10th INTERNATIONAL SEMINAR ON FLAME STRUCTURE

10 ISFS

Book of Abstracts

Novosibirsk, Russia
October 9-13, 2023

Siberian Branch of the Russian Academy of Sciences

Voevodsky Institute of Chemical Kinetics and Combustion SB RAS
Khristianovich Institute of Theoretical and Applied Mechanics SB RAS
Kutateladze Institute of Thermophysics SB RAS
Lavrentyev Institute of Hydrodynamics SB RAS
Boreskov Institute of Catalysis SB RAS
Novosibirsk State University
Russian Sections of the Combustion Institute

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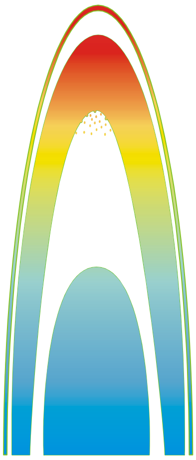

Novosibirsk

2023

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Preface

The Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, together with the Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, the Kutateladze Institute of Thermophysics SB RAS, the Lavrentyev Institute of Hydrodynamics SB RAS, the Boreskov Institute of Catalysis SB RAS and the Novosibirsk State University organized the 10th International Seminar on Flame Structure in Novosibirsk, held under the aegis of the Russian Section of the Combustion Institute. The Seminar is considered as continuation of 9 preceding workshops on flame structure: All-Union Workshop on Structure of Gaseous Flames, Novosibirsk, 1983; International Workshop on Structure of Gaseous Flames, Novosibirsk, 1986; Third International Seminar on Flame Structure, Alma-Ata, 1989; Fourth International Seminar on Flame Structure, Novosibirsk, 1992, Fifth International Seminar on Flame Structure, Novosibirsk, 2005, Sixth International Seminar on Flame Structure in Brussels, 2008, Seventh International Seminar on Flame Structure, Novosibirsk, 2011, Eight International Seminar on Flame Structure, Berlin, 2014, Ninth International Seminar on Flame Structure, Novosibirsk, 2017.

The objective of the Seminar is to provide an international forum for discussing the state-of-the-art achievements and perspectives in the experimental and computational study of the flame structure of both gaseous and condensed systems, the flammability limits and the applied aspects of combustion research, as well as to enhance international cooperation in these areas. The topics of the Seminar are: laminar and turbulent, premixed and diffusive flames of gaseous systems, flames of homogeneous and heterogeneous condensed systems, flame of polymers, composite materials, reduction of their combustibility, inhibition and suppression of flames and fires, electric-field assisted combustion and ion chemistry, chemical kinetics in combustion, self-propagating high temperature synthesis, catalysis of combustion, filtration combustion and microcombustion.

The 10th ISFS Organizing Committee has received over 90 excellent abstracts from Russia, China, France, Germany, Israel, Italy, India Kazakhstan, Sweden, and the United States, covering the entire domain of combustion from fundamental to technical aspects. The Scientific Program of 10th ISFS includes 16 plenary lectures, over 75 oral and poster presentations. We are grateful to all the authors who have contributed to the 10th ISFS.

We extend special thanks to the researchers from the laboratory of kinetics of combustion, the Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, who have made invaluable contribution to the preparation and organization of the Seminar. We are grateful to the sponsors of the Seminar: the Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, the Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, the Kutateladze Institute of Thermophysics SB RAS, the Lavrentyev Institute of Hydrodynamics SB RAS, the Boreskov Institute of Catalysis SB RAS, the Novosibirsk State University, LLC «ZIO-Energy», SIBALUX LLC, Joint Stock Company "Eberspächer Climate Control Systems RUS", Scientific Equipment Group of Companies. It was with their support that organization of the Seminar became possible.

Prof. Oleg Korobeinichev

Chairman of the 10th ISFS Organizing Committee

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- Siberian Branch of the Russian Academy of Sciences
- The Voevodsky Institute of Chemical Kinetics and Combustion SB RAS
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PLENARY LECTURES

Growth mechanisms of polycyclic aromatic hydrocarbons (PAHs) in benzyl radical (C_7H_7) reactions

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The mechanisms of the two- and three-ringed PAHs formation of in the reactions with C_7H_7 radial have been established using of molecular beams experiments combined with electronic structure calculations along with computational fluid dynamics and kinetic modeling. The temperature dependences of the rate constants for the C_7H_7+C_7H_7 and C_3H_3+C_7H_7 reactions in a wide range of pressures and temperatures were obtained (Fig. 1a). The formation of three-ring PAHs – phenanthrene and anthracene $C_{14}H_{10}$ in the reaction C_7H_7+C_7H_7, carried out in a high-temperature microreactor, was confirmed experimentally by the methods of molecular beam photoionization mass-spectrometry (Fig. 1b, mass-to-charge ratio m/z=178). The obtained dependences are in demand of the development of energy-efficient technologies for combustion of hydrocarbon fuels with low PAH and soot emissions and in astrochemical modeling of the nucleation and evolution of complex organic compounds in our Galaxy, including in the circumstellar envelopes of asymptotic giant branch stars.

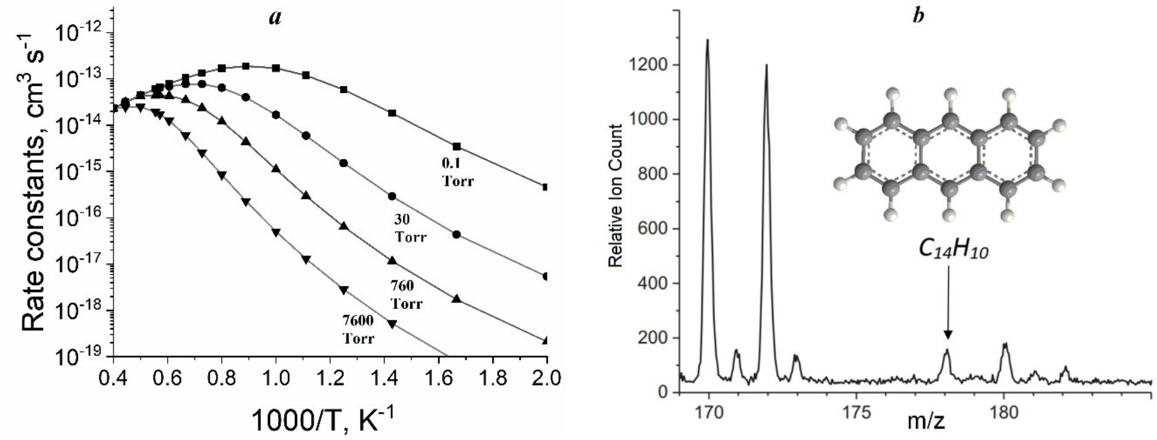

Figure 1 a – Reaction rate constants C_7H_7+C_3H_3 – from initial reagents to two-ringed products for different pressures in Torr; b – Mass spectrum of the molecular beam from the HTMR (T=1473 K), including the reaction products C_7H_7+C_7H_7.

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New insights into the cool flame oxidation of terpenes and surrogates: detection of highly oxygenated, polyunsaturated, and aromatic products using very high-resolution mass spectrometry

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Terpenes are hydrocarbons naturally released by vegetation. They constitute a large fraction of volatile organic chemicals present in the troposphere. In addition, because of their high-energy-density, this class of chemical compounds could be used as biojet fuel. Cetane numbers of monoterpenes have been determined to be of the order of 20. Then, one could also use them as drop-in fuels to reduce the carbon footprint in transportation. However, the use of terpenes as biofuel or drop-in fuel would undoubtedly contribute to increasing their concentration in the troposphere through unburnt fuel emissions and evaporation during transport and refueling. While the kinetics of oxidation of terpenes under troposphere-relevant conditions has been the topic of numerous studies, a good understanding of the multiple oxidation routes has not been reached yet. The chemical kinetics of combustion of this class of chemicals has not received much attention to date since only burning velocity in air and impact on ignition have been reported in the literature.

Recently, we tried to better characterize the autoxidation products of terpenes under cool-flame conditions. We investigate the formation of highly oxidized products, aromatics and polyunsaturated products. We carried out oxidation experiments in a jet-stirred reactor at 1 bar. Oxidation products were characterized using high-resolution mass spectrometry and soft ionization (+/– heated electrospray ionization –HESI– and +/– atmospheric pressure chemical ionization –APCI). As an example, we will present results for limonene-O_2-N_2 and α-pinene-O_2-N_2 mixtures oxidized in a jet-stirred reactor at 1 bar, in the cool flame regime, and fuel-lean conditions. Results obtained under the same conditions for a simple surrogate will be presented. Samples of the reacting mixtures were collected, dissolved in acetonitrile, and analyzed by Orbitrap mass spectrometry after flow injection or chromatographic separation by ultra-high-performance liquid chromatography and soft ionization. H/D exchange using D_2O and reaction with 2,4-dinitrophenylhydrazine were performed for probing the existence of hydroxy, hydroperoxy, and carbonyl functions in the products, respectively. A very large set of oxidation products, including highly oxygenated organic products with five and more oxygen atoms, was observed. Aromatic and polyunsaturated products were detected. Van Krevelen plots computed oxidation state of carbon and degree of unsaturation in products were used to rationalize the results.

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CH_4/Air laminar flame speed determination at high pressure and temperature using constant volume method

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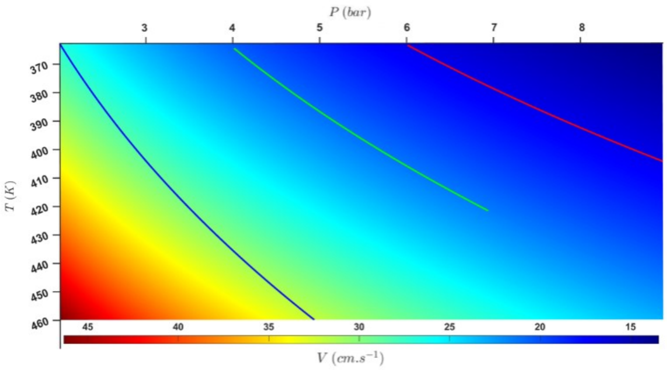
Due to experimental difficulties, most of the available flame speed database is for relatively limited thermodynamic conditions and for independent variations of pressure and temperature. These limitations may be overpassed by using spherically expanding flames with the constant volume method. This methodology, introduced in the 30s by Lewis and von Elbe, requires the knowledge of the pressure evolution in the combustion chamber. The isochoric method has been penalized for a long time because of the underlying assumptions (i.e. accuracy of the models for the burned mass fraction, stretch effects, influence of burnt gases equilibrium state and of radiation, or problems in flame instability detection). This method was recently revisited by Egolfopoulos with a coupled experimental / numerical approach integrating radiation and dissociation effects while maintaining moderate computing costs. The current study uses a new perfectly spherical isochoric combustion chamber with full optical access (OPTIPRIME) allowing the simultaneous recording of pressure and flame radius inside the chamber during the full combustion process. Flame speeds over large pressure and temperature domains are then obtained from these raw data with very good accuracy and S_L = f (T, P) maps can be generated (see figure). These new experimental targets allow constraining kinetic mechanisms under unprecedented conditions and the identification of key reactions needing improvements.



S_L = f (T, P) map for CH_4/Air mixture at $\varphi = 1.1$

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Use of biofuels to reduce PAH and soot emissions

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The use of alternative fuels (including biofuels) is an urgent task both due to the limited availability of fossil fuels and environmental problems associated with harmful emissions into the atmosphere. Currently, great prospects are associated with the use of various types of oxygen-containing biofuels. Their production has a "zero carbon footprint", and the presence of oxygen in the composition should lead to an increase in the efficiency of oxidative processes, which, in turn, can reduce the amount of polycyclic aromatic hydrocarbons (PAHs) and soot nanoparticles formed during incomplete combustion of fuel.

Linear and cyclic esters: furan C_4H_4O, tetrahydrofuran C_4H_8O, dimethyl ether C_2H_6O, diethyl ether $C_4H_{10}O$, dimethoxymethane $C_3H_8O_2$ and alcohols: methanol CH_3OH and butanol C_4H_9OH are promising representatives of biofuels. Therefore, it is of particular interest to study their effect on the formation of PAHs and soot.

The report presents the results of experimental studies of the effect of various biofuel additives on the formation of PAHs and soot in the processes of pyrolysis and combustion behind shock waves and in a standard McKenna premixed burner. To control the growth of PAHs and soot particles, a wide range of modern diagnostic tools were used, including methods of laser-induced fluorescence (LIF), laser-induced incandescence (LI), laser extinction (LE), as well as methods for measuring flow parameters (temperature and pressure) using appropriate sensors.

In addition to experimental measurements, the numerical analysis of the obtained data was carried out based on the most modern kinetic mechanisms (CRECK Modeling Group, etc.) using the OpenSMOKE++ software.

As a result of the work, the conditions were determined under which the use of certain biofuels leads to the most effective reduction in the formation of PAHs and soot, and the key kinetic pathways that determine the suppression (or stimulation) of their formation were identified.

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PLENARY LECTURES

Gaseous and heterogeneous detonation in water vapor: is it possible?

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Unlike conventional chemical propulsion systems based on controlled subsonic combustion of fuel in a combustion chamber, the operation process in pulsed detonation engines (PDEs) and rotating detonation engines (RDEs) is based on controlled combustion of fuel in the flow of an oxidizing medium in pulsed and continuously rotating detonation waves, respectively. One of the key issues in the design and operation of PDEs and RDEs is the choice of fuel possessing sufficient detonability in a particular oxidizing environment required for the sustainable and energy efficient operation process. In this contribution, the results of thermodynamic calculations of detonation parameters of boron- and aluminum-containing compounds in air and water will be presented. To verify the reliability of the calculations, we first compared the calculated detonation velocities of diborane, aluminum, and isopropyl nitrate in air with experimental literature data. Satisfactory agreement with the available calculated and experimental data is obtained. Thereafter, the results of calculations for (B, B_2H_6, B_5H_9, $B_{10}H_{14}$, Al, AlH_3, $Al(C_2H_5)_3$, and $Al(CH_3)_3$) are discussed. It is shown that all considered boron- and aluminum-containing compounds exhibit high detonation velocities both in mixtures with air and in mixtures with water: in the range from 1830 to 2020 m/s for stoichiometric mixtures with air and from 1880 to 2640 m/s c for stoichiometric mixtures with water. The highest detonability in mixtures with air is inherent in aluminum hydride, whereas aluminum exhibits the highest detonability in mixtures with water. The use of different sets of thermodynamic properties for $Al(C_2H_5)_3$ gives a spread in the maximum detonation velocity for mixtures with air from 1880 to 1900 m/s and for mixtures with water from 2150 to 2210 m/s, i.e., the relative spread of calculated detonation velocity values is 0.9% for explosive mixtures with air and 3% for explosive mixtures with water. Accounting for nitrogen oxides in the detonation products leads to a slight decrease in the detonation velocity from 12 m/s (for diborane) to 22 m/s (for aluminum), which is approximately 0.7 to 1.2%. The obtained results demonstrate the potential feasibility of using the compounds under consideration as fuels for PDEs and RDEs operating in the atmosphere and in water.

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Patterns and characteristics of the gel fuels ignition

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Composite fuels based on carbon-containing industrial waste, in-cluding those containing oil products, are promising for practical use in conditions of shortage and rising prices of traditional energy resources. The following various solid and liquid components can be used as fuel components: coal sludge, coal-refining waste (coal slurry), waste process oils, oil extraction and oil refining waste, chemical waste, various types of biomass.

Involvement of industrial wastes in thermal power engineering will reduce the environmental burden not only by reducing the area of landfills for waste storage, but also due to the reduction in greenhouse gas emissions. This effect is achieved by increasing the completeness of the slurry fuel components burnout due to the secondary atomization of inhomogeneous droplets during intense heating. Components (solid and liquid) of the composite fuel droplets are heated at different rates. As a result, local vaporization centers can appear at the boundary of their contact (including mutually insoluble liquids). An increase in stress near the interface between the components (especially solid and liquid ones) can cause a microexplosion, because of which a droplet is dispersed into tens and hundreds of finely dispersed fragments. Droplet fragmentation increases the surface area of heat exchange between the fuel and the heated air, thereby intensifying the evaporation and thermal decomposition of the fuel components, and, consequently, ignition and combustion. Unlike it is with liquid single-component fuels, combustion is initiated not in the immediate vicinity of the droplet but in a rather large area. This positively affects the development of subsequent combustion of the fuel and enhances the burnout of components. A significant difference between compositions containing carbonaceous particles and without them lies in the fact that as a result of the bubble collapse and droplet dispersion, vapors of combustible liquid and fine coal particles impregnated with it are blown into the high-temperature oxidizer medium. Therefore, the gas-phase ignition of the fuel containing fine solid particles occurs quite evenly in a large area.

In addition, the presence of water in the fuel is a favorable factor for intense oxidative reactions and neutralization of harmful substances occurring at relatively high temperatures in boiler furnaces. At a relatively high temperature, water vapor thermally dissociates, resulting in the release of oxygen and hydrogen molecules. These molecules intensify the oxidation process, thereby improving the completeness of fuel burnout. Additionally, favorable factors for replacing coal with composite fuels include a reduction in fire hazards (due to the presence of water in the fuel composition) at the stages of preparation, transportation and storage, as well as lower fuel costs.

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Influence of oxidation state of phosphorus on the flammability of polymers

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Because of their flammability, polymer materials are very easy to cause fire accidents, resulting in loss of life and property. At the same time, as polymer materials appear in more application scenarios, higher requirements are put forward for flame retardants, such as efficiency, environmental friendliness, etc. Compared with phosphorus flame retardants with higher oxidation state such as phosphates, organophosphine compounds have higher phosphorus contents and higher activity in vapor phase. In our work, the linear oligomer flame retardants were synthesized based on phosphorus containing monomers with different oxidation states. The effects of the structural differences of flame retardants on the flame retardancy and mechanism of unsaturated polyester resins (UPR) were systematically analyzed.

As shown in Figure 1, dozens of oligomeric flame retardants were synthesized for flame retardant modification of UPR. Compared with flame retardants with highest +5 oxidation state (PO-S, POEG), organophosphine flame retardants (PCH_3-S, PB-S, PBEG) have higher flame retardant efficiency, and 15 wt% of PCH_3-S or PBEG make UPR reach UL-94 V-0. In contrast, although the composites with 20 wt% of PO-S or POEG had higher phosphorus contents, their UL-94 levels were still lower than the former. Therefore, compared with the highest oxidation state of phosphorus structures, the organophosphine oligomers were more suitable for improving the flame retardancy of UPR. The analysis of flame retardant mechanism showed that the flame retardancy of organophosphine oligomers was mainly in gaseous phase, supplemented by condensed mechanism.

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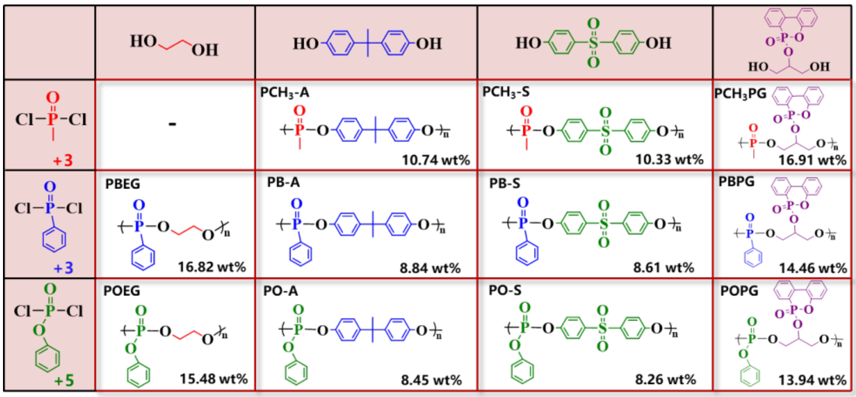

Figure 1 Synthesis of flame retardant oligomers for unsaturated polyester resins

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Associated Web site: http://sklfs.ustc.edu.cn/2017/0727/c12643a347098/page.htm
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Prediction of the diffusion flame spread behavior over the polymeric fuel surface

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Present level of the numerical study of the diffusion flame spread over solid fuel's surface relates to the following background of mathematical model (developed to the end of 1980s): elliptic formulation for the conservation equations for energy, momentum and mass, which are solved simultaneously both for gas phase and solid fuel; finite-rate chemical kinetics both for gas-phase combustion and solid fuel pyrolysis; radiation accounting (if necessary) both for flame and surface, and (most important) the coupled formulation providing the correct description of mutual interaction between gas-phase combustion and solid fuel thermal degradation, the heat balance between which ensures the self-sustained regime of flame propagation. Under this approach the reasonably well agreement between calculations and measurements has been achieved for the flame spread rate and mass loss rate as well as for temperature profile.

Here we would present some results of the prediction of flame spread over polymeric fuel with several modifications of the original model, which give better agreement with the experiments performed by the group of Prof. O.P. Korobeinichev of Voevodsky Institute of Chemical Kinetics and Combustion, the collaboration with which is highly appreciated by the authors of present paper. Flame spread over horizontal surface of PMMA has been studied numerically. Results showed rather good agreement with the experiments for the flame spread rate, mass loss rate and temperature field. It has to be noted that laminar flow approach assumed here is limited to the flame leading edge (at the distance of 10 mm order), while turbulent fluctuations occur downstream. For the comparison of concentrations profiles of basic components the following approach has been proposed: assuming that thermal degradation of MMA (as gaseous product of PMMA pyrolysis) in gas phase into lower-weight gas fuels has number of steps the molar weight of MMA is set to 50 g/mol instead of genuine 100 g/mol. While such an approach is of some heuristic nature, it gives better agreement with experiment. The downward flame spread over PMMA surface has been investigated. Unlike the generally accepted approach based on the one-step macro-reaction for combustion, proposed model employs the two-step reactions mechanism in the gas phase: solid fuel pyrolysis generates a gaseous product at the burning surface and, at the first reaction step, this relatively higher hydrocarbon decays into the lower-weight gas, which, in turn, reacts with surrounding oxidizer at the second reaction step, which is the combustion itself. The results showed that profiles of gas-phase temperature and concentrations obtained through the two-step reaction model fit experimental data noticeably better than customary one-step reaction. This two-step gas-phase reaction model has been applied to the flame spread over the horizontal surface of polyoxymethylene. Again, better agreement between calculations and measurements has been found. The downward flame spread over the surface of glass fiber reinforced epoxy resin (GFREP) has been studied. Here, the primary factor defining the flame spread behavior is anisotropic properties of solid fuel, which thermal conductivity is different in the flame spread direction and normal to the burning surface.

Work of second author (A.S.) was supported by Russian Science Foundation (Project 22-79-10066).

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PLENARY LECTURES

Burning characteristics of tropical forest litter

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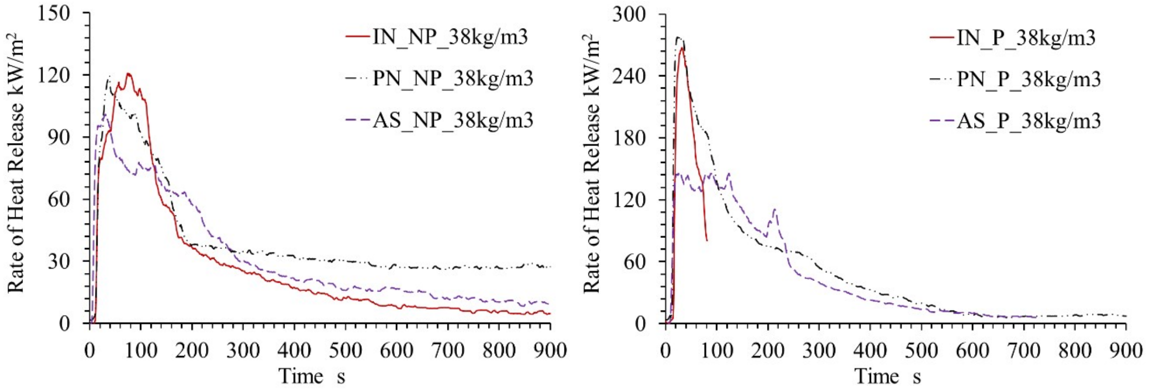
Forests in India are diverse ranging from Alpine, Temperate to Tropical forests. The number of incidents of fires has increased over years. Most forest fires start from litter at the forest bed especially during the pre-monsoon months of March-April. Here in this presentation burning characteristics and flammability of three species of forest litters in a cone calorimeter setup are reported. Figure 1 presents heat release rates for the three types of forest litters, two of these (Neem and Ashoka) have typical temperate/tropical broad leaf morphology and for comparison needle shaped leaf (Pine) litter is also tested. The tests are carried out in standard sample holder as well as a perforated wall sample holder to allow for ventilation that may be present in forest litter bed.



(a) (b)

Figure 1 Comparison of Heat Release Rates of three species of Indian forest litter beds, *Azadirachta Indica* (Neem, IN), *Pinus Roxburghii* (Pine, PN) and *Monoon Longifolium* (false Ashoka, AS) of density 38 kg/m^3 in cone calorimetry tests in (a) standard sample holder (NP) and (b) perforated wall sample holder (P).

For litter bed of identical density of 38 kg/m^3, the peak heat release rate for Ashoka is lower than for the pine bed but for Neem it is as high as that for pine. The peak heat release rate is more than doubled for Pine and Neem and to less extent for Ashoka litter bed tested in perforated walled sample older. The Ashoka leaf litter when tested in perforated sample holder exhibits multiple sporadic peaks in heat release rate in addition to the peak value. This is not observed for other litter beds.

The tests are carried out for fuel bed densities ranging from 25 kg/m^3 to 75 kg/m^3 in solid walled and perforated walled sample holders and the effect of bed density on heat release rate, ignition, flaming combustion duration, smoke generation and leftover residue are discussed. Critical heat flux is also determined and found to be comparatively higher for the tropical leaf litter.

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Liquid fuels with additives of vegetable oils: ignition and combustion characteristics

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Currently, there is a steady trend associated with an annual increase in the consumption of hydrocarbon fuels for use in internal combustion engines of cars and gas turbine units of air transport. In this regard, there is a need to find alternative solutions suitable for large-scale implementation. Despite the development of electric vehicles, their technological implementation remains imperfect and, in some cases, it is not possible to abandon internal combustion engines. Therefore, one of the promising options is the development of mixed fuels based on traditional energy resources with the addition of renewable raw materials, for example, various types of oils.

In this study, blended fuels based on traditional liquid hydrocarbon fuels (gasoline, kerosene and diesel) with additives of vegetable oils (distilled tall oil (DTO), rapeseed oil and waste cooking oil) were considered. The experimental setup was a combination of a Mettler Toledo TGA/DSC 3+ thermogravimetric analyzer and a laboratory tube muffle furnace used as a combustion chamber.

Fig. 1 shows the ignition delay times for fuels based on kerosene and various oils. It has been established that the addition of oils makes it possible to reduce the ignition delay time of the studied fuel mixtures. This result is caused by the effect of micro-explosive fragmentation of mixed fuel droplets due to different boiling temperatures of the components used. Micro-explosive fragmentation significantly increases the heat exchange surface area of a fuel droplet, thereby intensifying its heating and ignition.

