

## *Abstracts*

### **INVESTIGATION OF HYDROGEN–AIR MIXTURE IGNITION IN A HEATED STATIC REACTOR AT ATMOSPHERIC PRESSURE BY HIGH-SPEED COLOR CINEMATOGRAPHY**

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Spatial development of chain ignition of hydrogen–air mixtures in the vicinity of the third ignition limit has been investigated in a heated static reactor with the use of high-speed color cinematography. It was shown that spatial development of ignition is determined by the construction material and state of reactor surface; a primary ignition center always appears at reactor surface. Ignition of hydrogen–air mixtures surrounded by heated surfaces is shown to occur at the chemically active surface and propagate from the ignition center into volume.

### **CHEMICAL CONTROL OF COMBUSTION AND EXPLOSION OF METHANE–AIR MIXTURES**

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Suppression and prevention of combustion and explosion of methane–air mixtures at atmospheric pressure by adding chemical inhibitors has been studied experimentally. To enhance the action of inhibitors, the phenomenon of synergism is used. It is shown that combustion of methane occurs due to chain avalanche. The chain mechanism determines all specific features of methane combustion and explosion including the temperature dependence of the reaction rate.

### **PROMOTION OF HIGH-TEMPERATURE SELF-IGNITION OF HYDROGEN–AIR AND METHANE–AIR MIXTURES BY NORMAL ALKANES**

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The effect of small additives of heavy alkane hydrocarbons on spontaneous ignition and combustion of homogeneous mixtures of hydrogen and methane with air at high temperatures ( $\sim 2000$  K) has been investigated theoretically. Such

additives were shown to reduce the ignition delay due to thermal decomposition of the added hydrocarbon with the formation of atomic hydrogen and other radicals initiating chain reactions.

**INVESTIGATION OF REASONS FOR PREMATURE IGNITION OF GASEOUS MIXTURES AT ADIABATIC HEATING BY HIGH-SPEED PHOTOGRAPHY**

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Presented are the results of experiments on the visualization of self-ignition of stoichiometric methane–air and hydrogen–air mixtures in a rapid compression machine at temperatures of about 1000 K and a pressure of 0.8–1.8 MPa. The presence of particulate matter in the form of microparticles in the test section of the experimental setup was shown to cause premature ignition of gaseous mixtures.

**ON SPECIFIC FEATURES OF PROPANE IGNITION AND COMBUSTION WITH ADDITION OF HYDROGEN**

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Propane is considered as a prospective alternative fuel due to potential low HC and CO emissions compared with heavier hydrocarbon fuels like kerosene. In view of it, there are several issues to clarify. First, how the addition of H<sub>2</sub> to propane–air mixture influences NO<sub>x</sub> and other N-containing species emissions. Second, how it affects the self-ignition of propane at relatively low temperatures ( $T < 1000$  K). The objective of this paper is to analyze the kinetic mechanisms of the ignition of blended fuel comprising propane and hydrogen both at high and low temperatures based on a detailed reaction mechanism of propane oxidation.

**ON IGNITION OF PROPANE–AIR MIXTURE BY COMPRESSION IN PRESENCE OF LOCAL TEMPERATURE NONUNIFORMITY**

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Ignition of propane–air mixtures under compression in the presence of a local temperature nonuniformity in the test section of the experimental setup has been studied experimentally. Temperature inhomogeneities were shown to widen the ignition limits of both fuel-lean and fuel-rich mixtures.

**HOMOGENEOUS PYROLYSIS OF *n*-BUTANE  
UNDER PULSED ADIABATIC COMPRESSION**

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Thermal decomposition of *n*-butane has been studied under pulsed adiabatic compression in a temperature range 700–1250 °C. The major and minor reaction products have been determined. Among them, allene, methylacetylene, vinylacetylene, butyne-1, butyne-2, diacetylene, cyclopentane, cyclopentadiene, isoprene, and some other compounds were identified for the first time. The increase of pyrolysis temperature along with decrease of the residence time was shown to result in the growth of selectivity of ethylene formation and in the decrease of selectivity of methane and propylene formation. Soot was not found in the products.

**DETAILED KINETIC MECHANISM OF MULTISTAGE  
OXIDATION AND COMBUSTION OF ISO-BUTANE**

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A detailed kinetic mechanism of oxidation and combustion of iso-butane has been developed and validated. The mechanism is shown to describe satisfactorily both high-temperature and low-temperature (multistage) spontaneous ignition and laminar flame propagation in mixtures of iso-butane with air of different composition. The mechanism comprises 69 chemical species and 409 reversible reactions.

