

9th INTERNATIONAL SEMINAR ON FLAME STRUCTURE

9 ISFS

Book of Abstracts



**Novosibirsk, Russia
July 10-14, 2017**

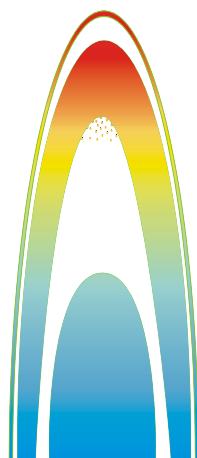
Institute of Chemical Kinetics and Combustion SB RAS
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Novosibirsk State University
Combustion Institute
Russian Sections of the Combustion Institute
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Preface

The Institute of Chemical Kinetics and Combustion SB RAS, together with the Institute of Theoretical and Applied Mechanics SB RAS, the Institute of Thermophysics SB RAS, the Institute of Hydrodynamics SB RAS, the Institute of Catalysis SB RAS and the Novosibirsk State University organized the 9th International Seminar on Flame Structure in Novosibirsk, held under the aegis of the Combustion Institute, Russian Section of the Combustion Institute and the Siberian Branch of the Combustion and Explosion Council of RAS. The Seminar is considered as continuation of 8 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.

The objective of the Seminar is to provide an international forum for discussing the state-of-the-art achievements and perspectives in 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 diffusion flames, flames of energetic materials and polymers, detonation, experimental and numerical methods for studying the flame structure, chemical kinetics and mechanisms of flame reactions, inhibition and suppression of flames, formation of soot and synthesis of nanoparticles in flames, catalysis of combustion, solid flames, filtration combustion, and micro combustion.

The 9th ISFS Organizing committee has received over 100 excellent abstracts from Russia, Kazakhstan, Armenia, USA, England, France, Germany, Japan, China and India, covering the entire domain of combustion from fundamental to technical aspects. The Scientific Program of 9th ISFS includes 16 plenary lectures, over 70 oral and poster presentations. We are grateful to all the authors who have contributed to the 9th ISFS.

We extend special thanks to the researchers from the laboratory of kinetics of combustion, 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 Russian Foundation for Basic Research, the Institute of Chemical Kinetics and Combustion SB RAS, the Institute of Theoretical and Applied Mechanics SB RAS, the Institute of Thermophysics SB RAS, the Institute of Hydrodynamics SB RAS, the Institute of Catalysis SB RAS, the Novosibirsk State University, the Novosibirsk Technology Center “Schlumberger Research and Development Inc.”, Sigma-Pro LLC, BLM Synergie, Russia, JSC Machine-Building Factory of Podolsk (JSC ZiO), ZIO-COTES LLC. It was with their support that organization of the Seminar became possible.

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**Methods and results of experimental research of the dynamic regimes
of the condensed systems ignition**

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Studying of process of the condensed system ignition usually is carried out in the simplest conditions of heat input is constancy of temperature or heat flux on surface, that is in so-called "the static regime". In actual practice, as a rule, ignition is carried out at variables, time-dependent, values of heat flux. Forming of heated-up layer in this case is carried out in the complicated dynamic conditions and significantly depends on the mode of change of heat flux during heating of the studied sample (the induction period).

The analysis of the dynamic modes of ignition within the thermal theory was carried out by A.G. Merzhanov [1] who have shown that characteristics of process of ignition depends on dynamics of external heat flux. At the accruing heat flux influence of kinetic parameters for the period of ignition is significantly less, than in case of the constant or decreasing over time heat flux. The experimental research of this phenomenon is rather difficult in workmanship and therefore in available literature the number of the experimental data is limited [2].

The purpose of the presented study is development of methods and experimental research of the dynamic regimes of the condensed systems ignition.

As the condensed system it is chosen pyroxylin as the most studied substance with known kinetic and thermophysical characteristics. Dynamic heat flux regime is ensured by moving the test sample during its heating luminous flux along the optical axis of the elliptical reflector, the installation "Uran-1" [3]. Ignition delay times of pyroxylin in the conditions of heating increasing and decreasing heat fluxes in the range from 0.2 to 22 W/cm² are received.

It is shown that in the studied range heat fluxes the ignition delay time of pyroxylin at the increasing heat flux with the mean value equal to density of constant heat flux is, less, than at constant heat flux. With increase of heat flux density the difference in the ignition delay time decreases and asymptotically aims at zero at value of heat flux density, it is less than 8 W/cm². The found effect is connected, apparently, with features of forming of heated-up layer of condensed system in the conditions of the static and dynamic regimes of heating of the condensed system.

