrolysis of 1%–2% of benzene in argon were observed. The overall heat balance for the mixtures with 1%–2% benzene in argon was shown to be negative. The measured temperature at pyrolysis of 3 percent mixture of acetylene in argon was equal to the calculated temperature behind a reflected shock wave. The dependences of maximal optical density of condensed phase and final sizes of carbon particles on temperature were obtained.

PROCESSES, MECHANISMS AND KINETIC MODELS OF SOOT PARTICLE FORMATION AT PYROLYSIS AND OXIDATION OF VARIOUS MIXTURES OF ACETYLENE IN SHOCK WAVES

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Experimental and computational studies of soot particles formation in the pyrolysis and oxidation of various mixtures of acetylene and argon behind reflected shock waves as well as the study of the predictive capabilities of the new kinetic scheme of thermal decomposition and oxidation of acetylene with the formation of soot particle nuclei of different types have been conducted.

AEROSOL FORMATION DURING COMBUSTION OF ALUMINUM IN WATER VAPOR AND ITS INFLUENCE ON THE COMBUSTION RATE

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The combustion model for homogeneous gas compositions of Al and H_2O in adiabatic conditions is presented. Previous model of combustion process has been modified by inclusion of equations describing the coagulation process. As

a result of numerical calculations, the time dependence of mixture temperature and various gaseous species concentrations as well as the size distribution of Al_2O_3 aerosol particles have been obtained.

MIXED-MODE COMBUSTION OF ALUMINUM UNDER HYDROGEN GENERATION

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Flaky aluminum was shown to be capable of reacting in a wide pressure range with crystal hydrates containing bounded water. Combustion of samples containing such hydro reacting compositions and mineral oxidizers was observed and the mixed-mode combustion of such compositions was studied experimentally. Specific features of combustion at different values of governing parameters in various gas media were identified.

SPECIFIC FEATURES OF ALUMINUM COMBUSTION IN WATER ENVIRONMENT

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Combustion of flaky aluminum with liquid water was studied experimentally in a wide range of pressure. The effects of pressure, mixture composition, mixture density, sample diameter, and ambient gas medium on combustion characteristics have been studied. The anomalous falling dependence of the burning velocity on pressure in an argon atmosphere was obtained at pressures exceeded 50 atm.

COMPARATIVE FIRE RISK OF MICRO- AND NANO-SIZED AEROSOLS OF ORGANIC SUBSTANCES

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A computerized technique for calculating fire hazards of aerosols of organic materials has been developed. For three investigated substances — rezorcine, hydroquinone, and urotropine — of microsize (the particle size up to 100 μm) and nanosize (up to 100 nm) fractions, the fire hazard characteristics — pressure of combustion products, the maximum growth rate of pressure, flame propagation velocities, and lower flammability limits — were measured. The conclusion is drawn that the reduction of particle size results in increasing fire hazards of aerosols.

ON THE DYNAMICS OF WOOD DUST COMBUSTION IN A VERTICAL CHANNEL

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Combustion of fuel-rich pine-wood dust-air mixtures with dust particle diameter from 50 to 100 μm has been studied experimentally in the upgraded experimental facility ensuring more homogeneous mixture before ignition. The results obtained were shown to be in good agreement with those reported previously. In particular, the same strong dependence of burning rate and pressure rise on the time and position of the combustion front has been detected, thus implying that these dependences are governed by flame propagation rather than by the initial conditions before ignition.

MODELING OF PULSED MODES OF DECOMPOSITION OF ACTIVE FIRE-RETARDANT COATINGS

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Pulsed modes of decomposition were experimentally observed for active fire-retardant intumescent coatings subjected to high temperature. The proposed model describes the pulsed modes of propagation of the decomposition front. It is assumed that these modes occur due to an exothermal stage in the net endothermal reactions of decomposition. Upon reaching a critical surface temperature, a thin reactive layer is rapidly transformed into a char layer 1–2 orders of the magnitude thicker than the original one, and chemical reaction stops. With further heating, the temperature below the char layer reaches again its critical value and the process repeats itself. Equations for the thickness of char layer vs. time and the maximum time given to the fire-retardant coating of a given thickness to protect a coated object from fire are derived using the minimal number of empirical parameters.

A MINIMUM PARTICLES SIZE OF PROPELLANT BURNING CATALYST

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The minimum particle size of solid-propellant catalyst allowing effective increase in its burning rate is evaluated based on theoretical considerations, author's own experiments, and literature data.

EFFECT OF TITANIUM DIOXIDE ON THERMAL DECOMPOSITION OF HMX

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The influence of the specific surface area and the content of TiO_2 on HMX thermolysis has been studied experimentally. To elucidate the mechanism of action of titanium oxide on the HMX thermolysis, HMX thermal decomposition products were studied by mass spectrometry and thermal analysis.