**NEW TYPE OF LOW-CAPACITY GTL-PROCESSES BASED  
ON DIRECT PARTIAL OXIDATION OF HYDROCARBON  
GASES WITHOUT STAGE OF SYNGAS PRODUCTION**

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Most of modern GTL (gas to liquids) technologies for natural gas processing are based on preliminary production of syngas and are energy consuming and costly. Alternative low-capacity technologies without syngas production using direct conversion of hydrocarbon gases to liquid chemical products can be proposed. Among the most promising technologies is the selective oxidation of heavy components of hydrocarbon gases to C<sub>2</sub>H<sub>4</sub> and CO with their subsequent catalytic homologation.

### **OXIDATIVE CONVERSION OF HYDROCARBON GASES TO SYNGAS IN PERMEABLE VOLUMETRIC MATRICES**

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A new type of syngas reformers based on gas-phase conversion of hydrocarbon gases in permeable volumetric matrices is proposed. Some approaches improving the efficiency of the reformers including insertion of radiation screens, additional heat recuperation, and catalytic activation of matrix surfaces are discussed.

### **THERMODYNAMIC CRITERIA TO SIMPLIFY KINETIC MODELS OF COMPLEX CHEMICAL REACTIONS**

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The thermodynamic criterion for checking the adequacy of gas-phase combustion models has been proposed. The criterion is based on the concept of thermodynamic share of each stage of a complex chemical reaction mechanism.

### **MODELING OF COMBUSTION AND EXPLOSION BY POTENTIAL-FLOW METHOD**

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The potential-flow method is applied to combustion and explosion processes in a closed thermodynamic system. The method allows the dynamics of these processes to be modeled without *a priori* information on the detailed mechanism of chemical transformations.

### **METHODS OF CPU TIME REDUCTION FOR SIMULATION OF COMBUSTION WITH DETAILED REACTION MECHANISMS**

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Algorithms of *in situ* dynamic tabulation (ISAT) and dynamic adaptive chemistry (DAC) have been developed which are capable of significantly reducing the computer time of multidimensional gas dynamic calculations coupled with detailed reaction mechanisms. With ISAT, it was possible to reduce the total time of kinetic calculations by a factor of 12 when solving the problem of the operation process in a HCCI (homogeneous charge compression ignition) engine, whereas with DAC, the total time of kinetic calculations was reduced by a factor

of 20 when solving the problem of chemical transformations in a homogeneous reactor.

**CHAIN-THERMAL EXPLOSION AND ITS INHIBITION**

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Experimental studies of the development of branched-chain reactions in hydrogen–oxygen mixture within the ignition peninsula have been conducted at subatmospheric and atmospheric pressure. Extremely rapid increase in the maximum explosion pressure when moving from the self-ignition boundary of the peninsula has been detected.

**DIFFERENCE IN INHIBITION MECHANISMS OF COMBUSTION AT INITIAL AND DEVELOPED STAGES OF THE PROCESS**

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Minor additives of propane were shown to effectively inhibit detonation of hydrogen–air mixtures at atmospheric pressure. Controlled variation of inhibitor concentration allows deflagration-to-detonation transition to be prevented as well as a self-sustained detonation wave to be suppressed at a predetermined distance from its origin. The presented data indicate that both olefins and saturated hydrocarbons can be used as detonation suppressants.

**ANALYSIS OF FEASIBILITY TO SATISFY ICAO TARGET LEVELS OF NO<sub>x</sub> EMISSION AT ENHANCED PARAMETERS OF TURBOFAN ENGINE CYCLE**

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The factors determining emissions of nitrogen oxides in modern turbojet engines at high compression ratio and temperature at the inlet to the combustor have been analyzed and feasible ways to reduce the emissions have been suggested. The values of NO<sub>x</sub> emission indices at combustion of a model fuel (propane) have been calculated for fuel-lean and stoichiometric mixtures using various techniques. The increase in NO<sub>x</sub> emissions with the compression ratio was found to be governed by kinetics of NO and NO<sub>2</sub> formation.

**MECHANISMS AND KINETIC MODELS OF SOOT  
FORMATION AT PYROLYSIS AND OXIDATION  
OF ACETYLENE AND DIACETYLENE IN SHOCK WAVES**

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Presented are the results of experimental and computational kinetic studies of soot particles formation in the course of pyrolysis and oxidation of various mixtures of acetylene and argon behind reflected shock waves. Predictive capability of the modified kinetic scheme of thermal decomposition and oxidation of acetylene and diacetylene with nucleation of soot particles of different types has been demonstrated.

**ON THE ROLE OF HYDROGEN ADDITIVES IN SOOT  
FORMATION IN OXIDATIVE METHANE CONVERSION**

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Kinetic modeling is used to study the effect of hydrogen additives on formation of acetylene — an important intermediate product of oxidative methane conversion participating in incipience and growth of soot particles. The experimentally found effect of soot formation inhibition by hydrogen additives to rich hydrocarbon–oxygen mixtures is explained by an additional buildup, in the course of explosion development, of active light radicals and atoms that cause fast acetylene depletion and reduce, thereby, soot yield. The calculation results are supported by experimental observations.