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Numerical investigation of laminar one-dimensional counter-flow flames from product gas of woody biomass pyrolysis and gasification*F. Behrendt*

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Biomass thermochemical conversion processes are a promising alternative for decentralized biomass energetic utilization and waste treatment. In particular, processes such as pyrolysis and gasification offer the possibility of producing a fuel gas to be used, among other applications, in internal combustion engines or turbines for heat and power generation (CHP). However, these fuels present higher complexity than conventional gas fuels regarding their composition as well as higher heterogeneity depending on the conversion process. For this reason, a detailed characterization of their behaviour during combustion is still needed in order to improve the engine performance as well as to control and reduce emissions.

In the present study, the behaviour of several product gases is numerically investigated in a non-premixed laminar counter-flow flame. The influence of the product gas composition on the flame behaviour and flame structure is addressed and compared with the behaviour of a methane flame. 12 different biomass-derived product gas mixtures are used in the simulations with air as oxidizer: gasification gas, pyrolysis gas, landfill gas and syngas. These product gases are representative for several biomass sources (wood, charcoal, organic wastes) and conversion processes, i.e., pyrolysis, gasification, and as an add-on, fermentation in the case of landfill gas.

The Fortran code used code solves the governing equations for mass, momentum, energy and mass fraction for non-stationary laminar one-dimensional flames. In the simulations, 80 species have been taken into account with a reaction mechanism of 504 elementary reversible reactions.

Increasing the flow velocities results finally in aero-dynamic quenching of the flame. This extinction point can be identified clearly by tracing the maximum temperature as function of the strain rate. The higher the critical strain rate, the higher the resilience to quenching, making the flame more stable for a wider range of flow conditions. That is desirable for an industrial combustion system, since the turndown ratio of the burner could be therefore increased, allowing a wider range of firing rates and thus enhancing the flexibility of the system.

When compared with methane combustion, it can be stated that biomass derived gases with a hydrogen molar fraction higher than 5-10 % present a similar resilience to quenching as methane. There is a clear relation between the maximum temperature of the flame and the H₂ fraction in the fuels. Fuels with high contents of CO and CH₄ have also a high flame temperature. For high strain rates (high stretching or low Damköhler numbers), the flame is far away from a fast chemistry or equilibrium situation and therefore from the (maximum) adiabatic temperature. Results show a direct relation between the H₂ content in the product gas and the maximum possible strain rate prior to quenching of the flame.

The thermal NO mechanism is prevalent in the formation of this pollutant. Higher flame temperatures lead to higher NO emissions, which is the case for low strain rates. Close to extinction the only significant NO emission is in the case of pure methane or fuels with high methane content. Below temperatures of 1,500 K the thermal NO formation mechanism is not active anymore due to the high activation energy.

Prompt NO formation mechanism seems to have only slight relevance in fuels with high CH₄ content. The slight emission in NO in the case of fuels with high CH₄ in the strain close to extinction may be due to this prompt mechanism.

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Recent advances in fire retardancy of polyurethane*S. Bourbigot*

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Polyurethanes (PUs) are unique polymeric materials with a wide range of physical and chemical properties. Their applications are numerous but many of them require flame retardant properties and hence PUs must be flame retarded¹. To do so, flame retardants (FRs) are incorporated into them to limit their flammability or specific surface is applied on them. The talk will review the different methods to make flame retardant PUs (including thermoplastic PU, PU foams and thermoset PU) with the incorporation of FRs and by the application of FR coatings. The different mechanisms involving the gas phase (e.g. poisoning the flame by radical trapping) and the condensed phase (e.g. formation of a protective barrier) will be fully commented. A special emphasis will be done on intumescence².

Intumescence is a versatile method for providing reaction and resistance to fire to materials. When heated beyond a critical temperature, the intumescent material begins to swell and then to expand forming an insulative coating limiting heat and mass transfer. The talk will consider the use intumescence (coating and flame retardants) to make flame retarded PUs and fire barrier on substrates. Examples are: (i) the resistance to fire of steel protected by an intumescent PU coating², (ii) fire retardancy of thermoset intumescent PU³ (Figure 1 (a)) and (iii) the use of sol-gel process to flame retard PU foam⁴ (Figure 1 (b)). For all topics mentioned above, it will include a special emphasis on the mechanism of action involved in the fire protection and on the associated experimental method.