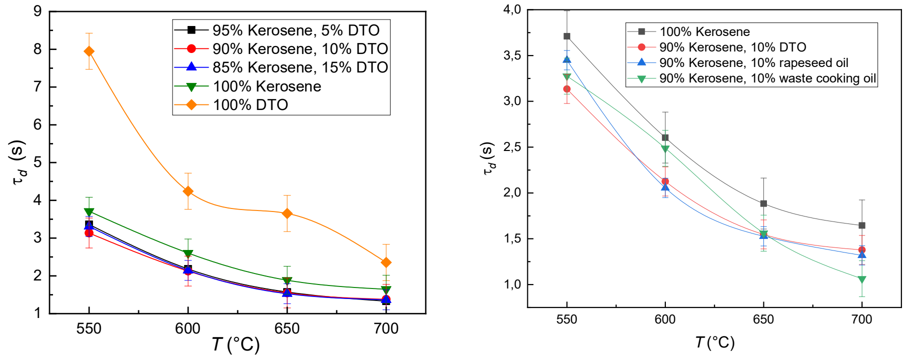

Figure1 Ignition delay times of fuel droplets depending on the temperature in the combustion chamber

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Combustion Patterns of Fire Whirl

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Fire whirl, a typical extreme fire behavior in wildland and urban fires, has received more attention over the past decade. A fire whirl is a vortex-shaped swirling diffusion flame, with significant increases in burning rate, flame temperature, and flame height, compared to a general buoyant flame of the same fuel dimension. It has been found that a fire whirl may undergo complicated combustion patterns with the change of the surrounding rotating flow. This lecture summarizes the recent research progress on the combustion patterns of fire whirl at SKLFS. In experiments, we used small-scale and medium-scale rotating screen facilities to control the imposed circulation and the fire heat release rate separately. It was found that laminar and turbulent buoyant flames within a large range of imposed circulation involve as many as nine combustion patterns. We have conducted in-depth research on the weak and conical fire whirls under weak rotation, and the cylindrical fire whirl under strong rotation.

Firstly, the linear hydrodynamic instability analysis demonstrated that the laminar and turbulent weak fire whirls form at critical dimensionless imposed circulations (Re) that depend on the heat release rates (B) by 1/4 and 1/3 powers laws, respectively. In addition, the formation of a real fire whirl also depends on the height of the initial generating eddy. Although the initial fuel velocity is low (10-2 m/s), laminar and turbulent weak fire whirls could exhibit flame lift-off behavior similar to jet diffusion flames. Stereo-PIV measurement results showed that the axial velocity followed an S-shaped distribution in the vertical direction of the lifted fire whirl. The stable equilibrium was achieved at the locations where the flame propagation velocity and the axial velocity were roughly balanced, and the axial velocity curve had a negative slope with height. For non-lifted weak and conical fire whirls, the centerline axial velocity increased by the 1/2 and 1/3 power laws of height in the continuous flame.

Second, the formation of cylindrical fire whirl is accompanied by the downward movement of the unstable flame bulge, and the propagation velocity agrees well with the predictions of the classical vortex breakdown theory. The physical analysis showed that the formation of cylindrical fire whirls would occur at specific critical values of Re/Bm, with m =1/4 and 1/3 for laminar and turbulent fire whirls, respectively. Based on the 3D instantaneous velocity field, two-celled vortex structures and central recirculation zones are found to form and move downwards with increasing imposed circulation in the plume region of cylindrical fire whirl. As the imposed circulation increases, the flame height and the centerline axial velocity at a specific height synchronously and rapidly decrease. A semi-physical flame height correlation is obtained from the radially-integrated momentum and mixture fraction equations, and a semi-physical flame width correlation is developed based on the concept of equal axial convection and radial diffusion times for the turbulent cylindrical fire whirl. The two models both couple the heat release rate and the imposed circulation, and agree well with the experimental data.

This lecture ends with a concluding discussion addressing the major challenging issues for fire whirl studies in the future.

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Formation of soot and nanoparticles in flames

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It is known that the formation and synthesis of fullerenes in the traditional method of arc evaporation of graphite and in flames are carried out at pressures below 40 Torr [1]. In [2] experiments were carried out at 40 Torr. The formation of fullerenes occurs at low pressures, and here it is important to consider the steric factor. It should be taken into account that the formation of such a graceful molecule as C_{60} requires the necessary spatial orientation of two C_{30} molecules. There are various models of C_{60} fullerene formation, one of which is realized by the zip-mechanism [3]. The necessary condition for such a mechanism is low pressures. With increasing pressure, i.e. with the transition to atmospheric and higher pressure, where triple collisions prevail, which complicates the formation of fullerenes and single-layer graphenes, the coagulation of PCAH with the formation of soot clusters occurs [4, 5].

Earlier, Bockhorn in 1994 [6] proposed a phenomenological scheme for the reaction of soot formation in homogeneous mixtures of premixed flames, where the intermediate products are PCAH. The sequence of formation of combustion products in fuel-rich flames was shown: CO, H_2, H_2O, aliphatic hydrocarbons, aromatics with the increasing number of rings, up to coronene, then nucleation of soot particles and their growth to the size of 50 nm.

Taking into account the new data PCAH can be considered as the basis for the formation of fullerenes and graphenes in the flame as precursors to the formation of soot particles. We developed a complete scheme of soot formation [4, 5].

Figure 1 shows the scheme of soot particle formation, supplemented by the stages of formation of fullerenes and graphenes. As shown in the scheme, at low pressures single-layered graphenes are formed, and at atmospheric pressure – multilayered ones.

A scheme for the formation of fullerenes, graphenes and carbon black in rich hydrocarbon flames has been developed, taking into account the pressure. It can be assumed that the synthesis in a flame of fullerenes, graphenes and carbon nanotubes is an alternative technology to the existing methods of synthesis in an electric graphite arc.

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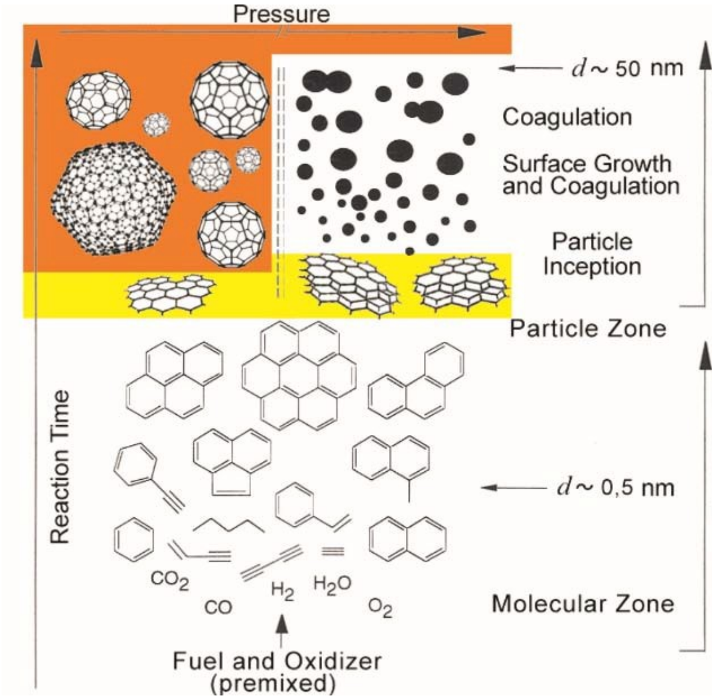

Figure1 Scheme of soot formation in a fuel-rich flame [4, 5].

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PLENARY LECTURES

Turbulent flow and flame structures in model gas-turbine combustors. Diagnostics and Control

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The present work provides a review on the current possibilities to study turbulent flows and combustion in model gas-turbine burners by using optical measurement techniques. Different existing experimental rigs provide optical access for the flames at atmospheric and realistic conditions at elevated temperature and pressure. These facilities are commonly equipped with point-wise and planar laser-based diagnostics tools for the measurements of local flow velocity, gas temperature, and main species concentration and for the visualization of pollutant formation zones (for soot and NOx). Coherent anti-Stokes Raman Scattering (CARS) and Spontaneous Raman Scattering (SRS) techniques are used for the measurements of local gas composition and temperature. The Planar Laser-Induced Fluorescence (PLIF) and Filtered Rayleigh Scattering (FRS) are now also used to evaluate the 2D distributions of temperature in a certain cross-section of the burner. For the liquid fuel combustors, the Shadow Photography technique is typically used for the visualization of spray shapes. The sizes and velocities of the droplets during the atomization of the sprays are monitored by Laser Doppler Particle Analyzers (PDA).

Nowadays, the PLIF is also commonly used for the visualization and concentration evaluation of liquid fuel droplets and fuel vapor in order to characterize the efficiency of the fuel spraying and mixing. Besides, the PLIF is also very efficient for the visualization of chemical reaction zones by exciting different kinds of molecules (OH, CH, NO, HCO, HCHO, etc.) in a selected cross-section of the flame. Solid tracer particles can be added to the flow to evaluate the velocity fluctuations in a point or 2D cross-section by Laser Doppler Velocimetry (LDV) and Particle Image Velocimetry (PIV) methods, respectively. The PIV and PLIF methods are often applied simultaneously to study the single- and two-phase combustion. A Laser-Induced Incandescence (LII) approach can be also used with the PIV and PLIF methods to visualize regions of soot formation and burnout. Besides, the LII method can evaluate the soot particles concentration in case of proper calibration.

Thus, there is a wide range of different optical techniques which have been successfully applied in the studies of model gas-turbine burners performance. They are used to understand the unsteady flame behavior, pollutants formation, possible blow-off or flash-back of the flames and also the ignition probability. In particular, unsteady combustion often appears in lean premixed burners. It is driven by a complex interaction of hydrodynamics flow instabilities, flame kinematics, fuel injection conditions, and acoustic modes of the combustor. The development of flow/flame control strategies relies on optical diagnostics of the mentioned complex interaction. The present work will provide the examples of recent studies on the unsteady combustion in swirling flows of model gas-turbine burners. Perspective strategies to control/avoid the unsteady combustion will be also indicated.

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Structure and stability of gas-phase flames in rotating flows

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Gas combustion in rotating flows attracts researcher's attention in view of creation of new industrial combustion technologies for energy production and research purposes. The industrial applications not only involve a variety of swirl combustors, like cyclone pre-furnaces, but also with explosions prevention in electrical motors, centrifugal separators, and turbo machines having cavities filled by rotating combustible mixtures. The fundamental aspects of flame-flow interaction in rotating media can be studied by using the tubular flames where the unburned mixture is injected diagonally into a cylindrical burner and the combustion products exit along symmetry axis. In the experiments or in the practical burners, the injection is made through some slits, but in the idealized model, one can suppose that mixture is injected through the whole periphery of combustion chamber with prescribed tangential and radial velocities. In the most of experimental and theoretical studies, the tubular flames had relatively small diameters, not exceeding ten centimeters. At the same time, the development of new energy technologies using large cyclone combustors, requires an investigations of large-scale tubular flames stability. One of the feature of large-scale flames is the possibility of developing hydrodynamic instability resulting in formation of large-scale perturbations. The analysis of the hydrodynamic instability of a cylindrical flame stabilized in a converging rotating gas flow simulating the flow in a cyclone combustion chamber is presented. In the stationary case, the gas flow is described by the solution for a rotating tornado-shaped vortex. The experimental measurements and the results of the theoretical modeling of the rotating gas flow in large scale cyclone is discussed.

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Numerical Simulations of Laminar Flames to understand their Characteristics

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Studies on laminar flames in various burner configurations using various fuels are important to understand their structure, stability and emission characteristics. Numerical simulations carried out using a validated numerical model will be able to provide significant insights on flow, temperature and species fields. These will be quite useful to understand the flame features and operating regime of the burner.

In this lecture, requirements of a numerical model for carrying out laminar reactive flow simulations are presented initially. These include thermal and transport data, chemical kinetics mechanism, radiation and soot models. Following this, case studies carried out using Ansys FLUENT are presented.

Characteristics of laminar flames fueled by biogas (mixture of methane and carbon-dioxide) and Liquified Petroleum Gas (LPG) are presented. Biogas is relatively non-sooty when compared to LPG. The differences in the structures of biogas and LPG flames are discussed.

Laminar flames formed over liquid MMA pool are reported subsequently. For simulating liquid fuel flames, coupling mass, momentum and energy boundary conditions are required to be specified at liquid-gas interface. The flame structures for cases with various ullages (distance from the pool surface to the burner rim) are presented. Soot generation in these cases are also discussed.

Finally, results from simulations of coal particle interaction with laminar methane-air premixed flame are presented. When coal particles of certain size and concentration are injected into laminar methane-air flames, the resultant laminar burning velocity is affected. The reasons for this observation is brought out using the numerical simulations.

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Critical conditions for micro-explosion of composite liquid droplets

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Fragmentation of inhomogeneous droplets as a result of their heating is a promising tool for increasing the efficiency of many technologies associated with the evaporation of atomized liquids. Determining the critical values of the input parameters that are sufficient to implement a micro-explosion is an important task for the effective prediction of the secondary decay of droplets and the controlled use of this phenomenon in engineering applications.

Modern physical and mathematical models of micro-explosion behavior are based on three criteria. *Criterion 1.* Overheating of the "water/fuel" boundary is based on the temperature rise in the zone of contact between the two components of the drop of the value corresponding to the state of water saturation. Overheating of the "water/fuel" contact boundary at the moment before the micro-explosion can be from 2 to 15 K. *Criterion 2.* Violation of the balance of forces on the surface of the drop. It is believed that until the moment of micro-explosion, the forces of atmospheric pressure and surface tension of the outer shell of the drop exceed the pressure of water vapor in the central part of the drop. *Criterion 3.* Critical dimensions of the drop due to its filling with vapor bubbles. In the numerical simulation of heating before micro-explosion using this criterion, it is necessary to set the interfacial transfer rate, the value of which is usually obtained from the results of experiments. The results of [1] show that the characteristic size of two-component droplets at the moment before the micro-explosion is $R=(1.2 \div 2.1)R_0$.

When choosing dimensionless criteria that would make it possible to assess the compliance of the parameters of a two-component drop with the conditions of its micro-explosion, it is necessary to take into account the most commonly used criteria for identifying this effect. Typical critical conditions for stable micro-explosion are presented in Fig. 1.

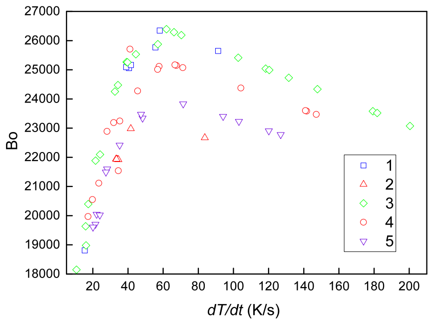

Figure 1 Values of the dimensionless criterion characterizing the growth of a vapor bubble in a two-component drop at different heating rates: 1 - Kerosene 50 vol.% - water 50 vol.%; 2 - Turbine oil 50 vol.% - water 50 vol.%; 3 - Rapeseed oil 80 vol.% - water 20 vol.%; 4 - Diesel fuel 80 vol.% - water 20 vol.%; 5 - Kerosene 80 vol.% - water 20 vol.%.

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Inorganic-Organic Hybrid Nano-materials: An Efficient Approach to Flame Retardation and Smoke Suppression for Polymeric Materials

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Over the last decade, inorganic-organic hybrid technology has attracted considerable attentions in the field of flame-retardant polymeric materials. In this context, various kinds of inorganic nano-materials like layered double hydroxide, graphene, and silica have been hybridized by organic molecules for enhancing the flame retardancy and smoke suppression of polymer composites. With a relatively low loading of inorganic-organic hybrid materials (< 10 wt%), the resultant polymer composites showed the significantly suppressed heat release rate as well as smoke and toxic gases release. For instance, the addition of 1 wt% and 3 wt% of boron nitride hybrids into the EP matrix results in the 47.2% and 53.1% reduction in PHRR, respectively. As well, epoxy composites containing 3 wt%boron nitride hybrids showed a approx. 40% reduction in smoke production rate (Fig. 1) [1]. In another study, the addition of 4 wt% melamine cyanurate/MoS_2 hybrid results in reductions in PHRR and total smoke production by 40% and 20%, respectively [2]. These studies demonstrated that inorganic-organic hybrid materials are one kind of highly efficient flame retardant in polymer composites.

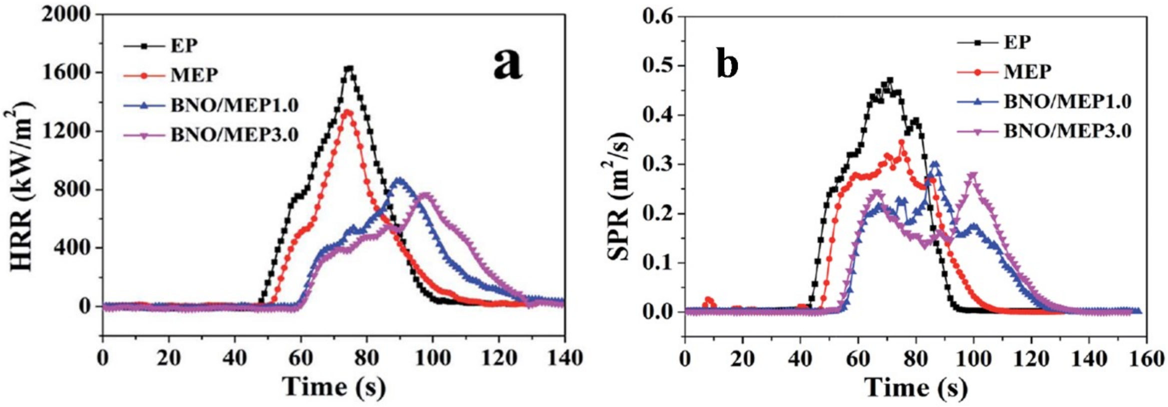

Figure 1 (a) HRR and (b) SPR versus time curves of epoxy and its composites.

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Effect of phosphorus-containing flame retardant and nanocarbon material additives on combustibility and physical and mechanical properties of composite materials based on polyimide binders

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Reinforced polymer composite materials (RPCM) are widely used in aviation, mechanical engineering, construction and many other areas of activity. The most widely used type of binder is epoxy resins, which has high physical and mechanical. However, this type of RPCM has a significant drawback – they have low temperature resistance and fireproofness. The combustion of this type of RPCM is accompanied by the release of a large amount of heat, smoke and toxic species released during the decomposition and combustion of the epoxy resin. Therefore, the improvement of the thermal stability and flammability of RPCM is important scientific task. Currently, one of the most widely used heat-resisting materials in the world are RPCM based on polyimide resins. Polyimides are a class of highly heat-resistant polymers of a heterocyclic structure, characterized by high physicochemical parameters, radiation and chemical resistance, good thermal stability in the temperature range from -150 to +350°C, and also have a relatively low cost of primary components. Despite the significant progress made in recent decades in optimizing the compositions of polyimide binders, the tasks of improving the manufacturability of processing, as well as increasing the maximum operating temperature, reducing flammability and increasing breaking strength, remain topical. One of the ways to reduce flammability of RPCM is the introduction of flame retardants of various types of action into the binder.

In order to study the effect of additives of phosphorus-containing fire retardants and nanocarbon materials, the RPCM samples based on a polyimide resin (SP-97k), glass fiber filler (glass fiber T-10-14), flame retardant additive DOPO-DDM (9,10-dihydro-9-hydroxy-10-phosphafenatrene-10-oxide-4,4'-diaminodiphenylmethane) and graphene nanoplates was prepared. To determine the flammability of the studied composites, the following tests were carried out: thermogravimetric (TG) analysis, limiting oxygen index (LOI), UL-94 and FAR-25. The strength characteristics of RPCM were also studied: modulus of elasticity, ultimate tensile strength, ultimate compressive strength, relative elongation at break, etc.

As a result of the research, new fire-resistant glass-reinforced plastics with a high LOI have been developed, which have already been introduced into the design of experimental aviation equipment, and can also be used as advanced structural materials, including in aviation and railway transport, as well as for building industry.

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Study of the Electrochemical Characteristics of a CH_4/H_2 Diffusion Flame

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Currently, the development of gas turbine systems capable of operating efficiently on mixtures of hydrocarbon fuel with hydrogen in the concentration range of 0...100% hydrogen in the fuel mixture is becoming relevant. However, to successfully meet these requirements, a radical change in the combustion chamber architecture will be required, since the vortex flame stabilization commonly used in gas turbines powered by natural gas can be disturbed by the addition of hydrogen. The development of new approaches and the search for technological solutions are required, which is impossible without a detailed study of the physical mechanisms of composite gas fuels combustion. The purpose of this work is to study the effect of dilution of methane with hydrogen on the physicochemical and electrical characteristics of diffusion jet flame.

The diffusion flame was formed when a laminar fuel jet flowed out of a quartz tube with an inner diameter of 3 mm. Two electrodes were placed symmetrically with respect to the jet axis at a height of 10 mm from the edge of the tube. The distance between the electrodes was 11 mm. The electrodes were cylinders 5 mm in diameter, the end of which was either conical with an opening angle of 45° or hemispherical, and located outside the flame front. The power supply (U=1.5 kV) operated in a repetitively pulsed mode with a frequency f=2 Hz and a duration $\Delta\tau \sim 15$ ms. The current flowing through the flame was recorded on an oscilloscope. The value of the average current per pulse in dimensionless form $\overline{I} = \frac{I - I_{H2}}{I_{CH4} - I_{H2}}$ was analyzed, where I_{H2} – is the average value of the current flowing during the combustion of pure hydrogen, and I_{CH4} – in the case of combustion of pure methane. When averaging, the regions of transient on/off processes were excluded.

For mixtures with a molar fraction of methane above 40%, the value of the flowing current depends linearly on the composition. This may be due to a change in the rates of chemionization reactions upon the addition of hydrogen. Note that during the combustion of hydrocarbons, the concentration of charges exceeds the equilibrium one by 3-4 orders of magnitude. Dilution with hydrogen with a molar fraction of methane in the mixture less than 40% leads to the fact that the dependence of the current on the composition becomes non-linear. In this case, the boundary of the transition from a linear dependence to a nonlinear one does not depend on the flow rate and the shape of the electrode. The results obtained indicate the existence of two regimes in which a significant difference in the kinetic mechanisms of diffusion combustion of a CH4/H2 mixture is possible.

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Modeling of the droplets cluster parameters at suppression fire by aviation technology

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The deposition of a cluster of droplets in a high-temperature gaseous medium is realized when the refrigerant is dropped into the fire from the aircraft. The volume of liquid released into the atmosphere breaks up into drops as a result of hydrodynamic instability. The droplet size depends on the physicochemical properties of the liquid and the parameters of the surrounding atmosphere. When a liquid-droplet aerosol cloud settles in a gravity field, it evolves, during which the shape of the cloud, the velocity of the center of mass, concentration, shape, size of drops, and other parameters change. The change in the characteristics of the aerosol cloud occurs due to the processes of dynamic interaction of droplets with the medium, coagulation and crushing of droplets in mutual collisions, as well as due to evaporation of droplets in a high-temperature environment.

This report presents the results of an experimental study of the regularities of gravitational settling and evaporation of a compact cluster of drops in a high-temperature environment, as well as a mathematical model for calculating the density of surface irrigation when a refrigerant is released into a fire. The dynamics of a liquid-droplet aerosol cloud is considered as the movement of a polydisperse cluster of droplets, taking into account the strength and direction of the wind, as well as an ascending convective column above the fire. This model in the Cartesian coordinate system is described by a system of equations including the equations of motion of droplets of each fraction, their heat exchange with the environment and the change in the size of the droplet due to evaporation.

Using the proposed model, including the experimentally obtained approximation dependences of the cluster parameters, a numerical study of the surface irrigation density during the discharge of refrigerant from the aircraft into the fire was carried out. It is determined that the length of the wetted surface is most influenced by the length of the primary cloud of droplets, and the smallest is the initial velocity of droplets and the distribution of wind speed in the atmosphere. It is determined that an increase in wind speed leads to an increase in the flight range of droplets of small and medium fractions, and, consequently, to an increase in the density of irrigation of the surface due to the ingress of droplets of large and medium fractions into the fire zone. Comparison of the results of mathematical modeling of the effect of aircraft flight parameters on the characteristics of the ground distribution of irrigation density and dispersion of water aerosol with experimental results confirms the possibility of using the developed model to determine effective conditions for extinguishing fires in various flight modes, as well as when using different types of aviation equipment.

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Composition solutions and regularities of pasty propellants burning

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One of the possible directions for improving chemical engines is the use of paste propulsion. Such engines have smaller weight and size characteristics and a higher level of reliability at similar costs in comparison with liquid propulsion systems and a higher energy potential in comparison with solid propellant propulsion systems.

A pasty propellant based on the following components has been developed: polyethylenepolyamine perchlorate plasticized with ethylene glycol, ammonium perchlorate (AP), octogen, and aluminum.

The quality of the propellant is largely determined by the characteristics of the burning process. With regard to the propellant under consideration, these characteristics include the burning rate law and the parameters of the agglomeration process. A study was made of the influence of various composition solutions on these characteristics.

These decisions do not affect changes in the content of the main components of the propellant. These solutions include the use of various additives and changing the particle size of the AP. The research was based on the experimental determination of the following characteristics of the burning process: fraction of original metal in the propellant used to form the agglomerates as a whole (Z_m^a); mass fraction of oxide in agglomerates; size distribution functions of agglomerates; burning rate (r_b). The pressure range (P) was 0.4–7.0 MPa.

The results obtained made it possible to establish the following. Composition solutions provide a change in burning rate law and the characteristics of the agglomeration process. The absolute value of the burning rate can change more than twice, the index ν in the burning rate law ($r_b=u_1\cdot P^\nu$) is in the range of ~ 0.2. The Z_m^a parameter can also change by more than a factor of two.

A research of the structure of propellants was carried out, within which the characteristics of such structural formations as "pocket" and "inter-pocket bridge" were determined. It is shown that the burning rate is affected by the number and size of "pockets", as well as the possibility of formation of a skeleton layer (SL) within them.

The presence of a peculiar of "pocket" mechanism of agglomeration for the investigated propellants has been established. When this mechanism is implemented, one agglomerate is formed within each “pocket”. However, the degree of involvement of the metallic fuel in the formation of the SL, and, consequently, of the agglomerates, depends on the size of the "pockets" and the value of the pressure.

The established regularities can be used to determine the optimal composition of propellant for engines for various purposes.

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Influence of size and morphology of titanium powder on agglomeration in composite model propellants

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Specific application of the technological combustion of titanium particles in air can be a pyrotechnic "generator" for creating a cloud of photocatalytic titanium dioxide in order to purify atmospheric air from local pollution with toxic substances. It is known that titanium, like aluminum, agglomerates in the combustion wave of a pyrotechnic mixture system, at elaborating this idea, problems arise similar to those that are solved for traditional aluminized rocket fuels. Namely, it is necessary to ensure sufficiently complete combustion of the agglomerated metal and its efficient transformation into a highly dispersed oxide with the required properties.

This study is aimed at increasing the yield of target products such as highly dispersed oxide particles. The results provide the basis and ideas for the development of propellant formulations intended for the generation of oxide aerosol by the "pyrotechnical" method. As a metallic fuel, we recommend using porous spherical titanium as small as possible.