**NATURAL-GAS FUELLED PULSE DETONATION BURNER:  
NOISE CHARACTERISTICS**

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Experimental measurements of the noise level in the room and in the vicinity of the vent outlet when firing a pulse-detonation burner (PDB) operating on a mixture of natural gas with air at a frequency of 1 to 4 Hz have been conducted. The maximum intensity of the noise in the room was 150 dB and did not depend on the PDB frequency. At a point in the vicinity of the vent outlet noise intensity

did not exceed 105 dB, which is below the threshold level of industrial noise allowed by existing standards.

**THREE-DIMENSIONAL CALCULATION OF OPERATION  
PROCESS AND THRUST PERFORMANCE  
OF AIR-BREATHING PULSE DETONATION ENGINE  
AT CONDITIONS OF SUPERSONIC FLIGHT**

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Comparative two-dimensional axisymmetric and three-dimensional calculations of thrust performances of a pulse-detonation engine (PDE) at conditions of supersonic Mach 3 flight at an altitude of 16 km have been conducted. The earlier conclusion about the superiority of the PDE over an ideal ramjet engine in terms of specific thrust by 20%–30% has been confirmed.

**EXPERIMENTAL STUDIES OF CONTINUOUS DETONATION  
COMBUSTION OF HYDROGEN IN ANNULAR COMBUSTOR**

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Continuous-detonation annular combustor with the outer diameter of 400 mm and annular gap of 30 mm has been designed, fabricated, and tested, using hydrogen as fuel and air as the oxidant. In the tests, sustainable modes of continuous detonation combustion with one, two, three, and five detonation waves were registered, the detonation velocity and the direction of detonation propagation, the height of the detonation front, and the thrust were measured. The measured specific impulse of hydrogen was on the level of 3200 s.

**PROBLEMS OF STABILIZATION OF HYDROGEN  
DETONATIVE COMBUSTION IN LAVAL NOZZLE**

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Calculations, theoretical and experimental studies of starting conditions of Laval nozzle in a supersonic flow of hydrogen–air mixture aimed at realization of steady-state detonative combustion have been conducted. It is shown that detonation of such a mixture can be stabilized in a Laval nozzle with a central body.

**THREE-DIMENSIONAL NUMERICAL SIMULATION  
OF CONTINUOUSLY ROTATING DETONATION IN ANNULAR  
COMBUSTOR WITH STATIC BLADE RAW**

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Numerical simulations of gas-dynamic and mechanical interaction of the flow in an annular continuous-detonation combustor with a fixed blade raw have been performed. The conditions of existence of the operation process with continuously rotating detonation and dynamic forces acting on the turbine blade in unsteady flow of detonation products have been determined. It is shown that the placement of the fixed blade raw downstream of the combustor may lead to changes in operating mode and even to its decay and to variations in the amplitude of flow pulsations. The influence of the turbine on the combustor operation mode depends on the angle of inclination of the blades relative to the combustor axis and on the direction of detonation rotation.

**NUMERICAL APPROACH FOR SIMULATION OF DIFFERENT  
COMBUSTION REGIMES IN HIGH-SPEED VISCOUS  
TURBULENT FLOWS: DEVELOPMENT AND VALIDATION**

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An approach to account for the influence of turbulent fluctuations on the average rate of chemical reactions in numerical simulations of turbulent flows with combustion has been suggested and applied to different modes of combustion in aircraft engines.

**MODELING OF NEAR-SURFACE EXPLOSION DYNAMICS**

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Near-surface explosion with complex interaction between incident and reflected blast waves is numerically simulated. The comparison between the solutions for near-surface and spherical explosions showed their similarity at the later stages of blast wave propagation.



**REDUCTION OF HIGH EXPLOSIVES BLAST WAVE  
BY MEANS OF ADDITIVES FIXATING GASEOUS  
DETONATION PRODUCTS INTO CONDENSED STATE**

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Effect of Zr/Al and Zr/Ti powder additives into the hot detonation products of detonating TNT charges has been studied. TNT charges were exploded in constant volume chamber together with the additives to reduce nitrogen contents in hot detonation products. Resulting effect of blast reduction was observed in experiments and discussed, including possible ways to reduce remainder gases in detonation products.

**BLAST WAVE MITIGATION BY MECHANICAL EFFECT  
ON EXPANDING HIGH-EXPLOSIVE DETONATION  
PRODUCTS AT SHORT DISTANCES FROM THE CHARGE**

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It is shown experimentally that the rigid polyurethane foam (with water inclusions and with distributed structure and density) covering a high-explosive charge is capable of reducing drastically the blast wave parameters in ambient air. The optimal foam block structure has been discussed.

**OBTAINING OF N<sub>2</sub> AND CO<sub>2</sub> SHOCK HUGONIOTS  
USING MULTICOMPONENT EQUATIONS OF STATE**

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Modern equations of state (EOS) of overcritical fluids have been adopted to simulate shock wave experiments with N<sub>2</sub> and CO<sub>2</sub>. Conclusions on the limits of applicability of modern EOS have been made.