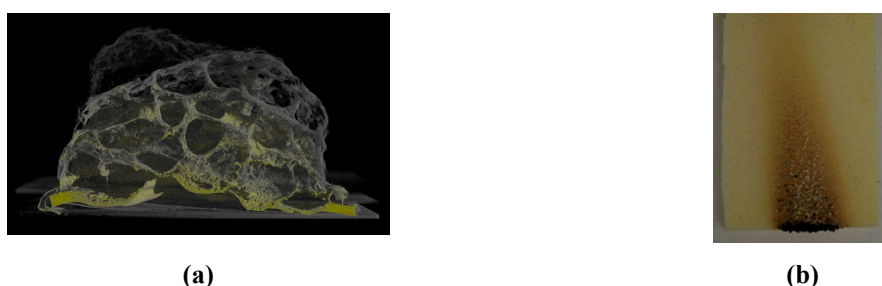


Figure 1. a) X-ray tomography picture of the internal char structure developed from an intumescent PU b) Char residue on PU flexible foam protected by sol-gel coating after UL-94 test.

This work has received funding from the European Research Council (ERC) under the European Union's H2020 – the Framework programme for Research and Innovation (2014-2020) / ERC Grant Advances Agreement n°670747 – ERC 2014 AdG/FireBar-Concept.

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Free radicals and the ions Mn^+ and MnOH^+ along flames of H_2 or C_2H_2 *N.A. Burdett^{1,2} and A.N. Hayhurst¹*¹Department of Chemical Engineering, University of Cambridge, Pembroke St, Cambridge CB2 3RA, UK²Nigel Burdett and Associates, Kelsale, Saxmundham, Suffolk IP17 2QT, UK

The ions Mn^+ and MnOH^+ have been studied along flat, premixed, fuel-rich flames of H_2 or C_2H_2 burning in O_2 and either N_2 or Ar at 1 bar and from 1800 to 2600 K. Ion concentrations were measured by continuously sampling the burned gas into a quadrupole mass spectrometer. Manganese was added to the gas fed to the burner by atomising an aqueous solution of MnCl_2 . Depending on the flame's temperature, an M/100 solution yielded a total mole fraction of Mn atoms of $\approx 2 \times 10^{-8}$ in the burnt gas, where conditions in the first 20 mm from the reaction zone were well defined. Manganese in these flames exists as molecular MnO ($\sim 25\%$), free atoms of Mn (Ionisation Energy 706 kJ/mol) and MnOH ($< 1\%$). Previous work showed that $[\text{Mn}]/[\text{MnO}]$ is constant along the burnt gas, because the reaction: $\text{Mn} + \text{H}_2\text{O} = \text{MnO} + \text{H}_2$ is equilibrated. Only two new ions, Mn^+ and MnOH^+ , were observed. Typically, $[\text{Mn}^+]/[\text{MnOH}^+]$ rose quickly to a maximum of ≈ 50 at 2 – 3 mm downstream of the reaction zone and then fell to $\sim 10 - 12$ at 20 mm, in accord with the equilibrium $\text{MnOH}^+ + \text{H} = \text{Mn}^+ + \text{H}_2\text{O}$ (I) shifting, as radicals recombine in: $\text{H} + \text{H} + \text{M} \rightarrow \text{H}_2 + \text{M}$ and $\text{H} + \text{OH} + \text{M} \rightarrow \text{H}_2\text{O} + \text{M}$. Here M is any molecule acting as a third body. The ratio $[\text{Mn}^+]/[\text{MnOH}^+]$ did not change, when the diameter of the sampling orifice was varied between 50 and 200 μm . This indicates that the measurements are not falsified by sampling and equilibrium (I) has a time constant exceeding $\sim 1 \mu\text{s}$, *i.e.* the time for a sample from the flame to enter the first vacuum chamber of the mass spectrometer and so become free of collisions between ions and molecules. The fall in $[\text{Mn}^+]/[\text{MnOH}^+]$ along a flame takes time (≈ 5 ms, depending on temperature) before reflecting the independently measured $[\text{H}]$, declining along the burnt gas. Measurements of $[\text{Mn}^+]/[\text{MnOH}^+]$ at 20 mm downstream enabled the equilibrium constant, K_I , of (I) to be derived. The values in flames hotter than 2100 K indicated an enthalpy change $\Delta H_I = -244 \pm 20$ kJ/mol, *i.e.* MnOH has an ionisation energy of 759 ± 25 kJ/mol. It is interesting that reaction (I) takes longer to equilibrate than: $\text{SrOH}^+ + \text{H} = \text{Sr}^+ + \text{H}_2\text{O}$, which was used to measure $[\text{H}]$ along these flames. Analysis of the profiles of $[\text{Mn}^+]/[\text{MnOH}^+]$ indicates that $\text{MnOH}^+ + \text{H} \rightarrow \text{Mn}^+ + \text{H}_2\text{O}$ has an activation energy of 137 ± 40 kJ/mol.