For the first time, we studied porous titanium particles with sizes in the order of hundreds micrometers. Porous spherical particles were obtained by rolling in an AGO-2 ball mill and they can be considered as a new type of titanium metal fuel.

The combustion characteristics of composite propellants were studied. The component composition of the propellants included 20% energetic binder, 60% ammonium perchlorate (AP, sieve fraction 180–250 µm), and 20% titanium powder. The fuel-binder is a methylpolyvinyl-tetrazole polymer plasticized with a nitroether-nitramine plasticizer. We used two types of titanium in the propellants: industrial grade PTM and porous rolled titanium with variable fineness in the particle size range of 32–500 µm. The combustion of composite propellants based on AP, an energetic binder, and titanium powder with a particle size of 32–500 µm was studied. It was established that the smallest sizes of agglomerates are formed from titanium powders of the smallest sizes. The smallest sizes of agglomerates were registered in the case of propellants containing PTM grade titanium powder with a fraction of <32 µm and porous titanium with a fraction of <71 µm.

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Modeling of the combustion of a PMMA sphere

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Polymethyl methacrylate (PMMA) is a synthetic polymer of methyl methacrylate (MMA, $C_5H_8O_2$), a thermoplastic transparent plastic widely used in industry, construction and everyday life. Due to its properties (transparency, resistance to moisture and microorganisms, electrical insulating properties) it is used as a structural, optical and decorative material. Its disadvantages include its low heat resistance. At temperatures above 200$_0$C, PMMA depolymerizes to form a monomer - MMA. Therefore, the study of fire propagation over the surface of such polymers is an important task. CFD (Computational fluid dynamics) - modeling is an accurate and currently available way to conduct such studies.

The aim of this work is to study the propagation of flame along a curved PMMA surface under conditions of free convection. The object of research was a sphere made of cast PMMA with a diameter of 40 mm. The flow calculation was performed on the basis of the complete system of Navier-Stokes equations for a multicomponent mixture, supplemented by a detailed chemical-kinetic mechanism taking into account heat transfer, convection and radiation in the ANSYS Fluent software package [1].

A coupled kinetic model has been developed that includes the surface reaction of PMMA pyrolysis and the reduced kinetic mechanism of gas-phase combustion of its methyl methacrylate (MMA) monomer. To optimize the calculations, the kinetic mechanism [2] was reduced. The chemical transformation of flame components was described by a kinetic model including 29 components and 44 reactions. The mechanism reduction procedure was carried out using the Mechanism Workbench software package (Kintech Lab) [3]. Satisfactory agreement between the experimental data and the results of 3D modeling of the chemical and thermal structure of the flame indicates the effectiveness of the proposed reduced chemical-kinetic model. This mechanism can be applied to describe the combustion of other objects, in particular, the combustion of PMMA slabs.

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Microwave controlled ignition, combustion and extinguishment characteristics of ADN-based ionic liquid propellant in single mode resonator

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ADN-based liquid propellants have attracted wide attention for its high performance, low toxicity, low cost and so on. The continuous progress of space exploration puts forward higher requirements for liquid propellant ignition methods. At present, catalytic combustion is mainly used in ADN-based liquid space motors. However, the working process of the ADN-based liquid space engine heavily depends on the catalytic decomposition process of the propellant in the preheated catalytic bed. Microwave ignition has received much attention in recent years and is promising to solve the problem of storing fuel and oxidizer separately in liquid motors. Different with traditional ignition methods, microwave radiation could interact with the material as a whole by penetrating the material. To date, research focuses on the microwave ignition of solid energetic material, mainly nanothermite. Compared with solid materials, liquid materials (especially ionic liquids) are natural microwave receptors on account of excellent molecule polarity, which could rotate hundreds of millions of times per second at typical microwave frequency (2.45GHz). Microwave can directly activate ionic structure in the liquid mixture, so that the material could be heated quickly and evenly and make the ignition possible. Meanwhile, the conductivity of IL also makes them heat up rapidly due to the resistance heating.

In this paper, to maximize the advantages of microwave heating, two kinds of ILs: ADN and 1-allyl-3-methylimidazolium dicyandiamide ([AMIM][DCA]) are used as oxidant and fuel of liquid propellant respectively. By varying the ratio between fuel to oxidizer, the most suitable propellant formulation which could be ignited by microwaves was found. Microwave-controlled and repetitive ignition and combustion of ADN-based propellant was achieved firstly in a customized single mode resonator. The result showed that the ignition process could be divided into two stages: ionic liquid propellant was first heated up and decomposed rapidly after absorbing electromagnetic energy, producing a lot of oxidizing and reducing gases into the air. Then gas phase ignition occurred and the flame quickly spread into the IL propellant. The ignition delay time decreased rapidly with the increase of power and stabilized within a fixed range finally (hundreds of milliseconds), while the extinguishment delay time under different power was relatively stable. In the case of repeated ignition at the same power, the subsequent ignition delay time decreased rapidly due to the previous heating of the system. This discovery is of great significance for further expanding the application of liquid propellant motors in the field of aerospace propulsion.

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The formation of water aerosol in an artificial analogue of the natural ball lightning

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A special type of pulsed electric discharge above water surface was detected in 2000 in the town of Gatchina. Since the discovery, this type of discharge attracts researchers' attention because a brightly glowing ball-shaped object (called plasmoid) is formed during the discharge. The lifetime of the glowing ball is rather long, reaching 0.6 s, while the typical time of galvanic contact of the formed plasmoid with the electrodes is about 0.1 s.

The results obtained in the studies of this formation, obtained in the laboratories of different countries, are discussed in the report. The major attention will be paid to the results of experimental studies carried out using the discharge set-up that was mounted at the ICKC SB RAS, to answer, by studying laser radiation scattering in the plasmoid, whether the aerosol is present in the plasmoid, and what its chemical composition and particle size distribution are.

The results of these studies show that laser radiation is clearly observed to be scattered by the aerosol particles of various sizes when a laser beam passes through the plasmoid. It has been established that the interior of the plasmoid is filled with water aerosol comprised by two fractions: one of them is composed of the particles of submillimeter size range, while the other contains medium-sized aerosol. The total volume of water aerosol particles in the plasmoid is estimated to be several cm^3.

In the report, several glow mechanisms are discussed for the object under investigation. There is hope that the results of this work will allow us to achieve advanced understanding of the processes that take place not only in plasmoids under consideration but also in natural ball lightnings.

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Investigation of particle size distribution in the condensed phase of the products formed in the combustion of energy-yielding materials using aerosol-based and optical methods

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Attention to the studies of the condensed phase (c-phase) arising during the combustion of energy-yielding materials serves as an impetus to upgrade and develop new experimental methods for its investigation. The particle size distribution and mass concentration of the c-phase formed in the combustion of energy-yielding materials, namely model fuels containing aluminium and boron, were studied with the help of measuring equipment designed and built at the ICKC SB RAS. The complex of equipment included the diffusion spectrometer of aerosol DSA-M, optical aerosol spectrometer, nephelometer, and optical microscope with a knife. The studies were carried out at atmospheric pressure and at increased pressure in a high-pressure closed vessel. The set of equipment allows us to determine particle size distribution, as well as the mass concentrations of the suspended dispersed phase within broad particle size and pressure ranges.

An experimental set-up for the studies of the combustion of solid fuel particles in the flame of a Bunzen burner has been also developed at the Institute of Chemical Kinetics and Combustion SB RAS. The parallel simulation of particle combustion in the flame of the burner allows us to compare the results of experimental observations and theoretical calculations for the purpose of modifying combustion models and their verification on the basis of the data obtained experimentally.

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Improving the prediction of C_3H_3+ abundance in hydrocarbon flames: theoretical, kinetic modeling and mass spectrometric analysis

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The flame is a weakly ionized plasma. Understanding the behavior of ions in flames is momentous for the development of new diagnostic methods and new ion-sensitive technologies for controlling combustion processes. In this work, the chemistry of $C_3H_3^+$, a key cation in fuel-rich flames, was revisited. The ion chemistry mechanism proposed earlier [1] involving cyclic $C_3H_3^+$ isomer only was augmented with the reactions for the linear isomer (l-$C_3H_3^+$). The thermochemical data for l-$C_3H_3^+$ were calculated and the reaction pathways of formation and consumption of both isomers were re-examined using the high-precision methods of quantum chemistry CCSD(T)-F12. The potential energy surface was constructed and the enthalpies of these reactions were calculated. It has been demonstrated that the role of reactions $C_3H_3^++H_2O=C_2H_3O^++CH_2$ and $C_3H_3^++H_2O=H_3O^++C_3H_2$ in the original mechanism is overestimated. The mechanism was improved accordingly and numerical calculations of the cationic structure of methane and ethylene flames, which were investigated experimentally earlier [1, 2], were performed using the Cantera software (V.2.6.0) [3]. The updated mechanism was demonstrated to correctly predict the relative mole fraction of the $C_3H_3^+$ and other key cations. It can be used as a basis for further development of the kinetic mechanism capable of describing formation of cations in fuel-rich hydrocarbon flames.

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Time Scale Analysis in a Laminar Methane-Air Flame

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The quality of predictions and modeling of flame propagation, acceleration and extinction depends on the knowledge of many regularities and, in particular, on the ratio of the gas-dynamic time scale to the characteristic flame time scale or the Damkëller number. In order to reveal the regularities that determine the interaction between the processes of molecular transfer and chemistry in the case of flame front deformation, we performed numerical calculations of the dependence of the characteristic time scale on temperature in an axisymmetric Bunsen flame. The results of calculations with one-stage kinetics were compared with experimental data. Time scale analysis was carried out by processing the vector field of velocities and calculating the dependence of the measurement of the local velocity of propagation of a laminar methane-air flame with $\varphi=1$ on the local strain rate. The experimental velocity field in the flame was measured by recording and processing stroboscopic images of particles in a selected flow section using the PIV system POLIS. The system consisted of two pulsed Nd:YAG lasers (wavelength 532 nm, pulse duration 5 ns, pulse energy 50 mJ, beams aligned to one axis), CCD camera (1360×1024 pixels, size of each pixel 4.65x4.65 μm) with 2-frame shooting function, Tamron SP AF 180 mm optical lens, sync processor and PC with “ActualFlow” software. To calculate the displacement of particles in the interval between a pair of laser flashes (100 μs), an adaptive iterative cross-correlation algorithm was used with a continuous displacement of the computational regions in the first and second frames. An analysis of the characteristic time scales of thermal conductivity, diffusion, and chemical reaction showed that the characteristic time of a one-stage reaction is several times longer than the time of preheating and diffusion of methane. With an increase in the initial temperature of the combustible mixture, the time scale of a chemical reaction becomes comparable with the times of molecular process.

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Determination of the minimum fire extinguishing efficiency of the powder by the pneumatic pulse method

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The topic of fire safety does not cease to be relevant throughout the ages. An important element of the fire prevention system, which should be created by a labor protection specialist at the enterprise, are portable fire extinguishers with powder extinguishing agents. For powder fire extinguishers, a mixture of an inert powder with various inhibitors in the form of metal salts, phosphorus and chlorine compounds, which in this case are called active additives, is used. A huge number of works have been devoted to the study of flame suppression by various fire extinguishers. The difference in the effectiveness of the action of one or another substance can reach more than tens of times. The aim of the work was to compare the normative, real and laboratory efficiency in extinguishing the flame of fire extinguishers. To assess the extinguishing ability of fire extinguishers from various manufacturers, as well as to test methods for enhancing the action of a shale barrier used in coal mines, in this article, a pulsed method of controlled pneumatic injection of powder into a class B microfire with an effective burning area of ~0.00636 m^2 was used. A numerical analysis of the movement of particles and gas was carried out using the pneumatic pulse method for determining the efficiency of the powder extinguishing agents using the Ansys CFX program. In the model, an air flow with a mass flow rate of 1.2 g/s and solid particles with a flow rate of 0.01 g/s exit from the outlet nozzle located above the microfire. The particle diameter varied. It was shown that a cloud of smaller particles moves in a wide jet, while large particles move in a narrow core, however, almost all particles pass through the microfire seat zone with an average speed of about 2 m/s. The presented research results showed that the normative, real and laboratory efficiency of powder fire extinguishing compositions are in good agreement. It was also shown that the difference in the extinguishing efficiency of different manufacturers can reach 2 times.

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Numerical Modelling of Filtrational Combustion Process in a Cylindrical Porous Layer With Axial Gas Supply

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The filtrational gas combustion in a chemically inert porous media allows create an intensive radiative heat fluxes compared with radiation from free flame. Other advantages of filtrational gas combustion burners over combustion systems with free flame are the higher burning rates, increased power dynamic range, extension of the lean flammability limits, and the low emissions of pollutants. Extensive experimental and numerical works were carried out and are still underway, to explore the feasibility of porous burners with filtrational gas combustion for energy production and others applications.

The filtration gas combustion in a cylindricalporous layer with injection of a combustible mixture through the end surface of a porous cylindrical tube is theoretically studied. The simulation of the filtration gas combustion was carried out in the framework of the two-temperature thermal-diffusion model. The influence of the gas flow rate , and the heat losses on the surfaces on the flame stabilization were studied. Comparison of the obtained results with experimental data showed a good agreement. High levels of radiative heat fluxes and wide range of operation condition with stable combustion shown feasibility of application of this type of porous burners for contactless treatment of different materials and fluids. This type of porous radiant burner can be used, for example, as a heat source for the thermal conversion of low-calorie liquid fuels. In this case, the optimization problem can be formulated as achieving the maximum conversion efficiency of the heated fuel. Another potential application may be the creation of a given field of thermal radiation, for various technological processes, for example, in the manufacture of glass. In this case, the optimization problem must take into account the conditions imposed by the applied technologies in order to achieve maximum efficiency. We hope that this work will contribute to the creation of new energy-efficient technologies. Further theoretical and experimental research in this direction will make it possible to formulate and refine a mathematical model depending on the field of application of the proposed type of radiant burner.

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MBMS probing n-heptane and toluene flames at elevated pressures

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This work involved experimental and numerical investigation on the combustion chemistry of the typical model components of diesel fuel (n-heptane and toluene) at pressures above atmospheric. The chemical structure of laminar premixed flames of n-heptane/oxygen/argon and toluene/oxygen/argon mixtures (φ=1.0 and 1.5, with 80% argon dilution) stabilized on a flat flame burner was studied at pressures ranging from 2 to 6 atm. For delivering and vaporizing of the liquid fuel at high pressures a new system was specially designed. The burner was located in a high-pressure chamber, which was connected to the flange of a molecular beam mass spectrometry (MBMS) setup with soft electron impact ionization. Gas sampling from the flames was performed via a conical quartz probe (~30 μm orifice diameter). The operating elevated pressure in the chamber was built up by nitrogen.

The CRECK mechanism was used as the basic kinetic model, and it was improved on the basis of modern data. Particularly, attention was paid to the chemistry of acetylene. The rate constants for the following reactions were revised:

$$C_2H_3+HO_2\leftrightarrow C_2H_4+O_2$$
$$C_2H_4+O\leftrightarrow CH_2CHO+H$$
$$C_2H_4+O\leftrightarrow CH_2+CH_2O$$
$$C_2H_4+O\leftrightarrow CH_3+HCO$$
$$C_2H_4+OH\leftrightarrow C_2H_3+H_2O$$
$$C_2H_2+H(+M)\leftrightarrow C_2H_3(+M)$$
$$C_2H_2+O\leftrightarrow CO+CH_2$$
$$C_2H_2+O\leftrightarrow HCCO+H$$

A total of 9 flames were investigated. New data on the mole fraction distribution of reactants (n-heptane, toluene, O_2), major products (H_2, H_2O, CO, CO_2), stable and labile intermediate compounds, including radicals H, OH and CH_3, were obtained. The improved kinetic model adequately described the measurement results.

The pressure variation exerted different effects on the maximum concentration of key components in the flame, but there is an overall tendency towards decrease. The maximum mole fractions of several C_2-C_5 intermediates were analyzed based on the utilized model and the obtained data. Special attention was devoted to the formation of indene and naphthalene as the precursors of heavier PAHs.

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Study of the kinetics of the thermochemical transformations of the energetic nitrogen-containing nickel complexes

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Energetic nitrogen-containing nickel complexes are promising components of gas-generating systems, which can be used in airbag inflators and fire suppression, and also for increasing the efficiency of marginal wells [1]. These compounds have been chosen due to their balanced composition, simultaneously containing anions-oxidizers and energetic ligands coordinated by the metal ion. Their high-temperature interactions result in the evolution of a large volume of gas.

The objects of this study were nickel complexes with ethylenediamine and imidazole as ligands and nitrate and perchlorate anions as counterions. The aim of this work was to establish the kinetic regularities of thermochemical transformations of these complex compounds under different heating rates based on the thermal analysis data, including in combination with the mass spectrometric analysis of evolved gases. It was shown that the use of the genetic algorithm results in the most accurate descriptions of thermolysis kinetics [2]. Moreover, combining it with the Nelder-Mead algorithm considerably decreases the time it takes to find a satisfactory result, which describes the experimental data with the highest accuracy. The acquired kinetic models were compared with the results obtained using the traditional kinetic description methods of Coats-Redfern, Horowitz-Metzger, Ozawa and Kissinger. Contrary to these methods, modeling using the genetic algorithm allowed revealing simultaneously occurring stages of the thermochemical transformations and determining their activation energies when varying the heating rate. Thus, it was established that the thermal destruction of these complexes undergoes several stages: (I) partial elimination of ligands from the nickel coordination sphere; (II) oxidation of the rest of the ligands by the anions-oxidizers; (III) high-temperature thermolysis of the products of the incomplete destruction of ligands under an inert atmosphere or their oxidation by oxygen in the flow of air. It was demonstrated that the ethylenediamine complexes of nickel have a higher activation energy than the imidazole complexes, supposedly due to the chelating bond. Moreover, the effect of the anion on the kinetics of the thermochemical transformations was shown, and it was noted that the nickel complexes with the perchlorate anions in the outer sphere are characterized by a higher activation energy of the thermal decomposition.

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Growth and transformation of soot particles in a flat laminar flame

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It is known that soot particles have a significant effect on the Earth heating, reducing the albedo of the planet's surface; cause the risk of respiratory diseases when penetrating the human respiratory tract and are raw materials in the production of rubber, lacquers and enamel. However, the structure and properties of soot particles may differ significantly depending on the conditions of their formation, such as the exposure time, reactor type, fuel mixture, temperature, etc. Thus, accurate knowledge of soot particle properties s is necessary for an adequate assessment of climate models that take into account the effect of soot on global warming; for calculating heat and mass transfer in combustion chambers and engines using hydrocarbons as fuel, and for optimizing the synthesis of carbon black, which will be involved in the production of rubber, enamel, etc.

The paper presents the results of an in-situ study of the optical and thermophysical properties of soot particles, as well as the results of an ex-situ study of their structure and chemical composition. As a reactor for the synthesis of soot, a standard McKenna-type burner was used, forming a pre-mixed flat laminar flame. The height above burner in this case is an analogue of the time of chemical reactions occurring in the reactor, including various stages of formation and growth of soot particles. Acetylene, propylene and ethylene with dimethyl ether additives (0-30%) were used as hydrocarbon in fuel mixtures with a different tendency to soot formation.

In-situ diagnostics of soot particles in the flame was carried out by optical methods of laser-induced incandescence (LII) and laser extinction (LE). The LII method at wavelengths of 532 and 1064 nm allowed to obtain data on the refractive index function of soot, on the sublimation temperature and on the coefficient of accommodation of ambient gas molecules on the surface of particles. The LE method, carried out in the wavelength range of 405-850 nm, allowed to obtain parameters such as the optical band gap and the dispersion coefficient of soot particles.

To analyze the reasons of changes in the properties of soot depending on the conditions of their formation, the internal structure and morphology of particles under these conditions were analyzed. For this purpose, soot particles were sampled at different heights above burner. The samples were investigated by transmission electron microscopy (TEM) and by Raman spectroscopy. They were used to obtain data on the parameters of the internal structure of soot (particle size, length and curvature of graphene planes, the average distance between graphene planes) and data on the chemical composition of particles (the ratio H/C).

The main conclusions of the study are the generalized dependences of the optical and thermophysical properties of soot particles depending on the conditions of their formation, as well as the determination of the parameters of the particle structure responsible for changing their properties.

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Research on Characteristics of Thermoacoustic Instabilities in Air-Methane-Ammonia Premixed Swirl-Stabilized Combustors

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As an excellent hydrogen carrier, ammonia is a very good clean energy source. However, due to the poor combustion performance of ammonia, other fuels can be blended to improve the combustion performance. In this paper, the combustion characteristics of ammonia/methane composite fuel and analyzed, and the ability of ammonia/methane ratio to alleviate the thermoacoustic instabilities of burners is discussed, which is of great significance for the development of low-emission and high-reliability combustors.

In this study, the pressure and heat release rate oscillation characteristics in the combustion chamber, and the evolution of the flame surface driven by velocity perturbation are investigated. The flow shape and instantaneous OH profile are measured with high-speed camera and OH-PLIF technique, respectively. Analysis shows that its vibration pattern and frequency are similar to the axial first-order acoustic mode; both the heat release rate and the pressure fluctuate at the same frequency. The inlet velocity perturbation leads to the reciprocating retraction and expansion of the flame front as well as the further change of the flame wrinkle. The spatiotemporal varying in the flame surface area are the key mechanism for driving the fluctuation of the heat release rate. When the swirling flame interacts with the combustor wall, the flame surface will be broken out, and the flame surface area will be extended to the maximum.

In addition, the stoichiometric ratio and ammonia/methane mixing ratio have a great influence on the thermoacoustic instability of premixed swirl combustion. As the equivalence ratio changes from the lean to the rich, the burner undergoes a transition process: from the stable combustion, quasiperiodic oscillation, limit cycle oscillation, quasi-periodical oscillation, until the stable combustion. Blending ratio mainly change the flame heat release power, flame shape, flame propagation velocity and the interaction between the flame and the combustor wall. As the ratio of ammonia gas increases, the burner changes from limit cycle oscillation to the stable combustion, and the flame heat release power also decreases.

Therefore, blending ammonia in methane is a good attempt to alleviate thermoacoustic coupling, and optimizing the overall airflow velocity, equivalence ratio and blending ratio is the key to get the best performance.

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Experimental study of filtrational gas combustion at the pore scale in a one-layer burner

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Nowadays, filtrational gas combustion is considered as a promising approach towards eco-friendly and efficient technologies of fossil fuel utilization in energy-related applications. Conductive and radiative heat recirculation through the solid matrix results in such advantages as extension of flammability limits, increase of the burning rate, and reduction of pollutant emissions. Although, many aspects of macroscopic flame behavior inside the inert porous media have been studied by means of experimental, numerical and theoretical methods, there is a gap in fundamental knowledge on the flame structure inside the porous media and its behavior at the pore scale.

In this work we propose novel design of optically accessible one-layered model porous medium aimed to make up for the deficiency in experimental data on flame dynamics at the pore scale. The burner consists of the one layer of solid balls sandwiched between two transparent quartz plates. Dynamical behavior of filtrational combustion wave inside the burner has been registered by photo camera, high speed camera and IR camera.

The results demonstrate that upstream flame propagation is accompanied with significant (hundreds of degrees Celsius) variations of the solid matrix temperature and the flame front can break up on separate fragments which subsequently rejoin. Herewith the average flame propagation velocity at large time intervals is nearly constant for the given mixture equivalence ratio and flow rate. Macroscopic propagation of the filtrational combustion wave in the upstream direction is accompanied with noticeable oscillations of the flame at the pore scale. Two different types of such oscillations can be distinguished, that are FREI-like pulsations and small-amplitude oscillations. The mechanism of FREI-like pulsations is identical to the flames with repetitive extinction and ignition in narrow channels with external heating. The small-amplitude oscillations are, apparently, have the same nature as the transitional oscillatory combustion mode between the steady flame and fully-developed FREI pulsations. It is found that these two types of flame oscillations clearly separates by oscillation frequencies and amplitudes. Typical frequencies of FREI-like pulsations are about tens of hertz, while for small amplitude oscillations it has an order of hundreds of hertz. Such oscillations can induce significant sound emission frequently accompanied the process of filtrational gas combustion.

Typical patterns of non-stationary flame behavior as well as relations between flame dynamic at macroscopic and pore levels was distinguished and generalized. Wide possibilities of modification of the proposed experimental system make it perspective for further research and verification experiments requiring studies of flame dynamics at the pore scale.

The research was carried out within the state assignment of Ministry of Science and Higher Education of the Russian Federation (state registration number 121030500154-2). The part of the work related to the high speed filming was carried out using the equipment of the Equipment Sharing Center "Mechanics" of ITAM SB RAS.

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SHS powder Ni-Al alloys of rounded shape

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Alloys based on NiAl, Ni_3Al intermetallic compounds have a unique combination of strength and oxidation resistance up to 1300°C, which allows them to be effectively used as part of the protection of combustion chambers, gas turbine blades, radiation burners and other high-temperature devices. In modern additive manufacturing of structural parts (SLM, EBM technologies), powder alloys with rounded particles are in great demand, which provide increased values of fluidity and bulk density of the material when it is laid in deposited layers. Traditional SHS methods make it possible to energy-efficiently obtain various dispersed intermetallic compounds, however, in most cases, the synthesized particles have an angular shape and, as applied to SLM, EBM, additional plasma spherization is required. In order to modify the morphology of the synthesized Ni-Al alloys, in this work, we studied SHS with the participation of fluid-forming additives $CaCO_3$, $Ca(OH)_2$ to the Ni+Al reaction mixture. Powder alloys were prepared according to the following scheme: SHS → grinding of the product in a vibrating grinder → washing the material in 10% HCl and distilled water. It is shown that an increase in the concentration of additives (β) initially leads to coarsening of material particles from $d_{90} \sim 0.1$ mm to $d_{90} \sim 0.3$–0.6 mm and a subsequent decrease in their size to $d_{90} \lesssim 0.1$ mm up to the SHS limit. In the region of $\beta > 10$ wt %, intermetallic compounds of various compositions ($L1_2Ni_3Al$; $L1_2Ni_3Al$ – $B2NiAl$ – $L1_0NiAl$) were synthesized, differing from $\beta = 0\%$ in the round shape of the particles (figure) and 1.6 times increased fluidity of the powder material. Based on video recording data, thermocouple and pyrometric temperature measurements, physicochemical studies of the final and quenched reaction products, an analysis of the mechanism of influence of $CaCO_3$, $Ca(OH)_2$ on the formation of the structure of intermetallic particles in the SHS wave was carried out.