**APPLICABILITY OF VAN DER WAALS ONE-FLUID MODEL  
IN COMPARISON WITH EXACT EQUATION OF STATE  
FOR BINARY MIXTURES**

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Limits of applicability of one-fluid model are investigated by comparing its predictions with those provided by the exact two-component model (2f-model) both at high pressures and at moderate pressures and temperatures. The conditions

when the one-fluid model fails to accurately predict the thermodynamic parameters of binary mixtures are identified.

#### **NONSTATIONARY OXIDATION REGIMES OF HETEROGENEOUS SYSTEMS**

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The simplest model of heterogeneous combustion systems is proposed. In this system, a nonlinear feedback between fuel and oxidant was shown to determine the basic characteristics of combustion, namely, ignition conditions, speed, and direction of combustion front propagation, etc.

#### **GODUNOV SOLVER FOR BAER–NUNZIATO EQUATIONS MODELING TWO-PHASE COMPRESSIBLE FLOWS**

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A system of Baer–Nunziato equations is a set of conservation laws for gaseous and dispersed phases supplemented with transport equation for the dispersed phase volume fraction originally proposed for the investigation of deflagration-to-detonation transition in heterogeneous explosives. To solve the Baer–Nunziato equations, the Godunov method is applied and tested against a number of Riemann problems with various initial conditions.

#### **ON THE COMBUSTION MECHANISM AND TEMPERATURE OF IRON MICROPOWDER IN GRAPHITE CUP AT ELEVATED PRESSURE OF OXIDIZING MEDIUM**

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New experimental results on heterogeneous combustion of iron micropowder accompanied by melt and iron oxide formation at different oxygen pressure are presented. Increase of oxygen pressure is shown to increase significantly the rate of heterogeneous combustion.

#### **SOME EFFECTS OF ELECTRICAL FIELD ON SURFACE COMBUSTION**

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The possibility of controlling thermophysical characteristics of surface combustion by applying electric field was demonstrated experimentally for fuel-lean and fuel-rich mixtures of natural gas with air.

**SPECIFIC FEATURES OF COMBUSTION ON THE SURFACE OF A FOAM METAL MATRIX WITH CERAMIC COATING**

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Characteristics of surface burning of natural gas on the foam metal matrix with the ceramic coating were studied experimentally. With the coating of low heat conductivity, the flame front was shown to immerse into the matrix, the effective temperature of the surface layer was shown to increase, and nitrogen oxides and carbon monoxide concentrations were shown to decrease.

**MODELING OF FLAME FRONT STRUCTURE IN POROUS MEDIA IN QUASI-ISOBARIC APPROXIMATION**

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The transient physical and mathematical model and the experimental method to study spatially inhomogeneous filtration combustion regimes in weak pressure gradient fields have been suggested. Under certain conditions, the flame front was shown to become unstable and exhibit a cellular structure.

**METAL COMBUSTION AS A METHOD FOR PRODUCTION OF ULTRAPOROUS NANOSTRUCTURED CERAMICS**

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Experimental studies on the mechanism of gas-phase synthesis of ultraporous nanostructured ceramic materials (aerogels and xerogels) at combustion of metal particles (aluminum, magnesium, zinc, titanium, and zirconium) have been performed. The dependence of the composition and morphology of the products on combustion conditions was determined.

**SAFFMAN–TAYLOR INSTABILITY IN FILTRATION COMBUSTION**

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The propagation of filtration combustion wave in two-dimensional thin channel was simulated numerically with due regard for a finite thickness of the combustion front and variation of porous medium heat and mass transport characteristics in the course of fuel conversion. At certain conditions, in particular, when the permeability of porous medium increases due to fuel conversion, the

planar combustion front was shown to become unstable and take a shape of a Saffman–Taylor finger.

#### **FIREPROOF INTUMESCENT PAINTS**

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Presented are the results of standard field tests of fireproof intumescent paint KHNA applied to the I-beam number 20 in fire conditions. The results are compared with a large variety of data on the same tests with other available fireproof paints.

#### **THE EFFECT OF NANOPARTICLE SHAPE AND SIZE ON PHASE DIAGRAM OF CARBON**

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A comparative analysis of contemporary knowledge on the phase diagram of carbon indicating significant uncertainty in the position of lines for carbon nano- and coarse particles has been conducted. The influence of carbon nanoparticles structure, size, and shape on the position of nanographite–nanodiamond phase transition lines was demonstrated by means of calculations.