COMBUSTION OF MICRO- AND NANOTHERMITES AT ELEVATED PRESSURE

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Combustion-wave propagation in Mg/Fe_2O_3 thermite compositions inside sealed steel tubes has been investigated experimentally to study the burning rate and combustion temperature at elevated pressure. The hot gas-phase products formed during thermite combustion in confined conditions result in considerable overpressure inside the tube that reverses the gas flow and leads to pressure-driven preheating effect of the burned-gas permeation. Convective origin of this preheating effect is discussed. The pressure–time histories and temperature distributions along the steel tube are obtained experimentally. The measured temperature of the external surface of the sealed tube is used to calculate the combustion temperature inside it to be compared with the adiabatic combustion temperature. Both micro- and nanosized components were used to prepare thermite compositions under study. The significant difference in burning parameters of micron- and nanosized thermites is observed and analyzed.

TRAVELING HIGH-DENSITY CHARGE OF CONVECTIVE BURNING IN THE HYBRID CONFIGURATION: NEW RESULTS

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New experimental data in the 23-millimeter laboratory smooth-bore setup for shots of hybrid configuration with the high-density modified propellant charge used as the traveling charge are considered. Varying properties of the traveling charge, the authors could raise considerably the muzzle velocity increment (in comparing to the shots of classic configuration) for two projectiles of different mass (factor $C_q = 3$ and 10), approaching ~ 340 m/s for the light 35-gram projectile. The muzzle velocity increment is accompanied by transformation of

the pressure profiles in flow behind the projectile. There are plateau or convex portions, and humps observed. Moreover, during some time the pressure at the projectile rare end can even be higher than the breech pressure.

CONVECTIVE BURNING AND TRANSITION TO EXPLOSION IN FINE MIXTURES OF AMMONIUM NITRATE AND ALUMINUM

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The conditions of convective burning and its transition to explosion in powder mixtures of ammonium nitrate and aluminum are studied experimentally. Convective burning of such compositions is shown to occur at relatively low pressures of about 1 MPa. High level of explosion sensitivity of fine mixtures of ammonium nitrate and aluminum has been detected. The critical height of the layer, at which transition to explosion occurs, is about 30 mm. The explosion pressure is on the level of 700 MPa. Of particular danger are the mixtures with submicron aluminum.

STRUCTURE OF COMBUSTION ZONE IN AMMONIUM PERCHLORATE AND ITS MIXTURES

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Temperature distributions in the stationary burning waves propagating in samples of pressed ammonium perchlorate (AP) crystals and solid mixtures, containing AP, were obtained by microthermocouple techniques. The rate parameters of gasification were obtained in terms of activation energy and preexponential factor. It was established that AP decomposition is the limiting factor for the burning rate of the mixtures. The values of heat released in the reaction layer of solid and the values of heat transferred from gas to solid were obtained. Dominant role of the solid heat release for the burning rates of the investigated mixtures was ascertained.

PHYSICS OF COMBUSTION OF AMMONIUM PERCHLORATE AND ITS SOLID MIXTURES

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Heat release rate distributions in burning waves propagating in pressed ammonium perchlorate (AP) samples and solid mixtures, containing AP, were found based on temperature distributions in the waves obtained previously. The temperature and heat release rate distributions are presented graphically. Main spe-

cific features of combustion physics of AP and its mixtures are discussed. Due to specific character of the derived functions, they are referred to as cascade-type functions.

HOT-SPOT COMBUSTION MODEL OF TWO-DIMENSIONAL NANOCOMPOSITES

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A model of combustion of thin metal or organic films coated with a nanoscale layer of oxidant is developed. In the case when the oxidant layer represents a system of discrete particles, the equation for burning rate has been derived and the analytical solutions of this equation were obtained and analyzed. The scale of burning rate for different film materials and different concentrations of oxidant particles on the film surface were calculated and discussed. Analysis of the model allows understanding the mechanism of influence of mechanical activation on the combustion and detonation of powder mixtures. The possibility of experimental verification of this model is discussed.

ENERGETIC PROPERTIES OF COMPONENTS OF LIQUID ROCKET FUELS CONTAINING HYDRIDES OF LIGHT ELEMENTS

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Presented are the results of calculations of fuel specific impulse and density for liquid rocket fuels containing additives of highly energetic components, such as aluminum hydride, aluminum boron hydride, and lithium boron hydride. These fuels are shown to be more efficient than those without additives or with aluminum powder additives, or even acetam, a novel fuel recently suggested for liquid rocket propulsion.

ANALYSIS OF ELECTROCHEMICAL REACTIONS IN SOLID OXIDE FUEL CELLS: A NEW APPROACH

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Discussed in the paper is the calculation of electromotive force (EMF) in a solid oxide fuel cell with due regard for changes in entropy and Gibbs free energy of inert substances as well as reactants and products not participating in electrochemical reactions. These effects are not taken into account in the Nernst equation; therefore, the traditional calculation of EMF based on electrochemical reactions is not strictly correct.