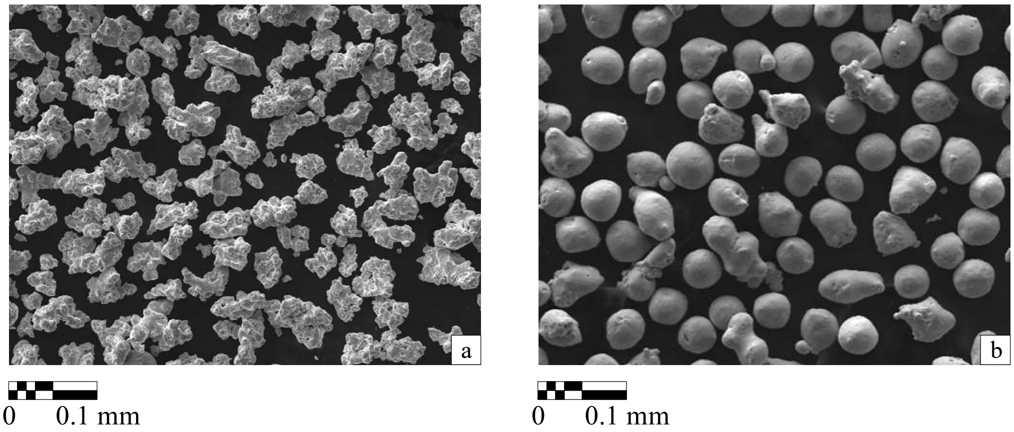

Figure 1 Morphology of Ni-Al powder alloys synthesized in Ni+20wt%Al (a) and (Ni+20wt%Al) + 18wt%$CaCO_3$ (b) mixtures.

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Modern Predictive Quantum Chemical Calculations for Thermochemistry and Decomposition Kinetics of Energetic Materials

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Highly accurate theoretical values of bond energies and activation barriers of primary decomposition reactions are crucial for reliable predictions of thermal decomposition and detonation-related phenomena of energetic materials (EM). However, due to the prohibitive computational cost, high-level ab initio calculations had been impractical for a large number of important EMs of medium size, including, e.g., CL-20. The widely used DFT calculations very often could not provide the uniform “chemical accuracy” (~1 kcal/mol) and, ultimately, the convincing mechanistic evidence on the decomposition pathways of important EMs.

Here we report on the advantages in the theoretical thermochemistry and kinetics of EM achieved with the use novel local modifications of the coupled cluster (DLPNO-CCSD(T)). These render feasible high-accuracy calculations on caged polynitroamino and polynitro EMs, e.g., CL-20 and octanitrocubane (ONC). For all important species studied, the obtained values of bond energies are at least 10 kcal/mol more accurate than those reported in the literature so far. We also studied in detail the gas-phase thermochemistry of novel high-energy polynitro derivatives of 5/6/5 heterocyclic frameworks comprised of fused tetrazine and two triazole or pyrazole rings. To this end, we proposed and benchmarked a “bottom-up” approach. First, highly accurate multi-level procedures W2-F12 and/or W1-F12 in conjunction with the atomization energy approach were utilized for smaller species. In turn, for medium-sized species (up to 24 non-H atoms), these values were complemented with the enthalpies of isodesmic reactions calculated using DLPNO-CCSD(T)/aVQZ. We obtained a set of accurate and mutually consistent gas-phase formation enthalpies for 12 energetic heterocyclic species. As a rule, DLPNO-CCSD(T) allows for routine QZ-quality coupled cluster calculations with reasonable turnaround computational times for the energetic species comprised of ~30-40 non-H atoms. In a more general sense, this offers a new level of predictive computational thermochemistry and kinetics for important EMs. The reliable DLPNO-CCSD(T) key thermochemical values comprise a viable step beyond the commonly used DFT procedures.

We also proposed a new approach for the determination of standard (solid) state enthalpy of formationof EM based on complementary high-level quantum chemical calculations (W1-F12 and W2-F12) of the gas-phase values and advanced thermal analysis techniques yielding sublimation enthalpies. We performed a massive benchmarking of the proposed procedure on a large set of EMs.

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Paraffin gasification under high-speed blowing by heated air flow

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Interest in hybrid and ramjet engines requires the use of proper high-energy systems/components. At high-speed blowing conditions, standard rocket propellant components exhibit relatively low gasification rate. As an alternative, it is proposed to use paraffin and compositions based on them. Paraffin is high-energy hydrocarbon with a low melting point leading to a high rate gasification in high-speed blowing conditions. The results of an experimental study of the combustion behavior of paraffin mixtures with various additives under conditions of intensive hot air blowing at a pressure of 1 MPa are presented. Stearic acid, nanoaluminium "Alex", aluminum hydride AlH3, B and mechanoactivated aluminum boride AlB2 were used as 10% by mass additives. Experiments were conducted using cylindrical samples with the central channel. Using the original design microwave gage the current diameter of a sample bore was measured during the experiment in real time with subsequent calculation of regression rate. Also the measurements of the gas flow parameters and temperature profile in the condensed phase were performed. Based on the data obtained, a physical-mathematical estimation of heat and mass exchange during paraffin fuel gasification under hot air blowing has been made.

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A structure of reaction zone in two-level model of coating synthesis

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Modern coating synthesis technologies often use chemically reacting mixtures together with moving high-energy heat sources. The chemical transformations occurring in this process can be divided into two groups. The first leads to the formation of strengthening particles. The second leads to the formation of the matrix composition. For example, in mixtures of Al-CuO, Al-TiO_2, Ti-Al-Fe_2O_3, Al+Ti+Cr_2O_3; Al+Ni+Fe_2O_3 the strengthening particles are formed as a result of metallothermic reactions

$$4Al+3TiO_2=2Al_2O_3+3Ti,$$

$$2Al+Fe_2O=A_2O_3+2Fe \text{ etc.}$$

The released metal interacts with other metals to form intermetallic compounds. This is used to build models of coating synthesis with a reduced chemical reaction scheme, as well as two-level models. Due to the heterogeneous nature of heating and complex thermal cycles, a wide reaction zone of a complex structure is formed during the synthesis.

In models of any type, it is possible to calculate the accompanying stresses and strains that affect the structure of the composite coatings being formed. Stresses can also be divided into physical scales corresponding to the scale levels of description.

The proposed models are implemented numerically.

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Ion chemistry in flames of dimethyl ether and ethanol

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Among many oxygenates, ethanol and dimethyl ether (DME), as substitutes for traditional hydrocarbon fuels, play a prominent role. Ions are formed during combustion in the chemionization reaction. Understanding the behavior of ions in flames is important for the development of new diagnostic methods and new ion-sensitive technologies for controlling combustion processes. In this work, the spatial distribution of positive ions (cationic structure) in premixed atmospheric pressure burner-stabilized dimethyl ether/oxygen/argon and ethanol/oxygen/argon flames was examined by molecular beam mass spectrometry in a wide range of equivalence ratios $\phi=0.5\div1.5$. Hydronium (H_3O^+) and acetyl cation ($C_2H_3O^+$) were detected in the flames of both fuels. In addition, fuel-specific cations were detected: in DME flames, these are CH_3O^+ and protonated DME, and in ethanol flames, protonated acetaldehyde and protonated ethanol. Numerical modeling of the cationic structure of flames has been carried out. For the calculations, a detailed chemical kinetic mechanism involving the reactions with a participation of charged species was used. The mechanism was developed using the ion chemistry model available in the literature for the flames of small hydrocarbons [1, 2]. The improved mechanism included the reactions involving the abovementioned cations. The thermochemical data for them were calculated by high-precision quantum chemistry methods (CCSD(T)-F12). The proposed mechanism was demonstrated to predict well the relative abundance of all key cations in the flames studied.

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Obtaining a "Crown" flame when burning flammable liquids

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Science knows both a flat - stationary flame and a new type of flame - the "blue whirl " - this is a small, stable, rotating blue flame that spontaneously arose in laboratory experiments when studying turbulent, fiery whirlwinds. In the form of a "blue whirl", a number of different liquid hydrocarbon fuels burn without producing soot, representing a previously unknown potential low emission combustion method. In this work, a fundamentally new type of flame has been obtained - the "Crown" flame, which differs both from the previously known types of flames, and from the new "blue whirl". In the "corona" flame, the mixture burns out only in a small area around the perimeter of the combustion source, while the flame does not close into the volume.

"Crown" flame when burning nonane

"Crown" flame when burning ethanol

"Crown" flame when burning hexane

"Crown" flame when burning acetone

This flame can be obtained from the combustion of any liquid, and the shape of the flame will always be the same, while the combustion of the fuel will occur until the products of complete combustion.

A patent for the invention No. 2782077 was obtained for the installation for the production of a “crown” flame. The principle of operation of the installation consists in the forced supply of heated air to the reaction zone, while at different air supply speeds the type of flame changes. And only in a small range of speeds the shape of the flame takes the form of a crown. A series of tests were carried out at the facility on various liquids: nonane, hexane, acetone, ethanol, kerosene. The result for all liquids is the same - the formation of a "corona" flame.

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ORAL PRESENTATIONS

Study of advantages of liquid hydrocarbons combustion with the superheated steam jet in comparison with other atomizers

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Improving the environmental friendliness of thermal cycles is one of the most important tasks in the study of combustion of hydrocarbon fuels. Emissions, which have the greatest impact on the environmental aspect of hydrocarbon fuel combustion, are particulate matter, CO, NOx. One of the solutions is the implementation of flue gas recirculation to reduce the rate of chemical oxidation reaction due to lowering the temperature of the combustion mixture and increasing the residence time of the particles in the furnace space in order to more complete combustion of the mixture, which simultaneously reduces the emissions of NOx and soot. Instead of flue gases, other substances, such as carbon dioxide, air and superheated water steam, can be used as diluent gas.

The purpose of this work is to identify the advantages of using superheated water vapor as a diluent atomizer over other diluent gases (carbon dioxide, air) when burning liquid hydrocarbon fuels. It was shown that the use of superheated water vapor as atomizer not only reduces the formation of "thermal" NOx, but also eliminates the problem of coking of fuel feed channels, allowing the combustion of liquid hydrocarbons contaminated with mechanical impurities and water.

To study the environmental and energy parameters of liquid hydrocarbons combustion in the presence of different diluent atomizers, the following parameters were experimentally studied: the flame temperature, composition of intermediate and final combustion products, completeness of fuel combustion.

As a result of studies of temperature profiles along the burner axis, it was obtained that the mode with air atomization has a higher flame temperature in the entire measured range compared to steam and carbon dioxide atomization, the maximum temperature is 1900 ° C, which is almost 150 ° C higher than in the modes with water vapor or CO_2 atomization.

Analysis of fuel combustion completeness showed that for all types of atomizer, high values of fuel combustion completeness were obtained. At that, the lowest content of carbon monoxide and nitrogen oxides were obtained in the mode with steam atomization, the highest emissions were recorded at air jet atomization. When comparing the values obtained with the normative values of DIN EN:267, it was found that in the case of steam and carbon dioxide they meet the most stringent - 3 class, and in the case of air - only 2 class.

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Experimentally observed double criticality in combustion of premixed gaseous mixtures

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On the basis of known and newly obtained experimental data the existence of two different kinetic modes of combustion of premixed gas mixtures at atmospheric initial pressure is shown.

According to the theory of a chain-thermal explosion developed by V. V. Azatyan, a combustible gas mixture ignites due to the fulfillment of the condition of chain ignition. The development of a chain avalanche is accompanied by significant self-heating. If both criteria of thermal ignition are met, a thermal explosion occurs. This implies the presence of two different kinetic modes of chain gas-phase combustion separated by a jump - like transition: the first occurs when the criteria of progressive heat accumulation is not met (maximum explosion pressure ΔP_{max} is relatively low), and the second, which corresponds to the simultaneous fulfillment of conditions of chain and thermal ignition (ΔP_{max} is substantially higher).

The predicted different kinetic regimes were observed during the combustion of both inhibited and non-inhibited mixtures of H_2, CH_4 and C_3H_8 with air, as well as $C_2H_4F_2$ with Cl_2 in presence of oxygen; the critical transition coincides with the concentration limits of detonation-capable mixtures. In Fig. 1 (the data obtained in a spherical bomb having a volume of 4.2 l with a central spark ignition) the two kinetic modes (zones I and II) are clearly visible in the flame structure.

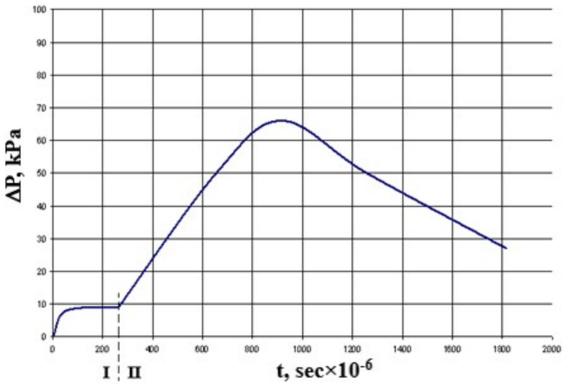

Figure 1 Flame structure in C_3H_8 (8 % vol.) - CF_3H (4 % vol.) - air (88 % vol.) mixture

The calculations of the upper flammability limit (UFL) based on classic thermal theory of combustion show an overestimated UFL value for the mixtures of methane and ethane with air in comparison with the experimental data obtained in the above described spherical bomb. The resulting discrepancy is explained on the basis of the chain – thermal theory.

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ORAL PRESENTATIONS

Studies on the fire resistance of epoxy resin with flame retardant additives DOPO and graphene

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Epoxy resin (ER) is widely used as coatings, composites and adhesives due to its exceptional mechanical properties, high chemical and thermal resistance. However, ER have a high fire hazard when used in the transport industry (aircraft, trains, ships, etc.) due to low fire resistance. During combustion of ER, a high rate of heat and smoke is observed, which can lead to serious consequences. For this reason, the world industry and science have recently paid attention to the modification of ER to improve its fire resistance.

At present, the addition of flame retardants to ER is an effective and widely used way to improve its fire resistance. With increasing attention to environmental protection, there is a trend towards the development of environmentally friendly and non-toxic flame retardants for polymeric materials, including ER. A modern alternative to halogen flame retardants is phosphorus-containing flame retardants. In this regard, many articles are devoted to the study of the flame retardant 9,10-dihydro-9-hydroxy-10-phosphaphenantrene-10-oxide (DOPO). At present, flame retardants based on nanoparticles are also gaining popularity - fullerenes, carbon nanotubes, nanosilicates, etc. However, the literature contains insufficient data on the effect of DOPO and graphene on the combustibility of ER, as well as their mutual influence on flame retardant properties.

The purpose of this work was to study the fire resistance of ER without additives of flame retardants and with additives of graphene and DOPO in laboratory conditions using UL-94 flammability tests, oxygen index, tests in a cone calorimeter and to study the effect of flame retardants on the rate of linear pyrolysis under the action of external thermal radiation. Linear pyrolysis rate experiments were carried out under a cone heater and compared with decomposition simulations using the open source software Gpyro. The input data for the simulation were the kinetic parameters of the thermal decomposition of ES, determined using a genetic algorithm implemented in Gpyro, for thermogravimetric analysis data. The data obtained indicate the effectiveness of the use of DOPO and graphene to improve the fire resistance of ER. Moreover, a synergistic effect was found to improve fire resistance with a mixture of these flame retardants due to their different mechanism of action.

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Effect of flame retardant additives DDM-DOPO and graphene on flame propagation through glass fiber reinforced epoxy resin under the influence of external thermal radiation

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The flammability of various materials used in industry is an important issue in the modern world. This work is devoted to the study of the flame retardants effect: graphene and DDM-DOPO (9, 10-dihydro-9-oxa-10-phosphaphenanthrene-10-oxide-4,4′-diamino-diphenyl methane) on the flammability of glass fiber reinforced epoxy resin (GFRER). Samples have been made without the additives and with additives of flame retardants: graphene and DDM-DOPO in various proportions. To study the flammability of the samples, standard flammability tests were carried out, such as thermogravimetric analysis, UL-94, limiting oxygen index (LOI) test, and cone calorimetry. The flame retardants have been shown to be effective in improving the fire resistance of the epoxy resin composites in these tests. In addition, in order to confirm the effectiveness of flame retardants in a real fire condition, the experiment on downward flame propagation under the action of two heaters was carried out. The flame spread over the surface of the sample almost uniformly, without acceleration. The flame spread rate had an almost linear dependence on the heat flux. An increase in the external heat flux lead to an increase in the flame spread rate, which was associated with the approach of the sample surface temperature to the epoxy resin pyrolysis temperature. An increase in the additive concentration of DDM-DOPO had almost no effect on the flame spread rate. A similar result was observed in UL-94 HB, where the flame propagation rate didn’t change with increasing the DDM-DOPO concentration. It’s worth emphasizing, that an increase of DDM-DOPO concentration had almost no effect on the mass consumption during downward flame propagation.

The numerical model of the downward flame propagation under the action of bilateral external heating over the fiberglass reinforced epoxy resins with and without the flame retardants DDM-DOPO and graphene was developed. The numerical model well predicted the temperature gradient in the condensed and gaseous phases, whereby the model well predicted the flame spread rate over the samples surface. Comparison of the flame structure from the model and from the experiment showed that the model for DDM-DOPO well predicted the trend towards a decrease in the length of the luminous flame zone. In the case of graphene, the model incorrectly predicted the trend, reducing the length of the luminous zone, however it correctly described the decrease in the flame spread rate and the surface temperature. Simplicity of the mechanism using in the model inevitably entails limitations and some disagreements with the experiment. The obtained data may be used for designing effective reinforced non-combustible composites applied in the aircraft industry and for determining a detailed mechanism of the effect of flame-retardant additives.

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Development and study of fire retardant composite materials promising for use in construction and aviation

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Reinforced polymer composite materials (RPCM) based on epoxy resin have a good strength, flexibility, thermal insulation properties coupled with a low density, that makes it a perspective material for aviation, machine industry, building and etc. Glass fiber reinforced epoxy resin (GFRER) is a perspective material. Rigid polyurethane foam (RPUF) is a perspective thermal insulation material. Flammability is one problem of these materials. To improve the RPCM fire resistance, flame retardants based on phosphorus-containing compounds (for example, DOPO (9,10-dihydro-9-hydroxy-10-phosphafenatrene-10-oxide), Disflamoll®51092) and nanocarbon materials (graphene, expanded graphite) were introduced into them. Several tests were conducted to investigate flammability, toxicity and mechanical properties such as: thermogravimetric (TG) analysis, limiting oxygen index (LOI), UL-94 and its modifications, measurement of fire resistance according to aviation regulations (AP-25 p.867 (a)), ASTM D 4986, tests on a cone calorimeter, measurements of the speed of propagation of flame on composites against the flow of the oxidizer, measurements of physical and mechanical properties using an electromechanical machine for testing materials Zwick / Roell Z100, determination of the smoke generation coefficient and toxicity in accordance with GOST 12.1.044-89. Along with the flammability tests (UL-94, LOI), experimental investigation and numerical modeling of GFRER with and without the fire retardants graphene and DDM-DOPO with max concentration 6% were carried out. It was stated, that graphene and DDM-DOPO are similarly effective in rate of flame spread (ROS) decrease. It's worth emphasizing, that 6% of DDM-DOPO addition in GFRER led to LOI = 26.5. For the first time the numerical model for GFRER incorporated by DDM-DOPO was developed, based on the gas phase DDM-DOPO action (because it contains phosphorous). The model for DDM-DOPO can satisfactorily predict the flame retardant effect on ROS decrease. In first time the numerical model for GFRER incorporated by graphene, based on the decrease of combustible fuel and increase of non-combustible volatile pyrolysis products. Obtained model for graphene with a good precision predicts effect of graphene on ROS decrease [1,2]. Phosphorus-containing acrylate ester binders A1, A2, A3 were synthesized to prepare RPCM samples. Two patents have been prepared for the use of A2 and A3 resins [3,4]. The use of a phosphorus-containing binder in

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RPCM allowed to significantly improve the most important characteristics of these materials - combustibility, heat release during combustion, physical and mechanical properties and reduce the toxicity of combustion products compared to a control sample based on epoxy resin. RPCMs based on A1, A2, and A3 have high LOI values (>31%), which is achieved due to chemically bounded phosphorus in the molecules of the initial oligomers. According to the combination of the fire hazard characteristics (heat release + smoke generation), A2 composition samples are preferable. The fire resistance test results according to AP-25 (clause 867 (a)) showed, that when the samples were exposed to the test burner flame with a temperature of 1100 °C, samples of RPCM based on ester acrylate resins A1, A2, A3 (dimensions 140x150 mm) retain their integrity for 5 minutes of direct flame exposure. Moreover, GFRER with addition of phosphorous containing benzoxazine based on cardanol (CBz) were prepared. This fire retardant is fully bio-based, that makes it environmentally friendly for industrial use. LOI and UL-94 test revealed, that CBz addition significantly reduces GFRER samples flammability resulting in LOI increase to 28.1. Glass fiber reinforced polyimide resins have been also tested by flammability tests showing very high LOIs of over 80.

As a result of the research, new slow-burning glass-reinforced plastics and rigid polyurethane foam with a high limiting oxygen index (>35%) have been developed, which can be used as structural and heat-insulating materials in construction and transport [5]. The addition of expanded graphite (EG) and Disflamoll®51092 mixture with a total mass content up to 15% to the composition of RPUF led to an increase in the oxygen index to 36.7%. At the same time, the sample with the addition of 15% RG showed the highest fire resistance among all RPUF samples. All RPUF with flame retardants are UL-94 HBF (low flammability for porous materials). In addition, compositions with a mixture of fire retardants 7.5% Disflamoll®51092 + 7.5% RG and with 15% RG successfully passed the test of aviation standards according to AP-25.

In Siberian Aeronautical Research Institute named after S. A. Chaplygin, work is underway to introduce new fire retardant reinforced composites to modernize existing and create new aviation equipment, including experimental ones. For this technique, structural elements, such as various thermally stable partitions inside the aircraft, hoods and elements of engine nacelles and engine compartment, from fire retardant materials with reduced smoke emission are made. This provides high operational, functional and technological properties that meet modern requirements for the safety of aviation equipment, manufacturability, and economic efficiency.

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Features of flame formation and propagation during laser ignition of boron-based high-energy compositions

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The combustion characteristics of metallized heterogeneous condensed systems are the determining factors for the implementation of sustainable and complete combustion of solid propellant, analysis and provision of optimal operating modes for propulsion systems and gas generators. The ignition serves as the initial stage of engine operation or a gas generating device, and in accordance with the technical regulations and the purpose of the device, requirements arise to ensure appropriate characteristics. The problems of stable combustion are solved by a detailed study of the ignition mechanism by a specific thermal effect on a model high-energy composition (HEC) containing various dispersed metal fuels. This paper presents the results of an experimental study of the additives effect of amorphous boron powder and aluminum borides AlB_2, AlB_{12} on the formation and propagation of the flame zone, and the time characteristics of HEC ignition during intense thermal heating.

Study of the characteristics of the flame appearance and ignition of cylindrical samples of HEC based on ammonium perchlorate and butadiene rubber with 15.7 wt. % with B, AlB_2, and AlB_{12} additives was carried out under the influence of a time-constant external radiant heat flux of CO_2-laser using high-speed video and thermal imaging cameras, a system for measuring the flame delay time and heat flux density. It has been established that at a constant q = 68 W/cm^2, the delay time, the rate of formation and propagation of the flame zone on the surface of the HEC sample depends on the nature and size of the metallic fuel particles. Pyrolysis of the components on the HEC surface is carried out when ~300–360 °C is reached, resulting in the formation of a gaseous cloud and a luminous spot on the surface of the samples. With an increase in T_s to 380–440°C, an intense outflow of gaseous products and luminous boron conglomerates or small metal particles is observed. The particle velocity is ~5–7 m/s. The appearance of a flash near the sample surface is recorded when the temperature reaches ~550–670 °C. In this case, the propagation velocity of the flame zone is ~6–8 m/s (depending on the nature of the additive). The maximum length of the flame zone is from 165 mm (B-HEC) to 180 mm (AlB_2-HEC) and 210 mm (AlB_{12}-HEC) and depends on the reactivity and diameter of the luminous metal particles.

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Regimes of combustion of hydrogen microjets

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Introduction

Alternative technologies of energy production from renewable energy sources have found various applications during the last decades and are still under development. One of such technologies is hydrogen power engineering, which implies burning of hydrogen extracted from water, and water resources on the Earth are almost unlimited. The reaction product is water again, which is an environmentally friendly product. Therefore, it is of interest to study the combustion of hydrogen jet flows formed by various burners and nozzles.

Experimental results.

1. *Flame Structure in the Case of Diffusion Combustion of Hydrogen Microjets*

The hydrogen jet flow and its diffusion combustion were studied with the use of nozzles of various shapes: circular and slotted nozzles. In both cases, a specific feature of the flow structure and combustion, i.e., a “bottleneck” was observed.

2. *Effect of the Jet Orientation in the Gravity Field on its Diffusion Combustion*

In addition to the geometric characteristics of the micronozzle, jet velocity profile at the nozzle exit, and hydrogen flow rate, the character of combustion depends on some other conditions, in particular, jet orientation in the gravity field. In the present experiments, we studied three variants of jet propagation: along the direction of the gravity force vector, opposite to it, and in the normal direction.

3. Dependence of Diffusion Combustion of Hydrogen Microjets on the Method of Jet Ignition

In addition to the conditions considered above, hydrogen microjet combustion depends on the conditions of jet ignition: near the nozzle exit or far from it. Diffusion combustion of microjets in these two cases was studied. In the case with ignition near the nozzle, the above-described flow structure with the “bottleneck” region near the nozzle exit is formed; the combustion process remains stable in a wide range of hydrogen flow rates, and the “bottleneck” region persists until transonic velocities of jet exhaustion are reached. In the second case (ignition far from the nozzle), this region is not formed, and “lifted” flame not contacting the nozzle is observed. In this case, a transition to stable combustion with supersonic jet exhaustion occurs.

4. Combustion of Hydrogen Mixtures with other Gases

The influence of gaseous additives (methane, helium, nitrogen, and oxygen) to the hydrogen microjet on its structure and combustion was studied in the experiments. A certain gas was mixed in various proportions with hydrogen at the entrance to the jet setup. The data were obtained for flows with an axisymmetric parabolic velocity profile at the nozzle exit.

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Heat transfer during flame propagation in a porous medium

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A study of the dynamics of gas temperature is carried out using the example of a single cylindrical channel of the Raschig ring placed in a porous medium of these rings. The temperature of the gas and the thermocouple filament on the channel axis was calculated, as well as the temperature distribution in the channel in two processes. The first process is an increase in pressure in a closed vessel during the propagation of a flame in a space free from a porous medium. The second process is the cooling of the gas after the passage of the flame in the channel.

Comparison with experiment is carried out. A V-shaped tungsten/rhenium thermocouple W/Re (5/25) with a diameter of $15\cdot10^{-6}$ m was placed in the channel on its axis. Measurements of the gas temperature and the equilibrium temperature of the gas and porous medium were carried out using this thermocouple in a cylindrical channel with a diameter of 2 mm and 7.5 mm long.

It is shown that in the process of gas compression at a constant speed, the thermocouple makes it possible to measure the steady-state temperature of the gas. But when reaching a steady value, it will lag the more, the larger the diameter of the filament. It has been established that in the process of cooling an instantly heated gas, the readings of gas temperature measurements using a thermocouple will be significantly underestimated. This is due to the high heat capacity of the thermocouple filament compared to the heat capacity of the gas in the pore. During the heating of the thermocouple, the gas has time to cool into the walls of the channel.

It is shown that pressure fluctuations significantly intensify heat transfer between the gas and the solid phase.