#### **PRELIMINARY RESULTS OF INVESTIGATION OF LIQUID FUEL PULSE DETONATION COMBUSTOR**

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The pulsed heterogeneous detonation regime of heptane + oxygen mixtures diluted with air has been implemented in the small-size combustor. The conditions and specific features of deflagration-to-detonation transition (DDT) are studied. The DDT and the detonation wave velocity were shown to depend on physical and chemical properties of the mixture and on design parameters of the pulsed combustor. In heptane + oxygen mixtures diluted with air, the detonation was initiated at distances of 250–600 mm from the igniter which is approximately 13–30 tube diameters.

#### **MAGNETOHYDRODYNAMIC EFFECTS OF HETEROGENEOUS MIST DETONATION**

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Experimental studies of magnetohydrodynamic (MHD) effects of pulse detonations in heterogeneous mixtures of liquid hydrocarbon fuel with oxygen gas have

been performed. A well repeatable pulse voltage with a frequency given by the pulsed detonation chamber operation was registered at all electrodes of the MHD generator.

**FORMATION OF CERAMIC COATINGS BY MULTICHAMBER DETONATION SETUP**

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A new method for creating a flow of detonation products for powder coating purposes has been proposed. The method allows the particles of sprayed powder to accelerate up to velocities exceeding 1000 m/s and coatings with new properties to be obtained.

**EFFICIENCY LIMITATIONS FOR FUEL-CELL BASED AVIATION POWER PLANTS CAUSED BY CHEMICAL PROCESSES OF FUEL TRANSFORMATION**

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Presented are the results of investigations of fuel cell application in aviation power plants. Estimations of fuel-cell battery parameters indicate that the efficiency of proton-exchanging membrane fuel cells is limited when aviation kerosene is used as fuel. These limitations are not applicable to solid oxide fuel cells (SOFC). Thus, application of modern SOFCs in aviation power plants makes it possible to reduce fuel consumption by a factor of two as compared to gas turbine power plant.

**KINETICS OF FAST HIGH-TEMPERATURE REACTIONS AT COMBUSTION AND EXPLOSION OF ENERGETIC MATERIALS**

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The reliable experimental determination of kinetic parameters of fast high-temperature reactions in condensed energetic materials (EM), which cannot be obtained by the extrapolation of low-temperature kinetic data into the high-temperature region, is of vital importance. Some new results dealing with the general theory of thermal explosion and quantitative comparative analysis of newly obtained experimental data with conclusions based on classical combustion and explosion theories for some EM are presented. The following topics are considered in detail: (i) maximum preheating under the critical conditions

of thermal explosion; (ii) kinetics of high-temperature decomposition, thermal explosion, and combustion of liquid explosives; (iii) analysis of the theories of the stationary combustion – explosive combustion transition for liquid explosives developed by L.D. Landau and V.G. Levich; (iv) comparison of data on kinetics and macrokinetics of high-temperature reactions in self-propagating high-temperature synthesis (solid flame) systems; and (v) kinetic data for fast reactions in some homogeneous and heterogeneous EM accompanied by significant heat release including processes occurring under static conditions and at high-speed impact.

### **CALORIMETRY OF ENERGETIC MATERIALS**

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Presented is the new reference calorimeter for thermochemical studies of energetic materials (EM), which is superior to all available domestic and foreign laboratory instruments in terms of metrological, technical, and performance characteristics. The calorimeter allows for performing a series of up to 5 experiments with small EM samples (0.5 g) and getting precise thermochemical characteristics of various classes of energetic compounds.

### **FORMATION ENTHALPIES OF AROMATIC RADICALS**

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A new scheme for empirical evaluation of bond energies in the energetic materials using available thermochemical data has been proposed and applied to calculate the dissociation energy  $D(\text{C}-\text{NO}_2)$  in nitrometilfurazane and nitrobifenile and the enthalpies of formation of the corresponding radicals.

### **A METHOD FOR ESTIMATING THERMOCHEMICAL PROPERTIES OF SALT COMPOUNDS**

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A method for calculating the enthalpies of formation and dissolution of compounds with molecular ions and heterocyclic-based ionic components has been proposed. The method is based on the assumption of additive contribution to the lattice energy, enthalpy of formation, and dissolution of salt structure compounds.

**SPECIFIC FEATURES OF REVERSIBLE PHASE TRANSITIONS IN ENERGETIC NITROCOMPOUNDS**

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The kinetics of phase transition (PT)  $\alpha \rightarrow \beta$  in polycrystalline 1,1-diamino-2,2-dinitroethene (DADNE) has been investigated by means of differential scanning and isothermal calorimetry. The kinetics of the reverse PT  $\beta \rightarrow \alpha$  in DADNE has been investigated using infrared spectrophotometry. The phase transition  $\alpha \rightarrow \beta$  was shown to follow the autocatalytic first-order kinetic law. The activation energy and the rate constant were determined. The kinetic law for the reverse PT  $\beta \rightarrow \alpha$  was shown to correspond to two parallel processes. Rate constants of both processes have been determined. Similar behavior was observed in reversible PT between  $\beta$ - and  $\delta$ -polymorphs of HMX. Possible reasons for the absence of self-acceleration in reverse PT are discussed.