OPTIONS OF CALCULATION OF SOLID PROPELLANT BURNING RATE UNDER PRESSURE DECAY IN THE SOLID ROCKET MOTOR

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In the framework of the inverse problem of internal ballistics, the nonstationary combustion rate at transients in a solid rocket motor caused by opening of an additional nozzle has been calculated in isothermal and adiabatic approximations based on the known pressure–time dependences.

ACCURATE PREDICTION OF ENTHALPIES OF FORMATION FOR HIGH ENERGY MATERIALS

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The *ab initio* Gaussian-4 (G4) composite method was used to calculate the enthalpies of formation of high energy compounds with available experimental data. This method when applied to atomization reaction tends to underestimate the enthalpy of formation values up to 20 kJ/mol, while the isodesmic reactions lead to reasonable results suggesting that this theoretical approach has an accuracy often comparable to the experimental data themselves. This approach is recommended for checking conflicting experimental data and prediction of enthalpies of formation of new high energy compounds.

ANALYSIS OF THE UNCERTAINTIES IN EXPERIMENTAL ENTHALPIES OF FORMATION OF HIGH ENERGY MATERIALS USING QUANTUM CHEMICAL CALCULATIONS

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The *ab initio* Gaussian-4 (G4) composite method coupled with isodesmic reaction approach was used to check the accuracy of experimental enthalpies of formations of nitro compounds, nitramines, azides, and other high energy materials. On the basis of theoretical evidence, the enthalpies of formation of some nitro compounds (trinitromethane, trinitroethane,1,1,1-trinitropropane, hexanitroethane, hexogen, and methyldiniroamine) may not be as accurate as cited experimentally. The accuracy of available data on azides is also discussed. The calculations give strong evidence that experimental enthalpy of formation of crystal 4,4′,6,6′-tetra(azido)azo-1,3,5-triazine may be overestimated by 300–400 kJ/mol.

THERMOCHEMISTRY OF AMMONIUM SALTS OF DINITRODIAZOLES

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The energy of combustion enthalpies of formation and the salt formation energy of ammonium salts of 3,4-dinitropyrazole, 3.5-dinitropyrazole, 2,4-dinitroimidazole(3), and 4,5-dinitroimidazole have been measured and estimated.

IISOMERIZATION ENERGIES OF NITRO METHYL DERIVATIVES OF TETRAZOLE

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The energy of combustion and the enthalpy of formation in the standard state were measured for the derivatives of 1,5 and 2,5 isomers of tetrazole. Based on the literature and available data, the thermochemical analysis of the effect of the chemical nature and place of attachment of functional groups on the isomerization energy of tetrazole isomers has been performed.

ENERGY PROPERTIES OF ALKYL NITRO FURAZANES

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The dissociation energies of the C–NO_2 bond in 3-methyl-4-nitrofurazane and 3-butyl-4-nitrofurazane and enthalpies of formation of the corresponding cyclic radicals have been determined. Also determined are the enthalpies of formation of these compounds in the standard state in the gas phase. The method of calculation of the dissociation energies of the C–NO_2 bond in cyclic compounds has been proposed.

EVALUATION OF THE PROPERTIES OF CERAMICS FROM ALUMINA AND ZIRCONIUM OXIDE BASED ON THE MODEL OF ADDITIVE MIXING

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Equation of state (ES) was derived for alumina–zirconia ceramics (Al_2O_3 and ZrO_2) based on the model of additive mixing and ES for the individual components. A good agreement between the calculated and experimental data has

been obtained. Thermal and thermodynamic properties of solid Al_2O_3 and ZrO_2 were calculated. Thermophysical, thermodynamic, and mechanical properties of the ceramics were predicted in wide ranges of pressure and temperature.

THEORETICAL AND EXPERIMENTAL STUDY OF ELECTROTHERMAL EXPLOSION IN GASLESS SYSTEMS PLACED INTO ELECTROCONDUCTING MEDIUM

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Electro-thermal explosion (ETE) in heterogeneous Ti + C system under quasi-static compression has been studied theoretically and experimentally. The technique for carrying out ETE in heterogeneous systems under quasi-static compression at pressures up to 100 MPa has been developed. The effect of electrical power and compression pressure on ignition temperature and the maximal temperature of sample heating were studied. The mathematical model of electrothermal explosion in cylindrical samples of pressed heterogeneous Ti + C mixture surrounded by a ring layer of the electroconductive medium and placed into a dielectric press-form has been developed. Critical conditions of the electrothermal explosion were determined.

KINETICS AND MECHANISM OF THERMAL DECOMPOSITION OF [1,2,5] OXADIAZOLE [3,4-E] [1,2,3,4] TETRAZINE-4,6-DI-N-OXIDE

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The mechanism of thermal decomposition of furazan-tetrazin-di-oxides has been studied experimentally and its thermal decomposition products have been identified.