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Diffusion combustion of liquid fuel in closed volumes

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In technological processes in closed volumes, combustible gas mixtures can be formed. To ensure the safety of such processes, it is necessary either to prevent the possibility of ignition of this mixture, or to provide for the strength characteristics of the vessel such that the vessel does not collapse during the combustion of the combustible mixture, or to organize the process so that the combustion wave cannot propagate through the combustible mixture. Working with an out limit mixture is often easier than creating conditions for the impossibility of igniting the mixture and it is not always economically feasible to make strong vessels or install protective devices. When the concentration of fuel in the mixture is greater than the upper concentration limit, the flame is unable to propagate through such a mixture. However, if there are leaks to the atmosphere, a combustible mixture may form. Given this factor, it is safer to work with extreme mixtures below the poor concentration limit. This communication presents the results of a study of combustion near and beyond limit mixtures from the point of view of their safe use. Two aspects were studied: the initiation of combustion in an out limit mixture and the developed pressures in a closed vessel. The experiments were carried out in a 3-liter thermostated bomb. Combustion was initiated by an electric spark or a heated coil in the gas phase. The pressure in the bomb was recorded using a pressure sensor DD10. The temperature of the gas and liquid phases was measured with a K-type thermocouple. The evacuated bomb was first filled with a combustible liquid through a hole in the bottom, and then, a nitrogen-oxygen mixture was added from above, ranging from air to pure oxygen to the desired pressure. The saturated vapor pressure of the fuel was controlled by changing the temperature of the bomb. The combustion of gas mixtures was studied, the concentration of fuel in which lay in the region of the lower concentration limit. The maximum pressures were determined from the obtained dependences of pressure on time. This made it possible to construct the dependence of the pressure on the composition of the mixture near the lower limit. Experiments have shown that at a fixed initial fuel temperature, an increase in the total pressure of the mixture, especially in an oxygen-enriched mixture, the maximum explosion pressure increased when approaching the lower limit, and combustion took place even beyond the lower concentration limit. The phenomenon of liquid fuel ignition by a spark located at a considerable distance from the liquid surface has been discovered. It turned out that a film of fuel is formed on the surface of the electrodes and the wall of the bomb. When combustion is initiated by a spark or a spiral in an out limit gas mixture, the combustion wave first spreads over a thin fuel film on the surface of the electrodes and the bomb wall. Next, ignition and diffusion combustion of the bulk of the liquid fuel occurs until oxygen is almost completely depleted. Since there is a lot of oxygen at the lower limit, this leads to a significant increase in pressure, exceeding the pressure increase at the lower limit of this fuel-oxidant gas mixture. For oxygen mixtures, this pressure increase can be higher than in a stoichiometric mixture. Thus, in the presence of a combustible liquid phase, even if the saturation vapor pressure is such that the resulting mixture has a vapor concentration corresponding to the lower concentration limit (or less), combustion is possible with a significant increase in pressure.

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Experimental study of flame spread over multiple thin fuel configurations

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In the present study opposed flow flame spread over multiple fuel configurations with thin cellulosic fuels are investigated experimentally in normal gravity and microgravity environments. The thin cellulose fuel (Kim wipes) is configured in different shapes as planar fuel, hollow cylindrical fuel, C- channel fuel, L channel fuel with the help of fuel sample holders and flame spread phenomena is observed over each configuration in normal gravity and microgravity environments at ambient oxygen concentration and 1 atm. pressure. The microgravity experiments are conducted using 2.5s drop tower available at the National Centre for Combustion Research and Development (NCCRD), IIT Madras, India. Over the flow speed range of 5 cm/s to 20 cm/s, it is observed that C channel configuration has the highest spread rate compared with other configurations in similar experimental conditions. Further each configuration shows a non-monotonic increasing-decreasing flame spread rate with respect to opposed flow speed.

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Flame propagation in the boundary layer of wood biomass particles during ignition

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As mentioned above, the theory of the processes of thermal preparation of wood biomass particles for ignition has been developed quite well. But the processes of direct flame propagation in a small vicinity of wood biomass particles are not studied. Also, to date, no analysis has been carried out of the effect of wood biomass particle sizes on the characteristics and conditions of flame propagation in the boundary layer. The latter is important for the development of the theory of substantiation of the optimal choice of boiler and auxiliary equipment of thermal power plants. For this reason, the main purpose of this work is the experimental study of heat and mass transfer processes occurring together under conditions of significant thermochemical transformations in the time period from the appearance of the first flame foci to the complete flame coverage of the particle when the latter is ignited under conditions of high-temperature heating in an oxidizing medium.

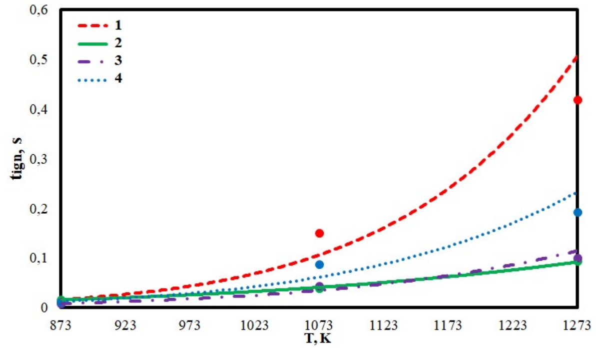

Figure 1 Dependences of the flame propagation time on the entire surface of the dry wood biomass particle on the ambient temperature for different types of wood: 1 – birch, 2 – pine, 3 – cedar, 4 – aspen

Figure 1 shows the dependences of the flame propagation time (t_{sf}) on the ambient temperature. The analysis of the t_{sf} dependencies shows that under conditions of low-temperature heating of wood particles, the type of the latter does not significantly affect the characteristics and conditions of flame propagation. However, with an increase in ambient temperature, the type of wood begins to have a significant impact on the characteristics and conditions of flame propagation. It can be noted that at T_g=1273K, the greatest flame propagation times (t_{sf}≈0.5c) for all variants of particle orientations in space are recorded in the case of ignition of birch particles.

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Features of gas dynamics and combustion of two colliding laminar jets

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The development of jet flows is associated with the appearance of various types of hydrodynamic instability. In the case of interaction of two jets, the flow pattern becomes much more complicated. At the same time, the use of colliding jets makes it possible, for example, to control the velocity parameters of the resulting jet, to form the shape of the flame, thereby influencing the combustion process. A feature of these studies is that the symmetry axes of the colliding jets are located at an acute angle to each other, and the transverse position of the nozzles changes from complete overlap of the jets, when the symmetry axes are in the same plane, to complete divergence of the jets, when the nozzles are separated in the transverse direction.

The experiments were carried out on a jet facility at the Khristianovich Institute of Theoretical and Applied Mechanics SB RAS. The setup consists of two identical cylindrical tubes 50 mm long and 0.4 mm in inner diameter, located at an angle of 50° between the axes of symmetry of the nozzles. The distance between the ends of tubes is 7mm. The experimental setup is shown in Fig.1. The used gas was a propane/butane mixture in a percentage ratio of 70/30. Liquefied gas was supplied from the balloon through the evaporator to the reducer, then to the mass flow controller, then it was divided into two parts. The gas flow rate through each nozzle corresponded to ½ of the set flow rate on the flow meter and was equal to 1.0×10-7m3/s.

The calculated velocity of the gas flowing through each nozzle is U1=U2=0.39m/s, which corresponded to Repropane=42, at the nozzle diameter 400 μm. At the current Reynolds number, the flame was laminar. When the velocity reaches U≥0.53m/s (Re≥55), the flame becomes turbulent and detaches from the nozzle exit. Figure 2 shows shadow photographs of the development of two colliding gas jets without combustion at different overlap. Photo 1 and 3 (Fig. 2) correspond to xy and yz planes, respectively, for case when the jets do not interact. Photo 2 and 4 (Fig. 2) show the same planes, for the case of overlap of the jets is ~ 100% of the cross-sectional area of each nozzle. Figure 3 shows the isosurface of velocity fluctuations at 100% jet overlap. As a result, characteristic features of the formation of the resulting jet and flame during diffusion combustion were obtained.

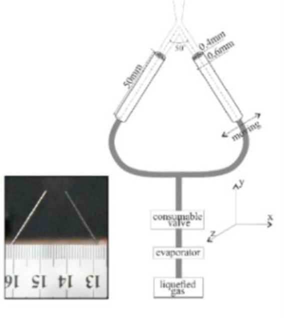

Figure 1. Setup.

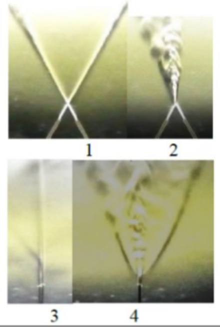

Figure 2. Shadow images

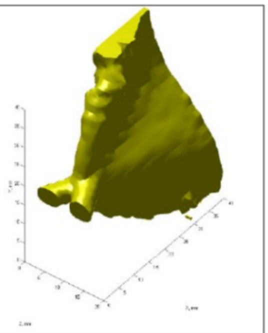

Figure 3. Hot-wire isosurface

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Extra energy release from nano-sized energetic materials via self-synchronization of collective atomic vibrations in low-dimensional nanocarbon-based transition interfaces

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High-end nano-sized energetic materials (nEMs) have recently attracted close attention due to a combination of the extraordinary properties set's and the promising effects that can be applied in the emerging areas of energy storage, designing new functional materials and high-energy additives, actuation in lab-on-a-chip devices and for the attitude control of micro/nano satellites. The incorporation of various nano-additives such as nano-catalysts into the nEMs formulations is a current research trend that are oriented to tailor properties, enhance the performances as well as safety and fully use their potential features. Over the past few decades, carbon-based nanomaterials and, specifically, low-dimensional nanocarbon allotropes have revolutionized the field of nanomaterials science. The discovery and synthesis of new forms of carbon and nanohybrid systems have always opened doors to new science and technology. Based on recently discovered fundamental phenomenon of collective atomic vibrations, manifested within transition domains of nanolayers, we developed a game-changing approach for predictive unlocking extra energy from nEMs, unlocking their new functionalities as well as environmental performance enhancement and safety level. The developed approach includes incorporation of the 2D-ordered linear-chain carbon-based multilayer nano-enhanced interfaces into the transition domains of nEMs nanocomponents through the multistage technological chain. This technological chain includes conversion of all components into the nanoscale, the ion-assisted pulse-plasma-driven functionalization and assembling of various carbon-based nanocomponents and catalytic nano-additives with multilayer nano-enhanced interfaces, the resonant acoustic mixing of all nanocomponents and growing the high-end nEMs elements by selective high-precision additive manufacturing. Predictive modification of the flat nano-enhanced interfaces into the 3D-shaped nano-interfaces with assistance of the surface-acoustic wave-based technique opens up fundamentally new opportunities for programming chemical and energy interactions in nEMs reaction zones. We consider a set of interacting 3D-shaped nano-enhanced interfaces as programmable nanodevices that serves as a smart gateway and weak-signals amplifier between nEMs nanocomponents via excitation and fine-tuning self-synchronization of collective atomic vibrations and phonon waves propagation. We have developed a combination of methods for predictive activation and fine-tuning synergistic effects such as self-synchronization of collective atomic vibrations, phonon waves propagation and energy exchange inside the 3D-shaped multilayer nano-enhanced interfaces. In particular, activation and fine-tuning mentioned synergistic effects is provided by energy driven initiation of the allotropic phase transitions, by using surface acoustic waves-assisted micro/nano- manipulation during the ion-assisted pulse-plasma functionalizing, by heteroatom doping, by initiating the directed self-assembly through application external high-frequency electromagnetic fields as well as by using the data-driven-based nanoscale inverse designing approach. The nanoscale inverse designing approach is based on the earlier developed and proven carbon nanomaterials genome approach for accelerating the discovery of the advanced hybridized functional materials with desired properties.

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Initiation of filtration gas combustion with open flame

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An experimental study of the unsteady process of filtration gas combustion (FGC) – the initiation of a wave of filtration combustion by an open flame of combustible gas filtered through an inert porous medium.

Similar processes occur during the operation of any device whose principle of operation is based on FGC and are insufficiently investigated at present.
The process is considered and the mechanism of the formation of a gas combustion wave is described. The presence of limits for the initiation of FGC waves by the gas filtration rate has been established. The influence of the external heat transfer coefficient on the mechanism of formation of the FGC wave is considered. The limits of the ignition of the FGC wave are determined, related both to the parameters of an inert porous medium (grain size, effective thermal conductivity of grains), with the coefficient of external heat transfer and with the filtration rate of the combustible gas. The figure shows the experimental and theoretical results of the study. The criterion of the limit was the absence of movement of the maximum temperature for 5 minutes.

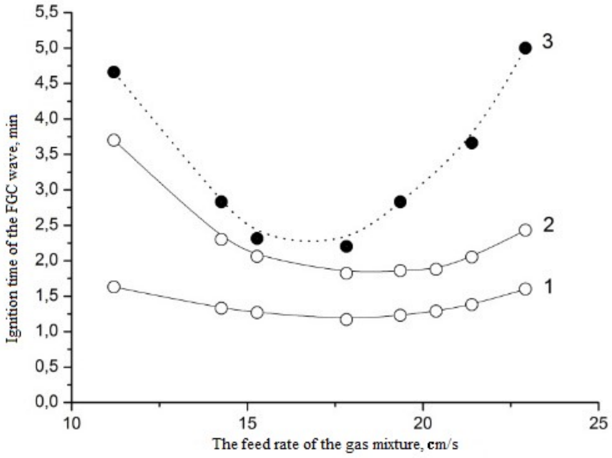

Figure 1 Dependence of the ignition time of the FGC wave on the gas mixture feed rate for a porous medium with an average grain diameter of 4 mm under various external heat exchange conditions. 1 – external heat transfer coefficient, α=0 W/m^{2}K; 2 – external heat transfer coefficient, α=250 W/m^{2}K; 3 – experimental data.

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Solid-state combustion synthesis of nickel-containing catalysts for CO_2 methanation using energetic nickel complexes

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One of the methods for the synthesis of nanomaterials is the solid-state combustion (SSC) of energetic complexes of metals. Besides metals, the complex compounds contain energetic organic ligands and oxygen-containing oxidizing anions, which ensure the initiation of the combustion process following a short-term heat exposure even in an oxygen-poor environment. Due to the high rate of the redox reactions the released heat is localized in a limited volume, creating a high-temperature zone, where metal-containing nanoparticles are formed. They are well crystallized and may be used as catalysts for several important chemical processes, such as CO_2 utilization by methanation, without an additional thermal treatment. It should be noted that usually metal-organic compounds are synthesized with the use of solvents, which have to be disposed of. The environmental impact of complex preparation can be reduced by using solvent-free methods of synthesis, which corresponds to the modern concepts of the development of the chemical industry.

This work suggests a new approach to the synthesis of metal-organic nickel complexes as precursors for the catalytically active phase of the CO_2 methanation catalysts. This method is based on the melting of nickel nitrate or perchlorate with imidazole, which is thermally stable and easily forms complex compounds with transition metals. The composition and structure of the acquired complexes have been confirmed by the elemental analysis, ATR-FTIR spectroscopy and XRD. The study of the solid products of their gasification in the SSC showed that they consist of nickel oxide and reduced metal. Their catalytic activity in the CO_2 methanation reaction was also studied. It was demonstrated that the sample acquired from the nickel imidazole complex with nitrate anions can be activated at 250 °C in the reaction mixture containing CO_2 and efficiently facilitates the interaction of CO_2 with hydrogen. The addition of lanthanides improves the catalytic properties in the low-temperature region.

A supported nickel-aluminum catalyst was prepared by the SSC method using the nickel imidazole complex with nitrate anions. It showed catalytic activity in the CO_2 methanation even at 150 °C, and achieved the CO_2 conversion rate of 69% at 350 °C, which is almost 3 times higher than the activity of the commercial catalyst NIAP-07-01, containing 1.5 times more nickel.

Thus, based on this research, a new solvent-free synthesis method for the nickel-containing catalysts for CO_2 methanation was proposed, which uses energetic nickel complexes as precursors of the catalytically active phase. In addition, the impact of the anion and additives on the catalytic properties of the products acquired by the SSC was investigated.

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Combustion synthesis of porous inert media burners

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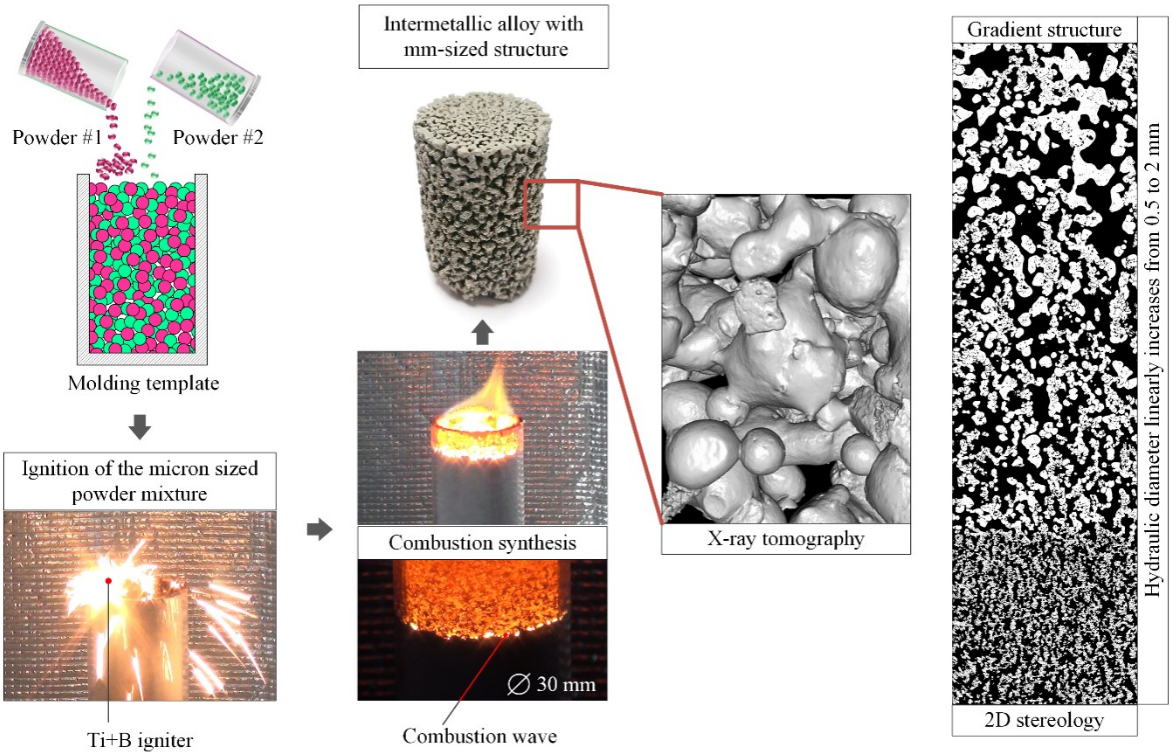
High gas-permeable materials with a pore channel from hundreds of microns to a few millimeters are widely used as a primary component of gas burners working on the principle of filtration combustion. The material selected as a porous media burner (PMB) must resist both thermomechanical stresses and the oxidative effects of combustion gases. The promising materials are intermetallic compounds based on the Ni_3Al phase. Combustion synthesis can effectively produce these compounds in one stage [1,2]. We will show the current results on the combustion synthesis of double-layer and gradient PMB and discuss their usefulness for utilizing ultra-lean mixtures of natural gas with air.



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Numerical Study of the Thermal Structure of Turbulent Diffusion Flame on the Horizontal Surface of PMMA

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The numerical study of turbulent diffusion flame on the surface of solid combustible material has been carried out. The predictions have been performed by employing the open-source software Fire Dynamics Simulator (FDS) employing LES technique for turbulent transfer modeling. Methylmethacrylate (product of PMMA pyrolysis) is assigned as the gaseous fuel component of gas-phase combustion reaction with corresponding values of molar weight and heat release.

The height from the burning surface of solid combustible material on which the turbulent eddies are formed has been determined based on the distribution of instant values of temperature. In the vicinity of burning surface where turbulent fluctuations do not occur, the temperature profiles agree with the ones obtained through the prediction in laminar assumption.

The algorithm for the coupled problem of flame spread over the surface of solid fuel is proposed. Entire computation domain is divided into two regions: relatively thin near-wall zone, where laminar flow occurs and the outer area, which includes the flame plume where turbulent regime is dominant. Thus, in near-wall zone the assumptions of laminar flow and two-dimensional formulation (if any) are accepted, which allow to use high resolution numerical grid. This results in accurate prediction of temperature gradient and correspondingly the heat flux from the flame to the solid fuel's burning surface.

As LES approach demands, the conservation equations in the outer area are three-dimensional and the size this area is much larger. These factors strongly restrict the number of grid nodes due to affordable computational resources, which resulting in rather coarse grid resolution allowed. The solutions in both regions are coupled by mutual boundary conditions at some surface, the position of which must ensure that laminar flow assumption is valid here.

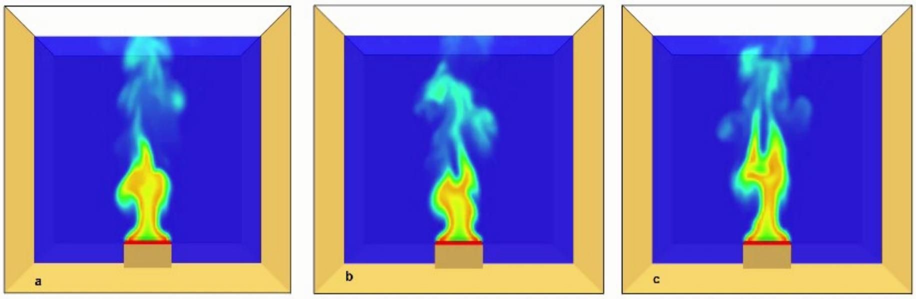

Figure 1 Turbulent flame structure at the time moments: a – 21.67 s, b – 21.73 s, c – 21.82 s

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Measurement of the overall activation energy of the methane-hydrogen mixtures

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In the modern world, pollution is seen to be an enormous problem, and other fuels, for instance, hydrogen, are considered to reduce the CO_2 emissions usually associated with hydrocarbons. Since hydrogen is very explosive, the next step towards this could be a methane-hydrogen mixture. In this work, we experimentally investigate one of the most important characteristics of the H_2/CH_4 mixture – the overall activation energy and its dependence on the equivalence ratio using the mixtures with different volume ratio of hydrogen to methane *a*. Similar experiment was conducted with methane as a fuel in our earlier work, and results show that the one-step model can be used to describe its properties according to the equation:

$$lnM = lnA - \frac{E_a}{2RT}$$

where M is mass flow rate of the mixture, A – pre-exponent, T – maximum gas temperature, E_a – overall activation energy. The experimental setup was created, which includes a plane flame stabilized on the flat porous burner equipped with the thermostat system and micrometric vertical stage. Gases are supplied through the mass flow controllers (Bronkhorst). Temperature is measured by thin filament pyrometry with infrared camera (OPTRIS PI) and SiC filament. A typical the dependence of T on M measured for ϕ=0.8 is illustrated in Fig. 1, which allows to estimate E_a. A dependence of E_a on the mixture composition is found by applying this procedure to different ϕ and a.

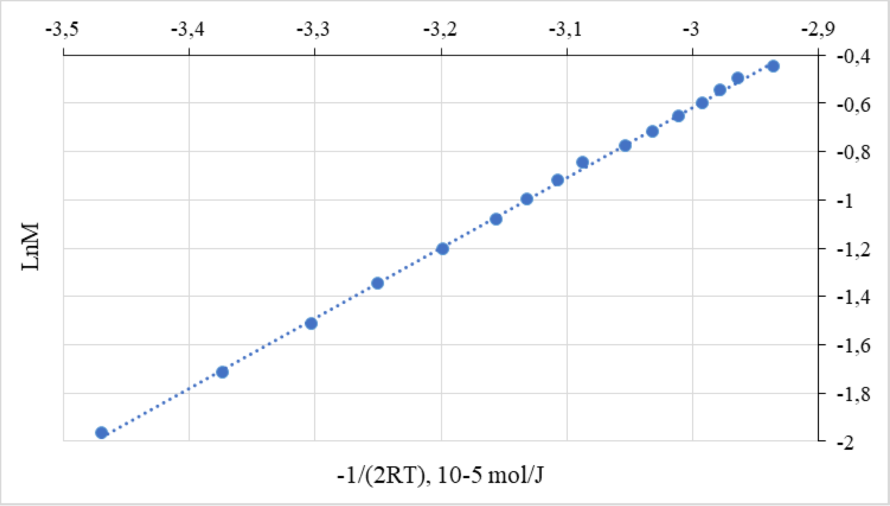

Figure 1 Activation energy is 291.4 kJ/mol for ϕ=0.8 and a=2

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Deflagration flame propagation over a fuel film under various conditions

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An experimental study of flame propagation over a thin film of various liquid fuels with a flash point below the ambient temperature has been carried out. The study was carried out on flat thin copper and thick glass substrates, as well as in porous monodisperse media made of steel, ceramics, and polyethylene. Fillings of steel balls with a diameter of 12.7, 9.5, 8, 6, and 3.2 mm, porcelain balls with a diameter of 6 mm, and high-pressure polyethylene granules in the form of ellipsoidal granules with a characteristic size of 3 mm were used in an environment with different oxygen content. In experiments with flat substrates, a number of normal alkanes (C_nH_{2n+2}) with numbers n=10, 11, 12, 13, 16, as well as alcohols: n-butanol (C_4H_9OH) and n-pentanol ($C_5H_{11}OH$) were used as fuels. In experiments with porous media, n-butanol was used as fuel. It is shown that the flame velocity increases faster with increasing oxygen concentration than the normal velocity of the corresponding homogeneous stoichiometric mixture. The range of flame speed change is 0.02 - 2.4 m/s when the proportion of oxygen in the mixture with nitrogen changes from 0.21 (air) to 1.

At flame propagation velocities above 0.3 m/s, the condition of thermal thinness is not met even for thin copper substrates. The flame propagation velocity ceases to depend on the properties of the substrate and the thickness of the fuel layer, and becomes dependent only on the properties of the fuel. The flame velocity increases linearly with the increase in the volumetric stoichiometric concentration of the fuel of a given homologous series. For all the studied fuels, the flame propagation velocity for this velocity range increases linearly with an increase in the thermal effect of a unit volume of a stoichiometric mixture of fuel vapors with an oxidizer and decreases with an increase in the difference between the temperature T_{st}, which forms a stoichiometric composition under equilibrium conditions, and the ambient temperature T_0.

It is shown that in porous media the flame velocity increases not only with an increase in the oxygen concentration, but also with an increase in the characteristic size of the porous medium element. At high speeds of flame propagation, the speed does not depend on the thermophysical parameters of the porous medium. At lower speeds (with less oxygen), the speed is higher in porous media with lower thermal conductivity. At high oxygen concentrations, the rate of flame propagation in a porous medium is higher than the normal velocity of a corresponding homogeneous stoichiometric mixture. The obtained experimental data are generalized in the form of a linear dependence of the Peclet number constructed on the characteristic size of the porous medium channel and the flame velocity v in laboratory system Pe_v on the Pe_{S_u} number constructed on the normal velocity S_u of the corresponding stoichiometric mixture.