**FORMATION OF IGNITION HOT SPOTS IN REACTIVE SOLIDS WITH IRREGULAR SURFACE**

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Reactive solids with rough surfaces possessing protrusions and other irregularities tend to ignite locally in hot spots. It is shown that the standard statistical description of a rough surface does not apply to ignition problems with the Dirichlet boundary conditions, because hot spots are formed at the places of the largest deviation from the mean values. The behavior of the solution in the vicinity of hot spot is studied and the ignition conditions of such hot spots are found. Due to rapid heating of protrusions, the ignition time and the characteristic size of the hot spot weakly depend on the initial temperature. This mechanism may give rise to pulsed modes of combustion of propellants due to repeated ignition and extinction of hot spots.

**CRITICAL DIAMETER OF DOUBLE-BASE PROPELLANT COMBUSTION FROM STANDPOINT OF SPOT-BURNING MECHANISM**

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Combustion and extinction of double-base propellant sample is analyzed. The analysis is performed from the standpoint of the spot-burning mechanism. It is shown that the determining factors are the limited number of burning spots

(with critical diameter having less than 3 spots) and their interaction through the gas phase.

### **BURNING RATES OF SOLID ENERGETIC MATERIALS AT PULSATING PRESSURE**

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Analytical formulae for instantaneous and average burning rates of solid energetic materials (SEM) at harmonic pulsating pressure were obtained. Calculations of the burning rates for different SEM (here, for double-base propellants and pressed HMX) in linear and quadratic approximations were performed. The average burning rates were shown to become equal to the rates of stable burning after a short transient period.

### **MODELING OF A CHEMICAL REACTION WAVE IN MECHANOACTIVATED POWDER MIXTURE**

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A numerical method to simulate propagation of chemical reaction in powder mixtures is proposed. The method involves two steps: simulation of powder structure followed by simulation of powder combustion. The results of parametric studies indicate that under certain conditions, the combustion of powder mixture proceeds nonuniformly in space and time: the curved combustion front exhibits leading points which can move significantly ahead of the average front. In addition, a period of active burning can be replaced by a relatively long period of stagnation followed by combustion process renewal. The velocity of reaction front propagation in nanopowders can substantially exceed the speed of sound in the gas filling the pores; thereby, mixture combustion can be followed by shock formation and onset of flow regimes similar to detonation.

### **MECHANISM OF INFLUENCE OF NANOSIZED OXIDES ON HMX THERMOLYSIS**

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The influence of various nano- and micro-sized metal oxides on HMX thermolysis has been studied experimentally. Nano-TiO<sub>2</sub> additive appeared to be the most effective. The mechanism of the catalytic effect of nano-TiO<sub>2</sub> on HMX decomposition is discussed.



**DROPLET CONCEPT OF SOLID FLAME PROPAGATION**

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Combustion of self-propagating high-temperature synthesis (SHS) systems is known to be often accompanied by partial or complete melting of reactants and/or products. It has been suggested that the motion of melts is governed by thermocapillary forces. In typical gasless systems, these forces are markedly stronger compared to other forces affecting melt motion. A modified droplet concept of SHS combustion wave structure and propagation is suggested which is based on some results of combustion experiments with inert-gas counterflow. According to the concept, flame front structure and propagation depend on the mobility of liquid droplets in a porous medium under the influence of thermocapillary forces.

**MATHEMATICAL MODELING OF ALUMINOTHERMIC MIXTURE COMBUSTION UNDER ARTIFICIAL GRAVITY CONDITIONS**

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The self-sustaining exothermic frontal process of chemical transformation in porous Ti–Al–CaO<sub>2</sub> aluminothermic composition under artificial gravity produced by centrifuge has been simulated numerically. As a result, spatial and temporal temperature distributions of individual groups of reactants, velocity fields of convective motion, fields of reactant concentrations, pressure (stress), and rates of exothermic chemical transformations of individual reactants were obtained.

**DESTRUCTION OF PARTS OF SATELLITES ORBITING THE EARTH**

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Experimental studies to explore the feasibility of using thermite compositions Al/CoO, Al/V<sub>2</sub>O<sub>5</sub>, and Al/Fe<sub>2</sub>O<sub>3</sub> for destruction of titanium fuel tanks of satellites orbiting the Earth when entering the Earth's atmosphere by initiating titanium alloy melting have been performed. It has been shown that titanium plate failure (melting) can only be achieved when using the Al/CoO composition.

**SYNERGETIC INTERACTION OF AMMONIUM  
PERCHLORATE WITH HMX: PRACTICAL APPLICATION**

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The feasibility of reducing the temperature of HMX decomposition in the presence of ammonium perchlorate (AP) and active fuel-binder was explored experimentally by coating HMX particles by AP. It has been shown that under certain conditions, the burning rate of such compositions can be varied within a wide range due to synergetic effects.