NONISOTHERMAL DECOMPOSITION KINETICS OF LIQUID AZIDES

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The goal of this paper is experimental investigation of thermochemical characteristics of high-temperature decomposition of liquid compositions based on organic and inorganic azides. The oversaturated aqueous solutions of sodium

azides and four types of liquid oligoglicidilazides were selected as subjects for such experiments with energetic materials.

THERMAL DECOMPOSITION OF AZO- AND AZOXI-DERIVATIVES OF FURAZANES

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Presented are the experimental data on thermal decomposition of some linear and macrocyclic representatives of azo- and azoxi- derivatives of furazanes.

HEAT OF EXPLOSION OF INSENSITIVE EXPLOSIVES AND THEIR BLENDS WITH POWERFUL EXPLOSIVES

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Heat of explosion of blends of insensitive explosives (IEs) with RDX has been determined experimentally. As a result of the analysis of authors' own experimental results and literature data, the method of calculating the heat of explosion of IEs has been proposed.

ENERGY CONTENT OF CL-20 MIXTURES WITH ALUMINUM

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The heat of explosion of aluminized mixtures of CL-20 explosive has been calculated and measured experimentally and the throwing ability of such compositions is evaluated.

INVESTIGATION OF THE EFFECT OF ALUMINUM AND OXIDIZER CONTENT IN MULTICOMPONENT CASTING SYSTEMS ON THEIR EXPLOSIVE CHARACTERISTICS AND FRAGMENTING ACTION

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Based on experimental studies, the effect of metal fuel (aluminum) and oxidizer (ammonium perchlorate) on explosive characteristics and fragmenting action of multicomponent casting explosives has been evaluated.

DEFLAGRATION-TO-DETONATION TRANSITION AND SENSITIVITY OF MECHANOACTIVATED MIXTURES OF ALUMINUM WITH POTASSIUM PERCHLORATE

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The production technique of mechanoactivated energetic composition (MAEC) based on aluminum and potassium perchlorate (PP) has been developed. The results of studies of explosive properties (deflagration-to-detonation transition (DDT), friction sensitivity) of MAEC are presented. It was shown that the detonation-like process in Al/PP composites is formed faster than in other types of solid oxidizer–fuel mixtures. The data on the influence of mixture ageing and time of mixture activation on sensitivity are obtained. Short DDT lengths and high sensitivity of MAEC makes it possible to consider them as perspective components of new igniting compounds for initiating devices.

THE STUDY OF SENSITIVITY TO SHOCK OF TEFLON–ALUMINUM POWDERS

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Experimental results on the initiation of pressed samples composed of finely dispersed teflon and aluminum powders by drop-hammer impact loading are presented. The light flash signifying the event of initiation and the impact pressure were recorded with a photodiode and a tensiometer, respectively. It was established that under typical condition of initiation of high explosives, the teflon–aluminum composition samples are deformed as brittle materials. At a certain pressure, after the stage of elastic compression, a rapid disintegration (within 30 μs) with the formation of local reaction initiation sites at shear surfaces of individual segments occurs. The results obtained are indicative of the mechanochemical nature of the interaction between teflon and aluminum under impact loading conditions.

THE GENERALIZED DEPENDENCE OF RDX DETONATION VELOCITY ON EXPLOSIVE CHARGE PARAMETERS

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Experimental measurements of a detonation velocity of cylindrical charges with different density of RDX powder were performed. The charge diameter was varied from 10 to 36 mm. Experimental results were analyzed in terms of the dependence of the detonation velocity on density and charge diameter.

THE STUDY OF THE EXPLOSION OF RUSSIAN STANDARD FRAGMENTING CYLINDERS CHARGED WITH OLD-20 AND GLA-15 EXPLOSIVE COMPOSITIONS USING THE METHOD OF PULSED X-RAY PHOTOGRAPHY AND A DEVICE FOR FRAGMENTS TRAPPING

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The paper presents the results of an experimental study of the fragmentation process of the Russian Standard Fragmenting Cylinders No. 12 made of stamped steel C-60. The cylinders were filled with new explosive compositions OLD-20 and GLA-15. Fragmentation of the cylinders was studied using the pulsed X-ray photography and the fragments trapping device.

THE DEPENDENCE OF FRAGMENT SPECTRA OF RUSSIAN STANDARD FRAGMENTING CYLINDERS No. 12 ON EXPLOSIVE COMPOUND CHARACTERISTICS

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The results of statistical analysis of fragmentation spectra of Russian Standard Fragmenting Cylinders No. 12 charged with different high explosives are presented. The possibility of establishing a correlation between the mass and number spectra of the fragments and the properties of high explosives has been explored.