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Catalytic methods for controlling the parameters of transformations of energetic compounds in the combustion wave

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The development of the component base for the energetic condensed systems (ECS) is aimed at the use of compounds with high values of density and formation enthalpy. New catalysts are needed for regulating the parameters of their combustion, which not only accelerate the oxidation processes by lowering the activation energy barrier, but also minimize its dependence on pressure. At the same time, they should not decrease the energy density of the condensed systems, thus it is appropriate to use stable metal-organic compounds of transition metals, containing energetic organic ligands and anions that play the role of oxidants. The balanced composition of the catalyst will facilitate the formation of nanoparticles of the catalytically active phase in the combustion wave, accelerating the process. However, there is still no unified theory explaining the mechanism of action of these catalysts.

In this work we analyzed the main tendencies of the research in the area of the catalysis of the transformations of energetic condensed compounds in the combustion wave and examined the current developments of the fundamental and applied studies on the effect of catalytic additives on the parameters of thermolysis and high-temperature oxidation of energetic compounds, depending on their nature. Using nickel, iron, and copper complexes with energetic ligands as examples, a catalytic effect on the combustion of nitroamine was shown.

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Kinetics and the mechanism of the chemical reactions of ammonia/hydrogen blends combustion and oxidation

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Ammonia is considered as a prospective hydrogen carrier as well as a carbon-free fuel. Its implementation enables to solve technical problems associated with hydrogen storage, transportation and distribution. However, pure ammonia has poor combustion properties, which include low burning velocity and high ignition energy. Hydrogen addition can be a possible solution. Moreover, hydrogen can be produced via ammonia cracking. The development of ammonia combustion and oxidation models requires experimental data obtained for different systems in a\ wide range of conditions. This study presents new experimental data on flame structure of ammonia/hydrogen flames as well as on the oxidation of ammonia/hydrogen blends in a jet-stirred reactor.

Flame structure was studied with the molecular-beam mass-spectrometric setup with soft electron-impact ionization. In the experiments, flames were stabilized at flat burner. Flame structure was measured at 1, 4 and 6 atm. Ammonia/hydrogen blends oxidation was studied in isothermal jet-stirred reactor in the temperature range from 900 to 1300 K. For numerical simulations, CHEMKIN package was used. Eight published mechanisms were tested on the experimental data obtained in this study.

It was shown that the addition of 30% of hydrogen shifts the onset temperature of intensive ammonia oxidation by 250 K towards lower temperature region. This nature of this effect is the increase of radicals' concentration, which take part in ammonia consumption process. The flame structure data revealed that the nitrogen-containing components, which are present in the post-flame zone in a significant concentration, are N_2 and NO, whereas N_2O and NO_2 concentration is negligible. Experimental data as well as numerical simulation showed that the transition from lean to rich conditions as well as the pressure increase reduce NO concentration in the post-flame zone as well as the peak concentration of N_2O and NO. The tested models correctly reproduce this trend. However, the quantitative discrepancies in the case of N_2O are larger compared to NO. For NO_2 models predict different dependence of its concentration on equivalence ratio and pressure. It was revealed that the submechanism of NOx formation and consumption needs further refinement.

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Effects of slope, wind velocity, flame retardant and spread direction on flame spread over a bed of Pinus silvestris pine needles

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Flame spread studies over forest fuel beds are important for understanding the dynamics of ground fire propagation. This data reports a systematic experimental and numerical study of important factors influencing the fire spread over a bed of pine needles from Siberian Boreal forests (Pinus silvestris). Factors such as slope of the fuel bed, wind velocity and direction of spread (coflow or counterflow), which play significant roles in determining the flame spread rate have been investigated. Careful measurements of gas phase temperature on and above the fuel bed surface, and total and radiative heat flux measurements are reported for coflow and counterflow flame spread under the influence of wind as well as for upslope flame spread in still air. This data serves as a validation of numerical model used for simulating the cases presented in this work. Numerical simulations have been carried out using a three-dimensional physics-based flame spread model available in Fire Dynamics Simulator Program package and the results are validated well against experimental flame spread rates. The validated numerical model is then used to simulate coflow and counterflow flame spread over a sloping fuel bed at wind affect. Predicted temperature, flow velocity and species concentration fields have been reported for selected experimental cases to understand the flow and flame dynamics in gas phase and within the porous fuel beds.

The effect of moisture and various commercially available fire retardants on the rate of flame spread over horizontally oriented single needles of pine litter in still air was studied. It has been shown that such an express method of analysis can be used to determine the effectiveness of a fire retardant on flame spread along a needles bed in still air. The influence of the type of the additive (water, 10% aqueous solution of fire retardant) and its loading concentration on the rate of flame spread over the bed of pine needles at the wind speed of 0 and 0.4 m/s was determined.

The obtained data can be useful for the development of effective fire extinguishing methods, as well as for the development of detailed numerical models describing the initiation, propagation and suppression of ground natural fires.

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Macro and microalloying of Ni_3Al-based porous SHS alloys to increase high-temperature oxidation resistance.

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A promising method to fabricate open porous intermetallics, ceramics and metal-ceramics with coarse porous structures is self-propagating high-temperature synthesis (SHS) or combustion synthesis. In this case porous material with given shape, pore structure and chemical composition is synthesized in one technological stage – combustion. The products obtained by this technology are widely used as the main functioning parts of solid oxide fuel cells, filters for flue combustion gases, flame arrestors, filtration combustion burners, catalytic systems, etc.

Modification of the chemical composition is the main way to improve the performance properties of materials. However, the SHS method is sensitive to changes in the initial conditions of synthesis, which often limits its applicability. To increase the high-temperature oxidative resistance of these alloys, it is necessary to carry out chromium macro-alloying and REM micro-alloying.

Following powders were used as starting reagents: nickel grade PNC UT-1 (Nornickel), aluminium grade PA-4 (Rusal), and chromium grade PCh1S (Polema) and aluminum PA-4 with Dy pre-deposited on its surface. All studied mixtures were doped with 0.05 wt% of an additive based on calcium salts that provide special conditions in the combustion wave needed to synthesize mm-sized structures.

In the case of micro-alloying of the REE of the green compact, there is a problem in the uniform distribution and the need to use a minimum amount of gasifying additives to prevent the volatilization of the microconcentration REE during the release of gases in the combustion wave zone. To do this, the powder mixture was premixed in mortar, after that, the required amount of aluminum with a Dy-coating on its surface powder was added. The resulting powder mixture was twice mixed in an SPD/0.5 three-dimensional shaker (Techno-center Elmash).

The report will highlight the latest results of the authors on the modification of the chemical composition of porous intermetallides based on the Ni-Al system used as porous infrared burners.

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Numerical study of flame burning velocity for ethanol/air mixtures in the presence of the ethanol dispersed phase

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Fuel combustion in engines and power installations often occurs in the presence of a dispersed phase. Although realistic combustors include turbulent flows and polydisperse droplets/particles, a fundamental investigation of the related physical and chemical processes can be performed for laminar flames with a monodisperse particle distribution. The combustion features of gaseous fuels in the presence of a sprayed monodisperse liquid phase are often studied for the model configurations, such as laminar counter-flow or stagnation flames.

One of the pioneer works is Burgoyne and Cohen [1], where the experimental evidence of the increase of flame propagation velocity in the presence of fuel dispersed phase was reported for conical flames. The effect was found for atmospheric burning of tetralin with droplets diameter typically exceeding 40 μm. Later, Hayashi et al [2] observed a similar effect for aerosol flames of ethanol and n-octane. An important observation was the existence of optimum droplets size resulted in maximum enhancement of the flame propagation speed. Neophytou and Mastorakos [3] in numerical one-dimensional study showed that under several conditions there was the possibility of reaching maximum flame propagation velocity in spray flame higher than maximum propagation velocity obtained in gaseous flame. Most of the subsequent works in numerical field were conducted for the model of counter-flow spray. However, to authors knowledge, there are still no numerical studies on laminar conical spray flame.

A three-dimensional numerical study of the combustion features of a laminar conical flame of ethanol aerosol in Euler-Lagrangian formulation was carried out on the basis of the direct numerical simulation approach. The burner represented an axisymmetric contraction nozzle. Two flame cases with the global equivalence ratio of 1.47 were compared, namely, when air/ethanol gaseous mixture with and without liquid droplets of ethanol issued from the nozzle. In the former case the droplets size corresponded to a monodisperse distribution with the diameter of 14 μm. The ethanol vapor concentration in air this case corresponded to the equilibrium concentration for the temperature of 23.8 °C, i.e. 0.134 g/l. The ratio between the gaseous and liquid ethanol mass flowrates corresponded 3.4:1. The Reynolds number for air flow without fuel was 1000. For the gaseous flame the laminar flame speed was 20 cm/s, whereas for the aerosol flame the speed was found to be 42 cm/s.

The study is carried out as the part of the state contract with IT SB RAS.

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On evaluation of temperature field in premixed flames based on thermally-assisted PLIF and two-line PLIF

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Gas temperature is very important for the understanding of combustion physical and chemical process, since it has a major impact on the rates of chemical reactions and, thus, on the combustion efficiency, pollutions formation and heat release rate. Reliable temperature measurements are required for validating numerical codes and theoretical models, as well as for the experimental diagnostics of flames. Despite the intrusive techniques, such as thermocouple probes, are easy to use, they distort the flow under the investigation. Laser-based methods are more relevant for the temperature measurements, as they are almost non-intrusive and have high spatial and temporal resolution. The planar laser-induced fluorescence (PLIF) technique can be successfully used for 2D temperature measurements.

PLIF method based on the excitation of two different transitions of the hydroxyl radical (two-line OH PLIF) can be implemented for thermometry in flames. The $Q_1(5)$:$Q_1(14)$ transition pair of (1-0) band of the $A_2\Sigma_+ – X_2\Pi$ electronic energy system is reported in many studies to provide the highest ratio of captured signals. The temperature evaluated with two-line PLIF is also known to be in a good agreement with the values of temperature obtained by other methods. However, performing the measurements using two-line PLIF, however, is associated by image processing difficulties, since two lasers are needed. A thermally-assisted PLIF approach is an alternative to measure 2D temperature distributions. This approach is based on a single-shot laser illumination and evaluation of the local ratio of intensity of two different vibrational bands emission. In particular, the ratio between the (2-0) band and (1-1), (0-0) bands provides almost linearly dependence on the temperature in the range from 1200 to 2200 K, when excited by the $Q_1(8)$ transition of the (1-0) band.

However, the proper interpretation of the fluorescence signal to remove different kinds of systematic errors is a key point to evaluate the temperature field from the PLIF images. The aim of this work is to demonstrate the signal processing algorithms and compare the temperature field measurements capability using the thermally-assisted PLIF and two-line PLIF for premixed methane/air, propane/air and ethylene/air flames. The PLIF measurements are performed for laminar Bunsen flames for the Reynolds number of Re = 1000 and lean mixtures. PLIF images are processed using a set of mathematical algorithms, including correction for spatial non-uniformity of the energy distribution in the laser sheet and the sensitivity of the recording camera matrices. Additionally, the procedure of background, dark current, and reflections removal is applied to the images. The spatial calibration of the PLIF cameras is performed using a calibration target.

This research was carried out in frames of the state contract with IT SB RAS.

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Pulsating instability of premixed methane-air flames stabilized on a flat porous burner

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It is known that the freely propagating premixed flames have intrinsic instability mechanisms, including hydrodynamic and thermo-diffusive instabilities. The thermo-diffusive instability arises due to an imbalance between the thermal and mass diffusivity of the mixture and their interaction with the curvature of the flame front, and is observed in mixtures with a non-unity Lewis numbers *Le*. In this case, for *Le* less than 1, the instability appears in the formation of cellular flames, while for *Le* greater than 1, pulsating instability is observed. Within a one-dimensional thermal-diffusion model with one-step chemistry and constant gas properties Sivashinsky's showed that for adiabatic unstrained planar flames the pulsating instability boundary is described by the criterion $Ze\ (Le - 1) = 4\ (1+\sqrt{3})$, where *Ze* is the Zel'dovich number. It has also been shown that heat losses enhance the occurrence of thermo-diffusive pulsating instabilities. A special case, which is studied in this work, in which heat losses can strongly affect the flame behavior is the case of flame propagation near the surface of a flat porous burner. In this case, at low flow rates of fresh mixture supply, the combustion front is located near the burner surface, where there are large heat losses to the walls, and because of the low inlet velocity, diffusion-thermal effects prevail and pulsating instability increases.

We analytically, numerically and experimentally investigated the onset and dynamics of thermo-diffusive oscillations of the combustion front stabilized over a flat porous burner, which occur when the stability boundary is crossed. The stability boundaries for a methane-air mixture depending on the fresh mixture flow rate, Lewis number and composition were determined. It was found that for system parameters selected near or moderately away from the stability boundary thermo-diffusive pulsations perturb the flame without changing its structure. It is noteworthy that, qualitatively the flame pulsation dynamics can be successfully predicted both by the model of a one-step irreversible reaction and by the system of nonlinear ordinary differential equations introduced in this paper, which models the evolution in terms of flame temperature and flame distance from the burner. In our opinion, this is only possible because the flame front behaves as a dynamically stable structure. However, as another result of this work shows, this is not always so. It is found that, as the system parameters shift from the stability boundary, the flame oscillation dynamics become more and more relaxational. In these highly relaxational modes of pulsation, the flame structure can be divided into two separate regions. The first one is characterized by low-temperature intermediates, such as HO_2 and H_2O_2 radicals. They form a reaction zone that is very close to the burner surface, and this reaction zone is weakly sensitive to perturbations imposed by thermo-diffusive fluctuations. Flame re-ignition occurs in this low-temperature region near the burner, and the pool of radicals existing here provides the chemical source for it. The other reaction region is located downstream of the first one and is characterized by high-temperature radicals such as OH, H, etc. This reaction zone is very sensitive to diffusion-thermal fluctuations. In the current setup this pool of radicals completely recombines and the buildup of a new pool of H and OH is happening after the flame reignites in the vicinity of the surface of the burner slightly downstream from the low-temperature reaction zone, like in a normal propagating combustion wave. This scenario is periodically repeated and the two reaction zones decompose and re-assemble during every period of oscillations.

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The flamelet approach for predicting polymer burning

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Generally, a numerical methodology of solid fuel combustion takes into account multicomponent fluid flow, gas-phase combustion, solid fuel pyrolysis and radiative heat transfer, with unsteady equations being formulated in two- or three dimensions. If a laminar flow regime is assumed, a model of gas-phase combustion is typically represented by one-step irreversible reactions with finite rate chemistry. This model reasonably predicts (in comparison with experiments) macroscopic (flame spread, mass loss of solid fuel sample) and local (temperature and species distributions, heat fluxes from gas to solid) parameters. It has to be noted, modeling of solid fuel combustion is not limited to one-step irreversible reactions, but reduced and skeletal mechanisms are applied as well. However, numerical solution of a stiff system of ordinary differential equations requires an extra computational time, which becomes unreasonable if a detailed chemical mechanism is applied.

One of the available approaches for reducing computational time is the flamelet concept, which separates the chemistry step from the fluid flow (convection-diffusion) step. Reacting gas flows in combustion systems mostly are turbulent. Nevertheless, in case of a flame spread over polymers experiments show distinct laminar flow regime in the flame front in the vicinity of the burning surface. This area governs most of heat transfer from flame to solid material, which forces flame to spread. Thus, an assumption of laminar flow regime for such systems seems appropriate, and the flamelet model can be applied here. Originally, the flamelet model was developed for turbulent combustion, but it can also be applied to laminar flow regime.

One of the main assumptions for derivation of the flamelet equations is two separate supplies of gaseous reactants — fuel and oxidizer — with fixed compositions and temperatures. However, such method can't be applied directly to the solid fuel combustion, because of non-uniform temperature of a burning surface, which supplies gaseous fuel.

Here, we propose a method to extend the flamelet concept to combustion of solid fuels by applying of existing non-adiabatic formulation of the flamelet model to take into account non-uniformity of gaseous fuel temperature. The numerical results of flamelet computations based on detailed kinetic mechanisms are to be compared with one-step irreversible chemistry model.

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An investigation of combustion of near-stoichiometric mixtures of flammable gas – oxidizer - fluorinated hydrocarbon in a closed vessel at various oxygen contents in the oxidizer

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An experimental study of an influence of an oxygen content in an oxidizer (mixture of O_2 and N_2) on the combustion characteristics of near stoichiometric mixtures of combustible gas (hydrogen, methane) – oxidizer – fluorinated hydrocarbons (HFC) (trifluoromethane CHF_3, pentafluoroethane C_2HF_5, perfluorobutane C_4F_{10}) was carried out. A concentration of oxygen in oxidizing atmosphere was 15, 20.6 (air) and 25 % (vol.). Dependences of a maximum explosion pressure ΔP_{max}, a maximum pressure rise rate on the explosion $(dP/dt)_{max}$ and a laminar burning velocity S_{ui} on a content of the fluorinated hydrocarbons were determined at various oxygen concentrations in the oxidizing atmosphere.

Experiments were carried out on a spherical set-up having a reaction vessel of an internal diameter of 20 cm (volume 4.2 dm^3). Gaseous mixtures were created in a preliminary evacuated reaction vessel by partial pressures and ignited by an electrical spark in a center of the vessel. Parameters of an explosion were measured with a pressure detector.

It was shown, that at relatively low contents of the fluorinated hydrocarbons C_d (up to 30 – 50 % from those in peak points of flammability curves) a maximum explosion pressure elevates from its value in an absence of HFC. It was found that the lager is the molecule of the fluorinated hydrocarbon the higher is its inertization ability is relation of such parameters as $(dP/dt)_{max}$ and S_{ui}. A qualitative interpretation of the obtained results is given, based on the concept of an additional heat release during chemical transformations the fluorinated hydrocarbons in a flame front. These chemical reactions are the following:

$$CHF_3 + 0{,}5O_2 = 0{,}5CF_4 + 0{,}5CO_2 + HF + 240\ kJ, \qquad (I)$$
$$C_2HF_5 + O_2 = CF_4 + CO_2 + HF + 478\ kJ, \qquad (II)$$
$$C_4F_{10} + 1{,}5O_2 = 2{,}5CF_4 + 1{,}5CO_2 + 739\ kJ, \qquad (III)$$
$$H_2 + 2CHF_3 = 0{,}5CF_4 + 4HF + 1{,}5C + 166\ kJ, \qquad (IV)$$
$$H_2 + 2C_2HF_5 = 1{,}5CF_4 + 4HF + 2{,}5C + 247\ kJ, \qquad (V)$$
$$H_2 + C_4F_{10} = 2CF_4 + 2HF + 2C + 228\ kJ, \qquad (VI)$$
$$CH_4 + 2CHF_3 = 6HF + 3C + 172\ kJ, \qquad (VII)$$
$$CH_4 + 2C_2HF_5 = CF_4 + 6HF + 4C + 252\ kJ, \qquad (VIII)$$
$$CH_4 + 2C_4F_{10} = 4CF_4 + 4HF + 5C + 228\ kJ. \qquad (IX)$$

The obtained result is qualitative close to that fined for near mixtures of the same composition.

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Combustion initiation in a flow by simultaneous action of laser radiation and an external electric field

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The use of plasma to initiate and stabilize combustion has the potential to reduce the need for mechanical flame stabilizers. After mechanical flame stabilizers, as a rule, stable, subsonic combustion zones are installed, which stabilize combustion in a cocurrent high-velocity flow. With an increase in the flow rate, the stabilization of combustion deteriorates. The additional introduction of an injector or stabilizer will lead to an increase in total pressure losses, which increase with an increase in the free flow velocity.

Experimental modeling. An experimental study was made of the initiation of combustion in a supersonic flow of a hydrogen-air mixture under the simultaneous action of focused repetitively pulsed CO2 laser radiation and an external electric field. Combustion in a supersonic jet was studied on the basis of data on the intrinsic glow of the flame at the wavelengths of radiation of excited OH* radicals. In the experiment, the shape of the incident radiation pulse was recorded, as well as its temporal characteristics at different frequencies, and the shape of the incident radiation pulse was fixed. Two cases of ignition initiation of a hydrogen-air mixture in a flow were considered: 1 - ignition and stabilization of the mixture by an optical discharge, 2 - ignition and combustion stabilization by an optical discharge, in the presence of an electric discharge.

Numerical simulation. A mathematical model of diffusion combustion of hydrocarbon fuel in flat and axisymmetric channels is constructed. The non-stationary problem of ignition and combustion in a high-speed flow of a homogeneous air-fuel mixture (H2+air) is considered. The problem is solved using two-dimensional Navier-Stokes equations. At the initial moment of time, a high-temperature region is set in the flow in the form of a circle with a Gaussian temperature distribution. The mathematical model of the energy source describes the physical phenomena characteristic of pulsed energy supply using focused laser radiation directed perpendicular to the flow. The speed of the incoming hydrogen-air mixture varied in the range u=100--500 m/s. At the initial moment of time, a region with an instantaneous heat supply is modeled in this flow. It has been found that with an increase in the oncoming flow velocity, the growth rate of the ignition region diameter slows down. At the maximum free flow velocity considered (500 m/s), an increase in the diameter of the ignition region was practically not observed.

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Development of the chemical-kinetic mechanism of pyrolysis and combustion of triphenyl phosphate: the structure of the $H_2/O_2/Ar$ flame with the addition of TPP, quantum chemical calculations, numerical simulation

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Synthetic polymeric materials have many advantages, however, most of them are combustible substances, so this disadvantage significantly limits their scope. The main method for reducing the flammability of polymeric materials is the introduction of flame retardants into them. An effective search for effective flame retardants requires information on the chemistry and mechanism of their transformation in a flame.

In order to establish the mechanism and kinetics of chemical reactions of the conversion of the model phosphorus-containing flame retardant triphenyl phosphate (TPP), the high-temperature pyrolysis of its vapors in Ar was studied experimentally and by quantum chemistry methods, and the conversion of TPP vapors in $H_2/O_2/Ar$ flame at a pressure of 1 atm was also studied. The mass spectra of the products of thermal decomposition of TPP vapors in a thermal flow reactor in the temperature range of 300–1000 °C and the spatial distribution of the concentration of TPP and phosphorus-containing products of its transformation in a flame of a stoichiometric mixture of $H_2/O_2/Ar$+0.1% TPP stabilized on a flat burner were measured by probe molecular beam mass spectrometry. Using the B3LYP method in the framework of the density functional theory (DFT) with the 6-311G(d,p) basis set, calculations were performed to optimize the geometry of all structures on the considered potential energy surfaces of TPP and products of primary and secondary decomposition of TPP. Also, the kinetic rate constants of the thermal decomposition of TPP and its reactions with the participation of H, OH, and CH_3 radicals were calculated using the Rice-Ramsberger-Kassel-Marcus theory and the basic kinetic equation method (RRKM-ME) implemented in the MESS software code. The thermochemical parameters for TPP and products of primary and secondary decomposition of TPP in the temperature range 200-6000K was calculated.

Based on the results of calculations, as well as the mechanisms of transformation of the phenyl and phenoxyl radicals from the literature, a combined detailed chemical-kinetic mechanism was developed that describes the pyrolysis of TPP vapor in an inert medium, as well as the conversion of TPP vapor in a hydrogen-oxygen flame. Comparison of the results of numerical simulation of the concentration profiles of TPP and the main products of its conversion in a $H_2/O_2/Ar$ flame showed that the developed mechanism satisfactorily describes the chemical structure of the studied flame, including the concentration profiles of intermediate phosphorus-containing TPP conversion products. The developed mechanism of TPP transformation can be used for numerical simulation of flame propagation through polymeric materials with the addition of phosphorus-containing flame retardants.

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Development of a Genetic Algorithm Tool for the Optimization of Chemical Kinetic Model for the Methanol Oxidation

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This work focuses on the development of an optimization tool based on genetic algorithm and the open-source software Cantera for the chemical kinetic model. The chemical kinetic model of 72 species and 610 reactions developed at Technical University of Munich has been optimized for the CH_3OH oxidation. Uncertainty analysis and modification have been carried out for 54 parameters including reaction rate constants and third body efficiencies for 40 key reactions.

Experimental data of ignition delay times measured in shock tubes and concentration profiles measured in jet-stirred reactor and plug flow reactor were collected for the model validation. The 0-dimensional reactor models of 'Ideal Gas Reactor' and 'Constant Pressure Ideal Gas Reactor' were used for the simulations of ignition delay times and concentration profiles.

54 reaction rate constant parameters of the initial model are modified by the genetic algorithm. The prediction ability of the model has been improved for the simulation of ignition delay times and concentration profiles of CH_3OH oxidation. The developed genetic algorithm tool and optimization strategy was proved to be useful and efficient for the optimization of the detailed chemical kinetic models.

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Synergistic effects in flames of mixtures of methane and carbon monoxide with air

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Numerical simulation has shown that replacing a part of methane by carbon monoxide in a rich mixture while maintaining the equivalence ratio leads to a decrease in the superadiabatic temperature effect due to the competition of chemical reactions. This is explained by a decrease in the H content in the combustible mixture and a decrease in the superequilibrium concentration of water in combustion products. Using numerical tracer simulation and a comparative analysis of the rates of consumption of CH_4 and CO, it has been found that the consumption of both fuels in the CH_4/CO/air flame is a competitive reaction path and CO monoxide does not act as an inert component in the low-temperature region of the front (contrary to the statements of a number of authors). Furthermore, the rate of consumption of CH_4 is much higher than that of CO due to the larger number of consumption reactions of CH_4 and their higher rates. The main contribution to the increase in the concentration of H atoms in the flame in passing from a methane–air mixture to a CH4/CO/air mixture is due to the same reactions that increase the heat release rate: $O + CH_3 = H + CH_2O$ and $CO + OH = CO_2 + H$. The results obtained and their comparison with literature data lead to the conclusion that the increase in the heat release rate and, hence, the flame propagation rate should be greater in rich mixtures since there the thermophysical effect is higher.

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Experimental study of diffusion combustion of interacting hydrogen microjets

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Scenarios of diffusion combustion of a hydrogen microjet flowing from an elongated cylindrical tube into a flooded space are described in [1]. The objectives of this experimental study: 1) to determine the main features of the combustion of a hydrogen microjet flowing out together with an air flow from a nozzle apparatus with a coaxial arrangement of nozzles in a direct and reverse flame configuration; 2) to determine the main features of the combustion of single microjets oriented at a small angle to each other, the flames of which interact to form the resulting flame. The scheme of the experiment with a nozzle apparatus providing the supply of air and hydrogen from coaxial micronozzles is shown in Fig. 1, and the scheme of the experiment for interacting microjets is shown in Fig. 2.