**SYNTHESIS, PROPERTIES AND BURNING LAWS OF SIMPLE  
ESTERS AND DIMETHYLOLNITRAMINES**

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Presented are the detailed physicochemical and explosive characteristics and burning law parameters for alkyl esters and cyclic ethers of dimethylolpolynitramines.

**TEMPERATURE PROFILES IN THE COMBUSTION WAVE  
OF LIQUID NITROESTERS**

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Temperature distributions in the combustion wave propagating in nitrate ester plasticizers — nitroglycerin, nitroglycol, and diethyleneglycol dinitrate — have been measured by tungsten-rhenium microthermocouple to determine their boiling temperature in pressure range 0.04–2 MPa. The burning surface temperature of these plasticizers was shown to be determined by the boiling temperature, i. e., the combustion process is governed by gas-phase reactions.

**STUDY ON THERMAL DECOMPOSITION AND COMBUSTION  
OF 4,4''-DINITRO-TRIS-FURAZAN**

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Thermal decomposition of 4,4''-dinitro-tris-furazan (NTF) in isothermal and nonisothermal conditions has been studied experimentally. The thermal stability of NTF was found to be higher than that of HMX while the burning rate of NTF was close to the burning rate of CL-20. The NTF vapor pressure was determined from manometric measurements.

**COMBUSTION OF NANOCOMPOSITES BASED ON ALUMINUM AND NITRAMINES: NEW DATA**

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The effects of aluminum particle size, type of coating, and age as well as the effects of component mixing on the combustion characteristics of HMX and ADNA compositions with aluminum have been studied experimentally. It has been shown that proper surface modification of aluminum particles and proper preparation of composition can be used for controlling ballistic properties of such compositions in a wide range.

**THE EFFECT OF HUMIDITY ON THE BURNING OF POWDER AND GRANULATED Ti + 0.5C MIXTURES**

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Burning of powder and granulated Ti + 0.5C mixtures in coflow filtration mode with and without argon purging has been studied experimentally at different humidity of initial mixture. The experiments showed that the combustion front velocity decreases with mixture humidity due to the growth of impurity gas release, whereas granulation results in a significant reduction of the effect of impurity gases on the combustion front velocity.

**CONVECTIVE MODE OF REACTION ZONE PROPAGATION: A NEW MECHANISM OF GASLESS COMBUSTION**

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A new convective-conductive model of gasless combustion is proposed to explain the experimental results which seem to be abnormal from the viewpoint of the combustion theory. The main factors affecting the combustion wave propagation are established with due regard for the limiting role of melt penetration into the initial green mixture.

**INFLUENCE OF GRANULATION ON COMBUSTION OF 2Ti + C MIXTURE IN NITROGEN COFLOW**

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Combustion of granulated 2Ti + C mixtures in active gas coflow was studied experimentally for the first time. Possible combustion regimes of granulated

mixtures related to a more complex scale hierarchy (micro, macro, and meso) as compared to powders (micro and macro) are analyzed. Considerable (several times) increase in the burning rate of the granulated mixture as compared to powder of the same structure is observed. It is shown that in contrast to  $2\text{Ti} + \text{C}$  powders, combustion of granulated  $2\text{Ti} + \text{C}$  mixture in nitrogen coflow exhibits only one combustion front due to the leading role of titanium nitridation reaction in the course of combustion front propagation. The essential role of radiation in combustion front propagation through the granulated  $2\text{Ti} + \text{C}$  mixture is outlined.

#### **SHORT-PULSE PROJECTILE SETUP OPERATING IN LOW VELOCITY DETONATION MODE**

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Chemical conversion of high explosive (TNT/RDX 30/70) in low-velocity detonation mode in the short-pulse projectile setup has been studied experimentally. Recorded are the thrust impulse, projectile trajectory, and pressure in the charge chamber. These characteristics have been used for calculating the muzzle velocity and a degree of chemical conversion of the high explosive. Effects of charge and projectile masses and chamber length on the thrust impulse, muzzle velocity, maximum pressure, and the completeness of chemical conversion have been considered.

#### **NUMERICAL MODELING OF GUN-BARREL THERMAL STATE AT A SHOT**

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Mathematical models, numerical algorithms, and computer software were developed for numerical modeling of the thermal state of a gun barrel at a shot. The numerical model involves internal ballistics processes coupled with the gun barrel thermal state in the axisymmetric geometry. The internal ballistics processes are simulated based on the mathematical model of multiphase multicomponent two-velocity gas-powder continuum motion taking into account burning of powder grains and interphase interaction. The gun barrel can have a multilayer structure. Also, the thermal state of projectile casing can be taken into account. The calculations can be carried out either for one shot or for the sequences of shots. As an example, numerical simulations for a 100-millimeter gun barrel are discussed.