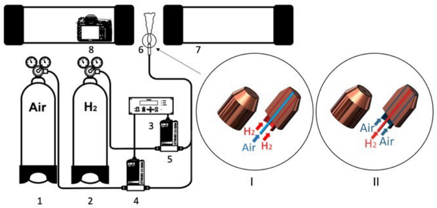	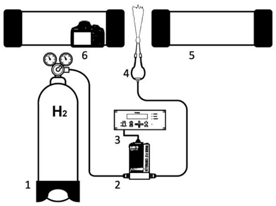
Fig. 1. 1 – cylinder with compressed air, 2 - cylinder with compressed hydrogen, 3 – 2-channel flow meter controller MKS PR4000B (MKS Instruments) 4, 5 – flow meter valve MKS 1179B (MKS Instruments), 6 – coaxial nozzle apparatus, 7 – IAB-451 shadow device, 8 - Nikon D7500 digital camera with AF-S NIKKOR 18-105mm lens, 9 - CEM DT-9897H thermal imager.	Fig. 2. 1 – cylinder with compressed hydrogen, 2 – 2-channel flow meter controller MKS PR4000B (MKS Instruments), 3 – flow meter valve MKS 1179B (MKS Instruments), , 4 – pair of nozzles d*1* = *d2* = 200 μm, 5 – IAB-451 shadow device, 6 - Nikon D7500 digital camera with AF-S NIKKOR 18-105mm lens, 7 - CEM DT-9897H thermal imager.

Fig. 3 shows the scenarios of diffusion combustion of a hydrogen microjet flowing out together with an air flow coming from the annular slot, and Fig. 4 shows the shadow patterns of the inverted flame when the supersonic air flow comes from the microjet, and hydrogen from the annular slot. Fig. 5 shows the results of experiments in the case when 2 single hydrogen microjet interact.

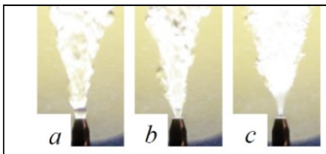	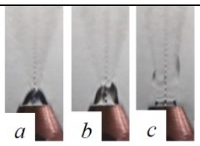	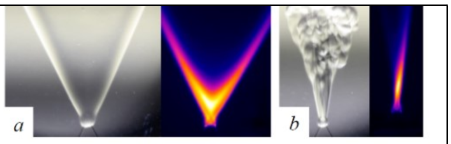
Fig. 3. Diffusion combustion of hydrogen direct flame	Fig. 4. Diffusion combustion of hydrogen inverted flame	Fig. 5. Interacting two single microjets of hydrogen

As a result, new combustion scenarios for interacting microjets were obtained.

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Temperature field measurements in a Bunsen flame in a weak DC electric field

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Stabilization of flames in burners and combustion chambers is typically provided by organizing local flow recirculation or stagnation zones. However, such zones can lead to local overheating of the combustor parts and increased hydraulic losses. Moreover, for lean premixed combustors, which are now commonly used for low-emission fuel burning (for NOx and soot) in gas turbines, large recirculation zones should be avoided to prevent long residence time of the hot combustion products, which contain nitrogen and oxygen. Thus, the development of alternative flame stabilization methods for burners combustors are of interest. The application of an electric field to hydrocarbon flames has been proven to increase the flame stability (e.g., see [1]). Different physical and chemical mechanisms that may affect the flame have been discussed in literature. While most authors agree that weak electric fields can significantly affect the flame propagation speed, there is a lack of data on the changes in temperature distribution. Further research is needed to investigate this topic.

The aim of the present study was to investigate the effect of a constant electric field on the temperature distribution in laminar cone-shaped premixed flames of different mixtures (methane/air, propane/air). The fuel equivalence ratio of the mixtures was 0.92 and 0.85, respectively. The focus was placed on the comparison of the temperature distribution for the flames with and without the electric field. The flames were organized by a burner, which represented a contraction nozzle, made of caprolactam polymer, with the nozzle diameter of 15 mm. The Reynolds number of the non-reacting flow corresponded to Re = 1000. A constant electric field with strength of 62.5 kV/m in the transversal (normal to the cone axis) direction was applied by placing two parallel metal plates. A two-line planar laser-induced (PLIF) method was used to measure the flames temperature based on the fluorescence of OH molecules for different excitation transitions of the (1-0) vibrational band of the $A_2\Sigma_+$–$X_2\Pi$ electronic system. The PLIF system was composed from a pulsed tunable dye laser, pumped by a pulsed Nd:YAG laser, an intensified sCMOS, equipped with intensified relay optics, lens and filter, and from a synchronization device.

During the experiments, photographs of the flames were captured, as well as the OH PLIF images for $Q_1(5)$, $Q_1(8)$ and $Q_1(14)$ transitions. A number of image post-processing routines have been used to account for image background, non-uniformity of the laser light in the measurement plane and others. Besides, the linearity of the PLIF regime has been tested for each excited transition. Finally, the temperature fields were obtained based on the ratio $Q_1(5)$:$Q_1(14)$ for flames both with and without the electric field. It was observed that the electric field changes the flame shape inclining and deforming the cone in the direction normal to the plates. The differences in the OH temperature behind the flame front are planned to be discussed during the presentation.

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Influence of H_2O concentration on hydrogen combustion in a hot vitiated air coaxial jet

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Results of numerical studies of the water vapor concentration effect on the ignition and combustion of a round hydrogen jet in a coaxial jet of hot vitiated air expanding into a still space are presented. Numerical simulation was carried out in ANSYS Fluent 2020 R1 on the basis of the transient Favre-averaged Navier-Stokes equations for a multicomponent viscous heat-conducting gas, supplemented by the κ–ω SST turbulence model and the detailed kinetic scheme of hydrogen combustion in air [1]. Comparison of the calculated profiles of the flow parameters and species mass concentrations with experimental data [2] (Fig.1) have shown qualitative and quantitative agreement. In Fig 1, x stands for a distance from the jet exit, and d_j is the diameter of the hydrogen jet.

The paper presents a detailed analysis of the instantaneous, average and pulsating flow parameters as well as the species concentrations and reaction rates in a wide range of the water vapor mass fraction in the air jet ($0 \leq Y_{H2O} \leq 0.2$). Plots of the H_2 combustion efficiency for various water vapor mass fraction are presented in Fig. 2. For all calculated cases, the combustion efficiency coefficient reaches a constant value of approximately 1 in the jet farfield $x/d_j > 50$. However, in the jet nearfield ($x/d_j < 20$), significant differences are observed in the combustion efficiency due to the influence of the H_2O concentration in the oxidizer composition.

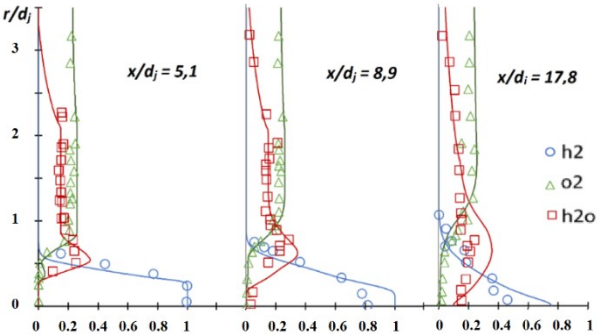

Figure 1. Comparison of calculated and experimental profiles of species mass fraction for $Y_{H2O} = 0.15$.

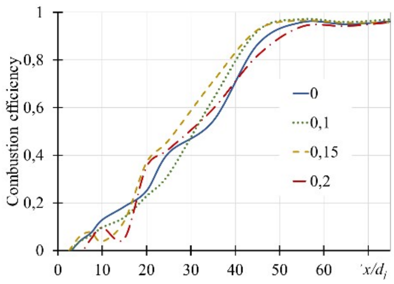

Figure 2. Combustion efficiency for different Y_{H2O} in air jet.

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Is the Arrhenius Formula for Ignition Delay Exact for Detonation?

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For ignition processes, the heating of the initial and intermediate substances to temperatures at which they begin to glow is characteristic. The appearance of their radiation can be detected experimentally, therefore, the time interval from the "start" of a chemical reaction until the moment the glow appears is called the ignition delay of the combustible mixture.

Traditionally, τ is measured in adiabatic compression setups (low temperature T) and shock tubes (high T behind incident and reflected shocks) and is represented by an well known Arrhenius-type formula. Numerical coefficients – E_{act}, A, n_i, , … are obtained by approximating experimental data on τ under the assumption of homogeneity and invariance of gas-dynamic parameters in the range $0<t<\tau$. Then, the kinetic coefficients obtained in this way are formally transferred to the detonation conditions and, using them, the characteristic temporal and spatial scales of detonation waves (DW), critical initiation energies, etc. are calculated.

Today in most cases we have to talk only about the qualitative behavior of the detonation parameters calculated using these coefficients, quantitatively these values diverge noticeably, especially for fuel-air mixtures. This is clearly demonstrated by the gradual dilution of fuel-oxygen mixtures with nitrogen and the transition to fuel-air mixtures: for most of the studied combustible gaseous systems, an increasing discrepancy between the experimental and calculated values is observed as the nitrogen concentration increases. This discrepancy noticeably reduces the reliability of the calculated predictions of the behavior of detonation in combustible systems.

Note that the problem of a priori determination of the kinetic coefficients for detonation conditions has not yet been solved. This state is due, among other things, to the difficulties of experimentally determining the kinetic parameters for detonation conditions due to the fact that the structure of the detonation flow, due to its strong local inhomogeneity and nonstationarity, differs greatly from classical model representations (one-dimensional Michelson–Chapman–Jouguet and Grib– Zel'dovich–Neumann–Dering with smooth fronts).

The assumption of homogeneity and constancy of the parameters up to the moment of ignition of the mixture does not fit well with the idea that during τ, due to an increase in the number of particles in the system due to the decay of the initial particles and the formation of intermediate radicals, the molar concentrations of the initial components cannot be constant. Therefore, instead of the assumed Ci=const, the real concentrations c in the denominator of the Arrhenius formula should be noticeably smaller, which will lead to an increase in τ. Only taking this into account makes it possible to significantly bring the experimental and calculated data closer together.

Note that taking into account the increase in the number of particles in the system can significantly change all the coefficients of the Arrhenius formula, not only in relation to detonation, but also to the ignition of the mixture. It should be specially emphasized that the schemes of detailed kinetics currently existing (several thousand elementary stages for heavy hydrocarbons) are also based on the assumption ci=const in the range $0<t<\tau$.

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Oscillatory flame dynamics in porous media

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Research on unstable combustion is crucial as it directly affects the safety and reliability of burners in domestic and industrial sectors. Flames in porous media are prone to oscillatory behavior due to repetitive extinction and ignition (FREI). This phenomenon has been well-studied in narrow channels with external heating, but porous media burners have many channels, mostly irregular, making it unclear how oscillatory combustion works in such systems.

To address this, we conducted a pore-scale numerical investigation of flame dynamics in a two-dimensional pseudo-irregular packed bed of particles generated by Voronoi tessellation algorithm. The figure below presents the geometrical model in part “a.” Our mathematical model involved simulating mixture flow with chemical reactions, conjugate heat transfer, thermal conductivity, and radiation.

Our study found that the flame began to oscillate at around 18 cm/s velocity, with a transition between stable and FREI accompanied by transitional oscillations with small amplitude and incomplete flame extinction, but with significant variation of heat release rate. The stoichiometric flame demonstrated a lower region of transitional flame, and after reaching 2 cm/s, the flame stabilized again in the form of a weak flame (see a regime diagram for the case of $\varphi = 1$ in part "b" in the figure below).

Local perturbations in some pore channels significantly varied the local flow resistance during the oscillation cycle, resulting in a "hydrodynamical" interaction between flame fragments. In isolated pores, the adjacent flame front fragments oscillated synchronously, and coupling near critical flow velocity could be a source of stability loss in the entire combustion region. Multichannel systems play an important role in entire flame dynamics, unlike single narrow channels.

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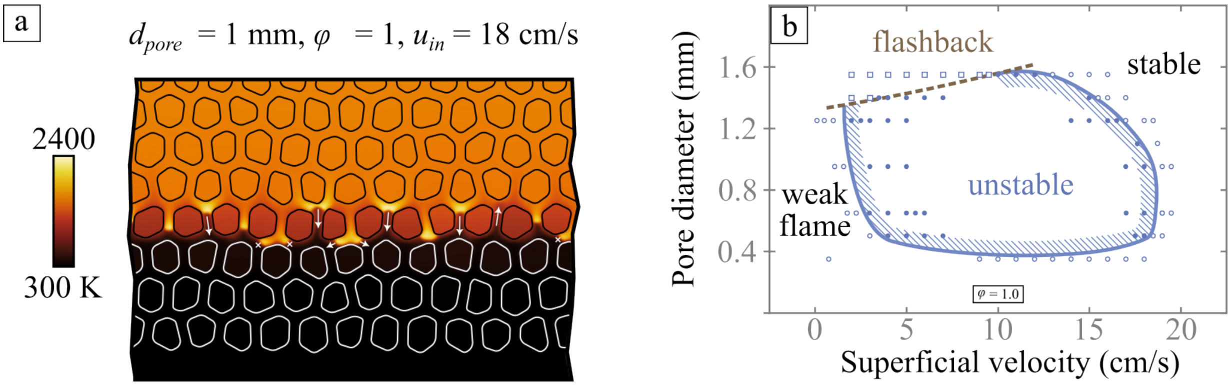

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Laminar flame propagation in Hele-Shaw cells of various geometry

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Hele-Shaw cells formed by closely spaced parallel glass plates are a specific type of channels having one dimension (gap size) much smaller than the other two (length, width). Laminar flame propagation in such channels is quasi-two-dimensional; yet, it exhibits many features of three-dimensional flames, including the development of instabilities, cell formation, transient behavior etc. Transparent channel walls allow easier study of such flames by video recording than in the full three-dimensional setup. On the other hand, flame propagation in narrow planar channels is of interest in such applications as micro-combustors, micro-engines, as well as fire and explosion safety. In this work, several configurations where premixed laminar flames are propagating in narrow gaps are presented, including recent experimental and numerical results on combustion in Hele-Shaw cells with or without internal obstacles. Experimental results are supplemented by corresponding three-dimensional numerical simulations.

For unobstructed narrow channels, cellular flame structure is studied experimentally, with the visible flame speed and cell size determined as functions of the channel gap width. It is shown that the flames propagating radially from the ignition point rapidly develop cellular structure, with the average lateral size of the cells about 10 times larger than the gap width. The cells are appearing and disappearing dynamically on the flame front as the flame radius is increasing. The paths of the cusps separating the cells are visualized by taking the long-exposure photos, demonstrating the propagation of stable cell pairs along straight trajectories, and complex interactions between the cells in the space between these lines.

Flame acceleration by obstacles is traditionally studied in application to deflagration-to-detonation transition problem, with the emphasis on the overpressure development. In this work, flame interaction with obstacles was studied experimentally and numerically in a Hele-Shaw cell having one or several internal obstacles separating the cell into chambers connected with small holes. These configurations are featured by very high blockage ratio; the studies are relevant to the problem of flame penetration through narrow gaps in fire and explosion safety. It is shown that flame propagation from closed to open channel end is promoted by the piston action of the gas due to the large pressure difference developing across the obstacle. Also, in this case the mixture in the open channel part is turbulized by the gas outflow before the actual flame penetration, which hastens its subsequent combustion. Flame penetration from open to closed channel part proceeds differently, with no significant turbulization ahead of the flame. Therefore, the concentration limits of flame propagation through small gaps depend significantly upon the channel geometry and ignition point location.

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Permeate combustion of 3D printed polymer grain for hybrid rocket engine

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The advent of various additive manufacturing technologies, such as 3D printing, has changed the structural design and preparation process of rocket fuels. In order to investigate the combustion properties of common polymer materials that can be additively manufactured by fused deposition, the combustion tests of hybrid rocket fuels prepared by 3D direct-writing (DIW) printing were carried out. These materials include polylactic acid (PLA), acrylonitrile-butadiene-styrene (ABS), acrylonitrile-styrene-acrylate (ASA), copolymers of nylon 6 and nylon 6,6 (CoPA), polycarbonate-polybutylene terephthalate (PC-PBT) and polyethylene terephthalateco-1,4-cylclohexylenedimethylene terephthalate (PETG). Thermogravimetric-differential scanning calorimetry (TG-DSC) analysis was carried out on these materials, the printing effect of the fuel grains were observed by three-dimensional X-ray microscopy (μCT) and the combustion performance of these fuels in gaseous oxygen flow (G_{OX}) was recorded by a high-speed photography at a constant pressure of 1MPa. The results show that the fuel grain manufactured by 3D printing produces a permeation combustion phenomenon which promotes regression rate well, and ABS is one of the best materials for polymer materials for fuel grain.

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Effect of fuel injection scheme on mixture formation and combustion processes in rotary engine

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The numerical simulation of mixture formation and combustion processes in syngas-fueled rotary engines was provided. The effect of different types of fuel injection on turbulent flame propagation was investigated. The idea of using port injection (PI) and direct injection (DI) simultaneously in a rotary engine is realized in a novel concept of dual injection with the integration of each injection type. It was shown that adjusting PI and DI timings could effectively control concentration stratification. In order to understand the effect of dual injection on mixture formation and combustion processes, the ratio R of fuel mass delivered by port and direct injection was varied from 0.0 (DI only) to 1.0 (PI only), including 0.1, 0.25, 0.4, 0.5, 0.6, 0.75, and 0.9.

The contour of equivalence ratio spatial variation and turbulent velocity fluctuation in the combustion chamber for ratios $R = 0.0$, 0.4, 0.9, and 1.0 is shown in Fig. 1. The complex individual structure of fluid motion is formed during the dual injection. The mixture homogeneity gradually decreases with the transition of R from 1.0 to 0.0, and the maximum non-uniformity is observed in the DI case. For cases $R = 0.0$, 0.4, and 0.9, the front side of the combustion chamber is occupied by a highly distorted air-fuel mixture with lean and rich regions. The specified direct injection process affects turbulence intensity enhancement or reduction. The fluid motion induced by the direct injector for each R interacts with existing fluid motion in a combustion chamber after port injection and air induction in a different way.

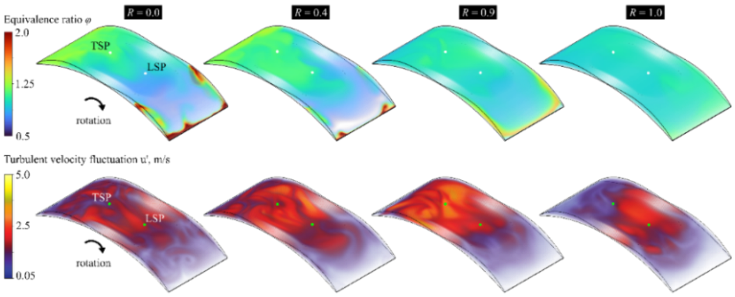

Figure1 Equivalence ratio and turbulent velocity fluctuation at top dead center for various dual injection ratios

Performance characteristics of the rotary engine increase linearly with the diminishing of the dual injection ratio. This effect was explained by an increased mixture mass charge in the wake of higher volumetric efficiency for the DI case. Minor portions of DI ($R = 0.75$ and 0.9) increase the fuel conversion efficiency by 7% and decrease specific fuel consumption by 6% in comparison with PI and DI schemes. Generally, the optimal fuel injection strategy in the considered syngas-fueled rotary engine is characterized by high-degree homogeneity along with advanced turbulence.

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Effect of temperatures on flame propagation of diethyl ether spray explosion

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The study aims to identify the flame propagation characteristics in the diethyl ether (DEE) spray explosion. Different ambient and material temperatures' effect on flame propagation and structure was investigated in a 20-L explosion vessel. Greyscale histograms are obtained from the high-speed images to distinguish the combustion and explosion zones. With the ambient temperature increased, the combustion duration showed a trend of first decreasing, then increasing, and then decreasing again. The combustion zone first increased and then decreased. The explosion duration showed an overall decreasing trend. The explosion duration was longer than the combustion duration, ranging from 152.75 to 307 ms. When the ambient temperature was 308.15 K, the combustion duration reached its minimum value of 13.25 ms, and the equivalent radius of the combustion zone reached its maximum value of 52.89 mm. With the increase in material temperature, both the combustion and explosion durations showed a trend of first decreasing and then increasing, with combustion durations ranging from 12.42 to 16.25 ms and explosion durations ranging from 106 to 117.5 ms, respectively. The difference in the equivalent radius of the combustion zone under different material temperatures was slight, and the influence of material temperature on the development of the combustion zone was relatively small. When the material temperature was 308.15 K, the combustion zone expansion rate reached its maximum value of 10.20 m/s, and the explosion zone expansion rate reached its maximum value of 13.36 m/s. The flame instability and flame propagation velocity in the explosion zone were both greater than in the combustion zone.

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Modeling of the behavior of uranium compounds during the burning of radioactive graphite in water vapor with the addition of oxygen

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As of 2022, according to data [1], 11 nuclear power plants with 37 power units are in operation in the Russian Federation, of which 9 are high-capacity channel reactors, which is about 25% of the total number of power units of the Russian Federation.

After decommissioning, radioactive graphite must be disposed of. One of the methods of disposal of radioactive graphite is combustion in water vapor with oxygen additives.

The physicochemical bases of processing radioactive graphite in the atmosphere of water vapor with the production of combustible gas are being developed [2], followed by the production of electricity. To change the composition of the gas, it is proposed to add oxygen to the water vapor. The calculation results allow us to understand the behavior of compounds of various radionuclides during such processing contained in radioactive graphite. For the purposes of scientific interest, uranium compounds were considered.

In this work, thermodynamic modeling of processes in the TERRA software complex occurring during heating and burning of radioactive graphite in water vapor with the addition of oxygen, namely the behavior of uranium compounds, is carried out.

Table 1 presents the results of thermodynamic modeling of the combustion of radioactive graphite in water vapor with the addition of oxygen in the temperature range from 573 K to 1073 K.

Table 1. Distribution of molar fractions of uranium compounds in the temperature range from 573 K to 1073 K.

Temperature, K	Uranium compounds, mol. %			
	UO_2(cond)	UO_3	$CaUO_4$(cond)	UO_3^-
873	99,47	$4{,}86\cdot10^{-16}$	0,26	$2{,}5\cdot10^{-8}$
973	96,87	$7{,}86\cdot10^{-13}$	1,56	$2{,}31\cdot10^{-6}$
1073	93,43	$3{,}74\cdot10^{-10}$	3,28	$8{,}81\cdot10^{-5}$
1173	92,44	$6{,}2\cdot10^{-8}$	3,78	$1{,}67\cdot10^{-4}$
1273	92,3	$4{,}53\cdot10^{-6}$	3,83	0,02
1373	92,29	$1{,}75\cdot10^{-5}$	3,81	0,05
1473	92,33	$4{,}08\cdot10^{-4}$	3,77	0,06
1573	92,46	0,06	3,64	0,07
1673	92,34	0,69	3,3	0,13
1773	87,98	5,8	2,54	0,53
1873	53,99	38,13	1,13	2,94
1973	99,47	$4{,}86\cdot10^{-16}$	0,26	$2{,}5\cdot10^{-8}$

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Pollution of the atmosphere by toxic combustion products in case of fires in the production of polyurethane foam

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In order to assess the environmental hazard of fires at enterprises producing polyurethane foam, studies were carried out to study the composition and quantity of fire products. To obtain the required data, methods for determining the qualitative and quantitative composition of fire products based on gas chromatography, chromatography-mass spectrometry, IR-Fourier spectrometry, etc.

Studies have shown that when a polyurethane foam product is ignited, up to 30 substances with a certain level of toxicity are released. The most dangerous among them are (in terms of unit mass): hydrogen cyanide - 1.0%; carbon monoxide - 15.5%; toluene diisocyanate (TDI) - 10.0%. When burning TDI, the main dangerous toxic component of fire products is hydrogen cyanide - 7.8%.

On the example of a typical enterprise, scenarios for the development of fires are considered and estimates of areas dangerous for gas contamination and smoke are given. The calculated scenarios of fires with the greatest environmental hazard are determined: fire over the entire area of the finished product warehouse; fire over the entire area of the warehouse of maturing blocks; fire over the entire area of the intermediate warehouse; spill and burning of TDI over the entire area of the warehouse.

The assessment of the possible environmental hazard of fires was based on the calculated values of concentrations of the main toxic combustion products of materials used in production.

The calculation of the maximum concentrations of toxic fire products for the selected scenarios of the maximum possible fire and in the worst weather conditions was carried out. The calculation of gas contamination zones during fires was carried out using a mathematical model of impurity transfer, taking into account the terrain and building density.

It has been established that concentrations of the fire products values are preserved in the surface layer of the atmosphere during the period of active combustion. In case of fire in the warehouse of finished products - 25-30 minutes; in case of fire in the warehouse of maturing blocks - 90-100 minutes; in case of fire in the intermediate warehouse - 55-60 minutes; in case of fire in the warehouse of TDI - 30 minutes.

The boundaries of hazardous gas contamination zones have been determined, the preservation of which in the surface layer of the atmosphere is determined by the time of fires. It is established that the greatest danger may be a fire in the warehouse of finished products. The zone of dangerous concentrations and elevated concentrations of fire products in this case reaches a distance of up to 150 m.

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Influence of the characteristic size of a woody biomass particle in the shape of a cube on characteristics and ignition conditions

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The modern "green" agenda makes significant adjustments to the development strategies of the energy sector in many countries. The latter primarily include wind power generators (wind farms) and solar panels, secondly, geothermal power plants, ocean power plants and wave power plants , etc. can be attributed to the URES. However, all these URES have one significant drawback – the generation of electricity with their help is significantly non-stationary and depends in a decisive way on weather conditions. In this regard, bioenergy is beginning to acquire a new impetus for development, in particular, technologies for burning wood biomass in furnace devices of boiler units of thermal power plants. Unlike other renewable energy sources, wood biomass combustion technologies do not depend on weather conditions and, accordingly, stably provide electricity generation in accordance with the load schedule of the power grid. In the world scientific periodicals, as a rule, great attention is paid to the study of the laws of flame propagation in relation to the spread of combustion processes of condensed substances over large areas (forest fires, indoor fires). Also, much attention is paid to the study of flame propagation processes during ignition of methane-air or hydrogen-oxygen mixtures. But it can be reasonably argued that the study of the processes of flame propagation in the zone adjacent to the surface of the particle during the induction of wood biomass has not been carried out to date.

The purpose of this work is to analyze, based on the results of experimental studies, the influence of the characteristic size of a particle of woody biomass of two types (cedar and aspen) made in the form of a cube on the characteristics and conditions of their ignition during high-temperature heating in an oxidizing environment.

Figure 1 shows the dependences of the ignition delay times t_{ign} of cubic particles of woody biomass (aspen and cedar) on the characteristic size L, at different ambient temperatures.

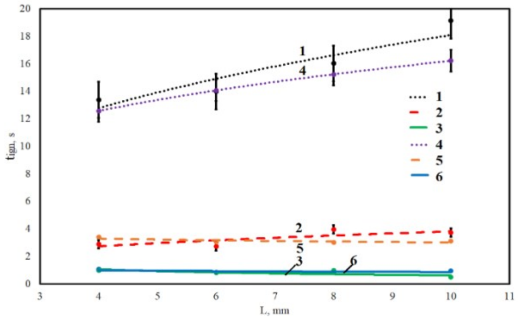

Figure1 Dependences of the ignition delay times of woody biomass particles made of aspen and cedar on the characteristic sizes at oxidizer temperatures: aspen 1 – 873 K aspen, 2 – 1073 K aspen, 3 – 1273 K aspen, 1 – 873 K cedar, 2 – 1073 K cedar, 3 – 1273 K cedar.

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Investigation of the flame retardants additives effects on the rigid polyurethane foam slabs combustibility

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Polyurethanes are an important class of polymers producing in the polyols and isocyanates reactions. Polyurethane foam is used in the aviation, automotive, construction industries. Despite the big number of good performances, polyurethane foams are highly flammable, that limits their usage. One of the best ways of combustibility reduce is the flame retardant (FR) addition. Flame retardants – are compounds that inhibits the combustion processes.

In this work the effects of the different flame retardant additions such as melamine polyphosphate (MPP), expandable graphite (EG), Tris(isobutylphenyl) phosphate (Disflamoll®51092) and biological flame retardant (bio) at concentrations from 1.5% (combustible) to 15% (fire-resistant) were investigated. Materials with small flame retardants additions were investigated for the downward flame propagation rate under the external heat flux influence. RPUF plates were inserted into a thin aluminum metal frame (sample holder) and installed on a non-combustible substrate, combustion was initiated using a torch. The radiant heat flux source was at a distance of 6 and 10 cm from the surface of the RPUF. The radiation flux was 2 kW/m^2 (6.5 cm) and 1.15 kW/m^2 (10 cm). During the experiment, the flame propagation rate, surface and 1 mm above the surface temperatures of the sample were measured. As a result, MPP and RG additives significantly reduce the burning rate and surface temperature of RPUF (about 50-100 degrees) in comparison with a pure sample.

Fire-resistant RPUF have been tested with LOI, UL-94 HBF, aviation rules (FAR-25), cone calorimeter tests. The addition of flame retardants EG and Disflamoll®51092 mixtures with a total mass content of up to 15% to the composition of rigid PU foam led to an increase in the oxygen index to 36.7%. At the same time, the sample with the addition of 15% EG showed the lowest flammability among all the RPUF samples, and lower than the sample with 7.5% EG + 7.5% Disflamoll®51092 and 15% Disflamoll®51092. All samples of rigid polyurethane foam with the addition of flame retardants have an HBF rating (low flammability for porous materials). Furthermore, formulations with a mixture of flame retardants 7.5% Disflamoll®51092+7.5% EG and with 15% EG successfully passed the test for compliance with aviation standards according to FAR-25. Therefore, the developed non-combustible rigid polyurethane foam samples can be recommended for practical use in the production of vehicle cabin elements, filling voids in aircraft wings, thermal insulation, etc. An application for a patent of the Russian Federation (application No. 202114491) was prepared for the resulting polyurethane foam compositions.

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Estimation of turbulence characteristics in a flame during a wildfire and the formation of induced atmospheric turbulence

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Widespread wildfires also impact global climate processes. Wildfires release a lot of thermal energy. Intense turbulent processes in the flame of a wildfire form turbulence in the convective column above the combustion source [1]. This affects meteorological parameters such as wind speed, air temperature, and humidity, induced by atmospheric turbulence. Turbulent processes in the atmosphere are characterized by internal and external scales corresponding to large eddies and small eddy structures, respectively.

In this work, we study the relationship between the scales of turbulence in a flame and the scales of induced atmospheric turbulence, as well as dissipative processes. Results of analysis and experimental data processing of turbulent processes in the flame of a model forest crown fire and in the atmosphere around the combustion source are presented. Experimental data were obtained using non-contact methods for measuring meteorological parameters and IR thermography using original techniques developed at TSU.

With increasing height, the internal scales of turbulence in the flame increase slightly due to expansion as a result of heat release during chemical reactions. They correspond to the inertial interval of the energy spectrum [2-3], and dissipative processes in the flame under semi-natural conditions of the experiment are not significant. Turbulent processes in the flame form induced atmospheric turbulence with characteristic frequencies of 0-2 Hz in the spectrum of air temperature fluctuations. Air temperature fluctuations with frequencies of 0.1 Hz correspond to the outer scale of turbulence corresponding to the measurement height.

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Investigation of the normal flame propagation speed of a hydrogen-enriched and water vapor-diluted methane-air mixture

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Highly efficient low emission combustion systems are being developed to reduce NOx emissions. However, the flame propagation speed of natural gas under lean conditions is slow, and there is a risk of flame extinction due to heat loss and stretch effects. This adversely affects combustion stability, which leads to an increase in hydrocarbons' and carbon monoxide emissions. Combustion under lean conditions can be stabilized by the temperature increase of the unburned mixture. This results in a higher burning velocity and a subsequent flame temperature increase and increased NOx formation.

Another important concept for combustion systems is the presence of water vapor in the combustion zone air. Water is one of the main combustion products, and water injection reduces the burning velocity of the mixture and, simultaneously, a lower adiabatic temperature is reached. This is another way to reduce NOx emissions.

The burning velocity of a water vapor-diluted mixture will be increased by enrichment of the flame with hydrogen. This results in a more stable flame. Flame propagation speed is an important characteristic of the air-fuel mixture. Accurate determination of the flame speed is important for the development of all types of combustion processes, as well as for the kinetic mechanisms validation. If the flame speed of hydrogen-enriched or water vapor-diluted methane-air mixtures has been previously studied, then the flame propagation speed of methane-air flames simultaneously diluted with water vapor and enriched with hydrogen have not been studied before.

This paper presents for the first time data on the normal flame propagation speed of water vapor-diluted methane-hydrogen-air mixtures obtained by the Heat Flux method. In addition, the flame speed of methane-air-vapor and methane-hydrogen-air mixtures are determined and compared with previously published data.

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Mathematical modeling of processes occurring during heating of gel fuel in the high-temperature oxidizer area

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Previously, we carried out experimental studies of the mechanisms and characteristics of the ignition of multicomponent fuels under dispersion conditions. A hypothesis has been developed and experimentally confirmed that the cause of the dispersion process is the nucleation, formation and growth of bubbles inside a heterogeneous fuel droplet. When a multicomponent fuel is heated, the components are separated – a combustible liquid and a water-thickener solution. Due to the difference in the surface tension of these components, a combustible liquid (more volatile component) is concentrated in the center (core) of a droplet, and the water-thickener solution (less volatile component) envelops it with a continuous shell, preventing contact with a gaseous oxidizer and monotonous evaporation of a combustible liquid with free surfaces. That is why it can be heated to a temperature at which vaporization centers nucleate. Due to the heterogeneous structure, further heating of the droplet leads to the formation of numerous centers of free interfaces (heterogeneous nucleation centers), which are located exactly at the interface between the liquid components of the fuel mixture (combustible liquid and thickener). Experimental studies show that the bubble formation process is affected by the difference in the characteristics of liquid fuel components (viscosity, boiling point), as well as the degree of overheating (i.e., a critical temperature difference must be reached). The most typical case is the heating of at least 10% of the interface between the components to the nucleation temperature, which is necessary for the subsequent manifestation of the dispersion effect (due to the collapse of bubbles containing vapors of a combustible liquid). For two-component droplets of immiscible liquids, such local overheating occurs due to the fact that the thickener shell has a much higher heat capacity and thermal conductivity than the inner subdroplet (combustible liquid).

On the basis of experimental and theoretical studies, a new approach to modeling the dispersion of a fuel droplet was developed. The essence of the approach lies in the fact that when developing a mathematical model, the criterion for the beginning of dispersion was the condition for reaching a temperature at the “combustible liquid / thickener” interface of the nucleation temperature, which is not equal to the boiling temperature of the combustible liquid, as is accepted in most existing models of puffing and microexplosion, and takes some value corresponding to the rate (intensity) of fuel heating. When developing a mathematical model, this approach makes it possible to more fully describe the processes that lead to the implementation of the dispersion effect and more reliably predict their characteristics for different heat supply mechanisms.

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Gel fuel particles ignition and combustion mechanisms under dispersion conditions

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A hypothesis was formulated on the mechanisms of ignition and combustion of gel fuels particles (melt droplets) of various component compositions under dispersion conditions. It is based on the assumption that the cause of the dispersion process (one of the most promising ways of enhancing the ignition and burnout of multicomponent fuels) is the formation and development of bubbles inside the fuel melt droplet by the heterogeneous nucleation mechanism.

Due to the multicomponent composition of gel fuels, they are characterized by melt droplet dispersion. The following set of interdependent physical and chemical processes in a condensed phase and gas medium was identified when a single gel fuel particle was heated in a high-temperature motionless oxidizer medium. The fuel particle exposed to radiant heating starts melting, and the liquid layer emerging on the particle surface evaporates. A combustible gas-vapor mixture forms in the vicinity of the particle. It does not ignite due to a relatively low temperature and due to the combustible vapor concentration. The liquid components of the fuel separate after its melting. Due to differences in surface tension, the thickener develops a layer on the melt droplet surface, and the combustible liquid is inside the droplet under the thickener layer. Due to the resulting structure, further heating of the droplet leads to the formation of numerous centers of free interfaces discontinuities (heterogeneous nucleation centers) precisely at the interface between liquids. This manifest itself as the formation and growth of single bubbles moving along combustible *liquid / thickener* interface. As the size of bubbles increases (due to an increase in the quantity of evaporated combustible liquid), they reach the combustible *liquid / thickener* interface. When the number of bubbles and their sizes exceed critical values, the thickness of the thickener shell decreases, the bubble collapse disrupts the thickener layer. The combustible vapors are blown into the gas medium of the heated oxidizer together with fuel microdroplets. They are blown quite far from the parent droplet surface, where the oxidizer temperature is higher than that around the droplet surface. Fine fragments, moving in a high-temperature medium, rapidly evaporate, thus increasing the concentration of volatiles which ignite in a rather large volume oxidizing area.

Also, the hypothesis is valid for fuel compositions with fine solid carbonaceous particles, with the exception of the following some features. The difference is that the formation of nuclei of a new phase occurs predominantly in the pores of solid particles located in the volume of the combustible liquid, and not at the combustible *liquid / thickener* interface. Carbonaceous particles have a porous surface structure and contain air bubbles in micropores, which can serve as centers of heterogeneous nucleation.

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POSTER PRESENTATIONS

Features of the interaction between meta-pyridyl and an oxygen molecule: a theoretical study

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Around the world, coal-fired power plants continue to play an important role in electricity generation, as coal is a less expensive, more abundant and reliable energy resource than oil and natural gas. In this regard, a detailed description of the process of coal combustion under various conditions remains an important and urgent task. The current state of computer technology makes it possible to theoretically calculate multi-stage and complex processes with high accuracy. In this regard, when considering the mechanisms of complex processes that are difficult to study by experimental methods, a great contribution is made by theoretical, including quantum chemical methods of calculation A pyridine molecule can be used as a model system for describing the process of coal combustion. This molecule is capable of forming three radicals during oxidation. At the same time, the main attention of researchers, both in theoretical and experimental works, is directed to the study of the oxidation of only one of the three possible pyridine radicals, ortho-pyridyl. However, the use of only one radical in the model does not make it possible to obtain complete information about processes and products formed. In this regard, we carried out a quantum chemical study of the features of the interaction of meta-pyridyl with molecular oxygen, determined the main paths and possible products of such interaction, and constructed the potential energy surface (PES) of the reaction meta-pyridyl + O_2.

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Experimental study of the regularities of titanium nickelide SH synthesis with a pre-mechanoactivated powder mixture

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Titanium nickelide, in addition to high strength and heat resistance at high temperatures, has a property of the "shape memory effect" and is widely used as porous implants and the basis of bioceramic composites. To realize the self–propagating high–temperature synthesis (SHS) titanium nickelide composition Ti - 55.06 wt%Ni, it is necessary to preheat the mixture to a temperature of 150-200 ^{0}C due to its low exothermicity. In this work, we study the possibility of using mechanical activation (MA) to carry out SHS of titanium nickelide without initial heating.

Mechanical activation (MA) of initial nickel and titanium powders mixture of (PNE-1, PTH-4-1) in a stoichiometric ratio was carried out in a planetary ball mill (60g, water cooling, steel balls 5 mm). Variable parameters: the ratio of powder mass to ball mass (M_P : M_b from 1:5 to 1:20), activation environment (gasoline, air), MA time (from 30 s to 10 min). After the MA, the pressed samples (diameter - 20 mm and a porosity - 45%) were placed in a constant pressure unit and SHS was carried out with the measurement of temperature and combustion rate.

The conducted studies have shown that mechanical activation of the low exothermic titanium – nickel system in gasoline makes it possible to realize SHS without additional heating of the entire volume of the mixture (Fig. 1)

It is revealed that the use of a highly energy planetary ball mill for 5 minutes or less allows for synthesis. The range of the maximum temperature of subsequent combustion under the specified conditions MA is from 1025^{0}C to 550 ^{0}C, and the value of the combustion rate is in the range of 0.23 – 0.51cm/sec. The XRD method established that in almost all synthesized samples, the product is multiphase with a predominance of the TiNi phase.

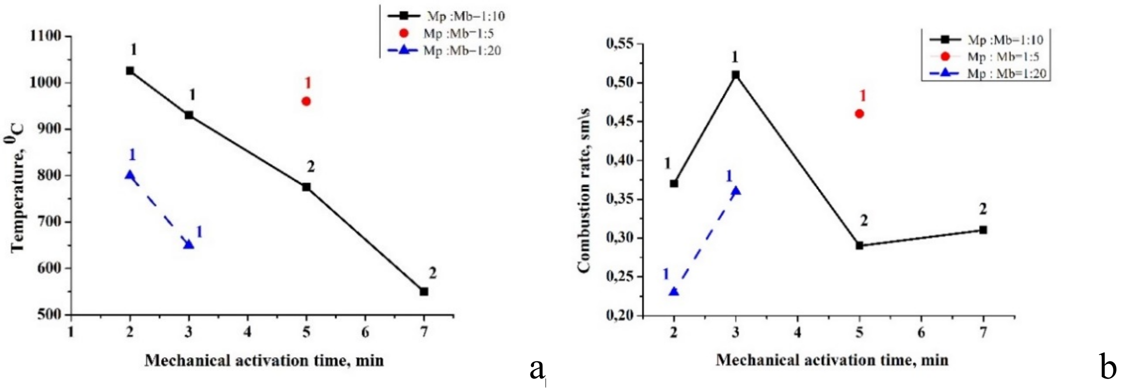

Figure1 The maximum combustion temperature (a) and combustion rate (b) dependences on the time MA in gasoline for different ratios Mp : M_b with the formation of different sets of synthesized phases: 1 - TiNi, $TiNi_3$, Ti_2Ni, 2 - TiNi, Ti_2Ni

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Study of the evolution of a titanium and nickel powder mixture after mechanical activation

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Titanium nickelide has many useful properties and is used for various fields of technology. To obtain titanium nickelide by self–propagating high–temperature synthesis (SHS) of the composition Ti - 55.06 wt% Ni, it is necessary to preheat the initial powder mixture to a temperature of 150-200 ^{0}C or to perform preliminary mechanical activation (MA), due to its low exothermicity.

Variety of phenomena happens in the powder mixture during MA, which lead the powder mixture to a state capable of combustion. Therefore, the study of changes occurring in the powder mixture during mechanical activation is important for understanding and regulating processes at the synthesis stage.

Mechanical activation of a mixture of initial nickel and titanium powders (PNE-1, PTH-4-1) in a stoichiometric ratio (TiNi) was carried out in a high energy planetary ball mill (60g, water cooling, steel balls of 5 mm, the ratio of powder mass to ball mass - 1:10, environment of the MA – gasoline, MA time 0.5 – 30 min). The morphology of the powder mixture was studied on JEOLSM-84, Axiovert 200.

It is shown that during mechanical activation of the powder mixture, agglomerates are formed, the external and internal structure and dimensions of which are constantly changing. The processes of grinding and agglomeration occur simultaneously, with variable predominance at different time intervals.

The average size of agglomerates increases from 15.35 microns after 0.5 min MA to 17.96 microns after 1 min MA and then decreases to 14.52 after 5 min MA. Further, due to the predominance of agglomeration processes, the size increases to 55.7 microns after 30 min MA.

The formed agglomerates consist of layers of titanium and nickel, which decrease with increasing MA time. The layered internal structure determines the growth of the size of the interfacial surface in agglomerates, which contributes to the subsequent self-propagating high-temperature synthesis.

Based on the experimental data obtained, a theoretical assessment of the rate constant of formation of the interfacial surface of titanium and nickel was carried out.

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Numerical investigation of the structure of a laminar premixed methane/air flame impinging on a flat cold obstacle

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In many industrial applications, fuel is burned in combustion chambers, where heat transfer to cold walls significantly affects the flame structure and chemical kinetics. Therefore, near-wall combustion often results in a higher level of pollutants. In addition, the heat from the flame may induce local temperature fluctuations at the wall surface, leading to additional thermal stresses in the wall material. Thus, studying near-wall combustion is relevant for more efficient and cleaner fuel burners in industrial devices.

We present the results of direct numerical simulations of a laminar premixed methane/air flame directed onto a cold flat surface, with a focus on detailed mechanisms of chemical kinetics. The flame was produced by a convergent axisymmetric nozzle (with the outlet diameter $d = 15$ mm), directed normally to the wall. Three cases were studied with the distance between the nozzle and the obstacle set to $1d$, $2d$ and $3d$, respectively. The Reynolds number of the flow was Re = 1000, and the equivalence ratio was $\varphi = 0.92$. The wall surface temperature was fixed at 371 K (in order to fit the experimental study). The computational domain was a sector of a cylinder with an angle of 5° (axial flow symmetry assumed). The computational grids used had adaptive refinement in the near-wall region and the flame front zone, with a maximum resolution of 5 μm.

The laminarSMOKE [1] package based on the open-source OpenFOAM code (www.openfoam.com) was used for numerical calculations. This package allows one to apply detailed kinetic mechanisms to chemical reactions by separating the steps of the transport evaluation and source terms. The reduced kinetic mechanism is provided as a set of elementary chemical reactions assembled into a single external file in CHEMKIN format. The GRI-MECH 3.0 kinetic mechanism includes 53 chemical compounds and 324 elementary reactions. The simulations were performed in transient formulation, taking into account the buoyancy effects.

The resulting flow velocity and temperature distributions were compared with the data from high-resolution stereo PIV-PLIF experiments for similar geometry and conditions. The flame shape was found to be in good agreement with the experimental results, whereas, for the temperature distributions, the simulation provided a slightly higher value of the temperature maximum. The differences are probably due to small errors in the cross-diffusion process of the discretization of different chemical species. Also, we investigated the evolution of the concentrations of intermediate radicals in the flame, which are essential for determining the rate of the overall chemical reaction.

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Development of a 4-Component Surrogate Model for Combustion of Gasoil, including investigation of PAH Formation

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The Gasoil fuel (also known as Diesel) is widely used in the power plant industry worldwide, particularly in the gas turbine system. Considering the combustion as the main thermo-chemical process in gas turbine cycle, its overall performance and environmental aspects, is highly dependent on identification of combustion behavior of the fuel. This proceeds through development of the Diesel Surrogate Model, which despite its particular importance, the number of existing researches focusing on diesel surrogate modeling, particularly a multi-component model, with desirable level of model uncertainly is still restricted.

The development of surrogate model follows from considering a reference model and an iterative procedure, starting from setting an initial formula, and continues until finding out the final composition, which should reflect the overall combustion behavior of properties of the real fuel. In this work, the modeling procedure starts from a reference model and its corresponding input formula, which is the Jet Surrogate Model, previously developed by the author and his coworkers [1]. The Model is also equipped with the newest acetylene [3] sub-model as the C_0-C_3 chemistry, and the latest cyclohexane kinetic model, also published by the author [3].

To this aim, the measurements related to fuel combustion characteristics, such as ignition delay time (IDT) and laminar flame speed (LFS) in different operational conditions, including various pressures ranges, and different equivalence ratios, are used for simulation and model validation. Among them, the IDT data in the low temperature range ($T<1000$ K) are specifically important due to appearance of two important phenomena of diesel combustion, i.e. Negative Temperature Coefficients (NTC), the pre-combustion ignition and the cool flame, where the developed surrogate model and the corresponding input formula showed an excellent consistency with experimental data.

By obtaining the final surrogate model and the final input formula, the effective roots of the formation of poly-aromatic hydrocarbons (PAH) in different operational conditions are investigated. This let us to conclude that, in lower temperatures the formation of the PAHs is mainly controlled by cascading dehydrogenations of all fuel contributions, meanwhile in higher temperatures it is dominated by C_0-C_3 reactions.

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Flameless combustion of wood long natural aging

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The change in the properties of wood of long-term natural aging is accompanied by complex physico-chemical transformations, as well as the transformation of its structure. Methods of thermal analysis (TG, DTG, DSC) have shown that as a result of prolonged aging of wood, its thermal stability changes. At the same time, the oxidation stage of the coal residue undergoes significant changes. The oxidizing ability of the coal layer increases 1.6 times compared to a sample of modern wood (the maximum reduction in activation energy in this area is from 331 to 240 kJ/mol). For the oxidation stage of the coal layer of wood aged in natural conditions, an increase in the rate of mass loss, an increase in the thermal effect of the oxidation reaction of coal and the rate of heat release of this process were recorded on the curves of DTG and DSC. It is shown that the structural organization of the coal layer is the determining factor in assessing the fire hazard and the intensity of smoldering combustion of wood. To establish the nature of possible structural changes in the wood of long-term aging, studies were carried out by the method of benzene vapor sorption. The maximum values of the adsorbate gain were obtained for a sample of pine wood coal with a service life of 150 years (26.76%), which is 2 times higher than the value of the adsorbate gain for coals for modern wood (12.8%). In addition, the values of the total pore volume and the specific surface of the coal residue for natural aging wood increase by 1.44 and 4.35 times, respectively. Using the electron microscopy method, a developed "honeycomb-like" structure was found for the carbon layer of aged wood.

The results obtained by thermal analysis methods are a reflection of experimental data on a modified muffle furnace under isothermal heating conditions, as well as during tests according to GOST 30403. By isothermal heating on a muffle furnace with a temperature of 800 ° C, charcoal samples were obtained. Under conditions of smoldering combustion of wood temperature on the sample surface and mass loss were recorded. It was found that the residual temperature on the surface of the coal layer of wood with a service life of 110 years increases by 14-20%, and the mass loss before the sample cools completely increases by 4 times. At the same time, the dynamics of reducing the residual temperature on the surface of natural aging wood is less intense.

During the experiment according to GOST 30403, it was found that with a fire exposure time of 45 minutes for enclosing wooden structures (service life of 81 years), the temperature was actually 50 ° C higher throughout the experiment compared to a sample of a modern wooden structure in both fire and heat chambers. At the end of the test, an abnormal glow of the carbon layer was observed for a wooden structure with a long service life associated with the active course of the reaction-oxidation process. Intensive heat generation for wooden structures of long-term natural aging is accompanied by a higher rate of burnout and charring (an increase in the rate of charring by 1.2 times or more), as well as an intensification of smoldering combustion.

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The determining role of heterogeneous reactions of atoms and radicalsin the combustion of gases at atmospheric pressure

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As is known, until recently, in the theories of combustion, explosion and detonation, as well as in investigations using the provisions of these theories: in monographs, encyclopedias and articles, the role of reaction chains in combustion processes with significant self-heating was ignored, and in some cases denied [1–4] . N.N. Semenov in his monograph [4], referring to the monograph [1], when discussing the third limit of ignition of hydrogen, states: “the agreement between calculation and experiment leaves limits no doubt that the third limit of mixtures of hydrogen with oxygen is thermal”. In his subsequent works, he also considered the third limit to be thermal, and not chain. After proving the chain nature of combustion at atmospheric and elevated pressures, as well as in self-heating modes (e.g. [5,]), new patterns of these processes become known.

The present investigation is devoted to the previously unknown determining role of heterogeneous reactions of atoms and radicals in the propagation of flame and explosion. Since the thermal theory did not consider the chain nature of combustion, it also did not consider the collisions of atoms and radicals with the surface. Meanwhile, during these collisions, not only momentum transfer occurs, but also chemisorption and recombination of active particles. In these reactions, free valences are destroyed, and, therefore, the reaction chains are broken. This affects chain combustion no less than heat removal. Since the features of heterogeneous reactions depend on the chemical properties of the surface, these reactions also determine the characteristics of flame propagation.

In the present investigation, in order to clarify the dependence of combustion on the chemical properties of the walls of the reaction we studied the propagation of a hydrogen flame with air in molybdenum glass tubes with varying ability of the walls to break reaction chains, as well as in a stainless-steel tube. In various experiments, the tubes were pre-rinsed with a solution of boric acid, distilled water, or a diluted thin suspension of magnesium oxide. Coefficients of heterogeneous recombination of the leading active combustion particles of hydrogen-containing substances, i.e. H and O atoms, the surfaces on the coatings created in this way are significantly different. The molybdenum tube was wrapped in black paper with four leeks along the axis for photo sensors. Four sensor windows were also on the stainless steel tube. Signals from the sensors were transmitted to a four-channel oscilloscope (“TEKTRONIX”, USA) and processed on a computer. Oscillograms were recorded as the flame passed past each of the four windows. From these oscillograms, x–t diagrams of the flame path were constructed (where x is the path traveled by the flame, t is time), which in this case are analogues of kinetic curves (Fig.1). It is also clear from x–t diagrams 3, 4 and 5 that the flame speed strongly depends on the chemical properties of the surface. It can also be seen that the surface properties change under the influence of flame.

Significant excess of the flame speed with weak heterogeneous chain termination over the flame speed with intense heterogeneous chain termination means that with intense

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heterogeneous recombination, the inhibitory effect of the surface on combustion is mainly due not to heat removal, but to heterogeneous chain termination. In a stainless-steel reactor, the effects of heterogeneous reactions are similar to those of MgO and are determined primarily by heterogeneous chain termination rather than by conductive heat removal. Chemiluminescence oscillograms from repeated experiments show that the kinetic pattern of the glow also changes under the influence of the flame. Thus, the patterns of flame propagation largely depend on the nature and rate of heterogeneous reactions of active intermediate particles and, above all, on the intensity of heterogeneous chain termination. In turn, the flame affects the chemical properties of the surface.

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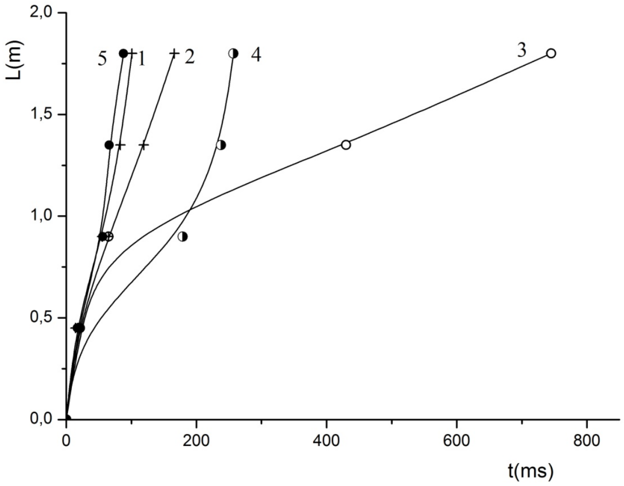

Fig.1. x–t diagrams of the flame path in a glass reactor above the surfaces: 1, 2 – boric acid; 3,4, 5 – magnesium oxide. Curve numbers. correspond to the sequence of experiments.

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