**HEAT OF EXPLOSION AND THROWING ABILITY  
OF MIXTURES OF HIGH EXPLOSIVES  
WITH INORGANIC OXIDIZERS**

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Presented are the computational and experimental studies of the effect of inorganic oxidizers (ammonium nitrate, ammonium perchlorate and ammonium dinitramide) on the heat of the explosion and throwing ability of blasting explosives based on mixtures of HMX and triaminotrinitrobenzene.

**MECHANOACTIVATION AND EXPLOSIVE PROPERTIES  
OF ALUMINUM AND AMMONIUM PERCHLORATE  
MIXTURES**

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The production technique of mechanoactivated energetic composition (MAEC) based on aluminum and ammonium perchlorate (AP) has been developed. The optimum conditions for mechanical activation were found so that the maximum homogenization of the mixture was provided in the absence of the reaction between reactants. The structure of MAEC was studied by X-ray diffraction analysis and scanning electron microscopy. Explosive properties (deflagration-to-detonation transition (DDT) in Al/AP loose-packed charges (80% porosity) and mechanical sensitivity) have been obtained. It has been found that DDT process goes through a stage of overdriven detonation with the maximum value of detonation velocity of 3200 m/s followed by the establishment of steady-state detonation with the propagation velocity of 2400 m/s.

**MECHANOACTIVATED ENERGETIC COMPOSITES  
Mg/FLUOROPLAST: THE EFFECT OF ACTIVATION DOSE  
ON THE STRUCTURE AND REACTIVITY**

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The effect of activation dose on the structure and reactivity of mechanically activated Mg/Teflon composites has been studied experimentally to determine the physical reasons for the increasing rates of interaction under shock-wave and thermal initiation of such composites.

**DEFLAGRATION-TO-DETONATION TRANSITION  
IN FINE MIXTURES OF ALUMINUM  
WITH AMMONIUM PERCHLORATE**

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The possibility of deflagration-to-detonation transition (DDT) in fine mixtures of ammonium perchlorate and submicron aluminum confined in low-strength glass tubes has been shown for the first time. Scenario and characteristics of the DDT process depending on aluminum content varied from 5 to 28 % (wt.) are considered. The smallest (20–30 mm) run-up distance to detonation is observed in fuel-lean mixtures with the aluminum content of  $\sim 5$  % (wt.). The DDT includes intermediate stages (convective burning and low-velocity detonation) and develops through the onset of a secondary pressure wave arising behind the leading flame front during the convective burning stage.

**DETONATION OF AN EXPLOSIVE CONTAINING  
PROPPANT — RDX CONTAINING WATER-SATURATED SAND**

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Experimental studies and thermodynamic calculations of a detonation in a mixture of RDX with water-saturating sand (explosive containing proppant) have been carried out. The detonation velocity of the mixture has been measured for the compositions with different RDX content varied from 14 up to 74 % (wt.), with different RDX and sand particle sizes, and with different initial temperature. The critical detonation diameter was shown to decrease with the RDX content attaining several millimeters for the RDX content of 30 % (wt.) and more. The calculation results are in a good agreement with measurements of the detonation velocity and the effect of the RDX content.

**SENSITIVITY TO IMPACT OF FLUORINOPOLYMERS  
AND MECHANICAL MIXES OF FLUORINPOLYMERS  
AT THEIR IDENTICAL ELEMENT COMPOSITION**

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Sensitivity to impact of fluorinopolymers prone to explosion-like chemical transformation is determined experimentally. It is shown that sensitivity of fluorinopolymers can differ considerably from that of binary mixtures of polymers at identical elemental composition. Such a behavior is caused by unequal strength

to compression for the corresponding charges and by spatial separation of fluorine and hydrogen atoms in the mechanical mixtures of polymers.

**INITIATION OF EXPLOSION BY IMPACT  
OF THE PASTE-LIKE MIXTURES ENRICHED  
WITH THE HIGH-STRENGTH INERT ADDITIVE**

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The effect of abrasive additive on the initiation of paste-like material based on ammonium perchlorate and nitromethane has been studied experimentally. The additive was shown to increase the sensitivity of the material. The initiation of the material before its fracturing was detected. This effect was more pronounced at higher speeds of load dropping on the material layer. The results obtained are physically interpreted.

**SHOCK WAVE LOADING OF CARBON NANOTUBES  
UP TO PRESSURE 100 GPa**

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Shock wave loading (SWL) of carbon nanotubes has been investigated experimentally. Carbon nanotubes (CNTs) samples were put in preservation ampoules and were loaded by impact of the aluminum flyer plates accelerated by high-energy charge. The maximal SWL pressures were 14, 19, 26, 36, 52, and 98 GPa. After SWL, the samples were examined by the methods of high-resolution transmission electron microscopy and Raman spectroscopy. The results have shown high durability of CNTs up to shock wave pressures exceeding 20 GPa.