Ions in a flame of H_2 and O_2 are shown here to be produced either by: $\text{Mn} + \text{OH} \rightarrow \text{MnOH}^+ + \text{e}^-$ or $\text{MnO} + \text{H} \rightarrow \text{MnOH}^+ + \text{e}^-$, *i.e.* involving the flame's radicals, just as with Ba or Sr as additive. If C_2H_2 is present in the fuel, it causes ionisation in $\text{CH} + \text{O} \rightarrow \text{CHO}^+ + \text{e}^-$, followed by proton transfer in $\text{CHO}^+ + \text{H}_2\text{O} \rightarrow \text{H}_3\text{O}^+ + \text{CO}$, yielding the major ion H_3O^+ . Although the reaction $\text{MnO} + \text{H}_3\text{O}^+ \rightarrow \text{MnOH}^+ + \text{H}_2\text{O}$ is capable of generating MnOH^+ , there is evidence that $\text{Mn} + \text{H}_3\text{O}^+ \rightarrow \text{Mn}^+ \cdot \text{H}_2\text{O}$ is faster. Evidently, the monohydrate, $\text{Mn}^+ \cdot \text{H}_2\text{O}$, is not stable enough to be observed. These processes in a flame of C_2H_2 result in the total concentration of every ion quickly reaching a maximum downstream of the reaction zone. Subsequently, ions and free electrons recombine in: $\text{MnOH}^+ + \text{e}^- \rightarrow \text{Mn} + \text{OH}$ or $\text{MnO} + \text{H}$, as well as in $\text{Mn}^+ + \text{e}^- + \text{M} \rightarrow \text{Mn} + \text{M}$. Values of the associated recombination coefficients for these 2- and 3-body processes have been measured and found to have the magnitudes expected.

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Bridge the gap between premixed and non-premixed flames: partially premixed flames over a wide range of premixedness*S. Chakravarthy*

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Over the past century of development of combustion science, considerable attention has been paid to two different kinds of flames, namely, premixed and non-premixed flames. In the present work, we attempt to bring them together within a common framework, where they are seen as extremes of continuum of states of partially premixed flames of varying degree of premixedness. A co-flow configuration is adopted, wherein the flame is submitted to varying degrees of stratification in the reactant concentrations, i.e., premixedness, by considering different stoichiometries of fuel-rich and fuel-lean mixtures in co-flowing streams that mix and react. Several aspects of these flames are considered, to bridge the gap across premixed and non-premixed flames. First, analytical solutions to a slowly varying triple flame of reactants with equal but significantly greater than unity Lewis numbers, and unequal but departures from unity Lewis numbers, are presented. These are compared with high-order accurate numerical solutions based on compact schemes. Next, the numerical solutions are explored in a larger parametric space of Damkohler number and full range of premixedness from non-premixed to premixed limits for both equal and unequal but significantly greater than unity Lewis numbers. It is observed that partially premixed flames exhibit large scale two-dimensional thermal-diffusive intrinsic instability, which convert into pulsating instability of weakly stratified and fully premixed flames at one end of the premixedness range. Third, experiments are performed in a slotted burner with methane-air mixtures, to bridge the gap between the laminar stoichiometric plane premixed flame speed and an asymptotic flame speed of edge flames in the non-premixed limit. A peak exists at an optimum concentration gradient of the reactants corresponding to maximum flame stretch that occurs out a balance of flame strain and curvature effects. The same experiments are performed subjecting the flame to nearly isotropic grid generated turbulence, and a correlation for the flame speed is developed to include premixedness, besides stoichiometry and turbulent intensity. Lastly, the contrast in sooting between premixed and non-premixed flame is experimentally investigated in a coaxial laminar burner to identify an 'S' shaped curve of soot volume fraction as the flames are advanced from the premixed to non-premixed end. The site of soot production is the tip of the fuel-rich branch of the triple flame, which advances upstream as one approaches the non-premixed end; simultaneously, the fuel-rich branch closes in on the diffusion branch, giving the appearance of the non-premixed flame as sooty. Similar data is also presented under turbulent conditions and also with introducing shear between the co-flows.

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To the theory of ignition, combustion and detonation of micro- and nanoparticles*A.V. Fedorov^{1,2}*¹Khristianovich Institute of theoretical and applied mechanics SB RAS, Novosibirsk, Russia²Novosibirsk State Technical University, Novosibirsk, Russia

The work is devoted to the review of some papers which were done in the domain of mechanics of reacting heterogeneous media (MRHM) of micro- and nano- structure. The review consists of three particles. In the first part we were investigated the problems of physical and mathematical modeling of melting of nanoparticles of Al, Fe. We use the methods of molecular dynamics to describe the problems. This allows to determine the melting temperature, the heat capacity and some other parameters of the melting nanoparticles. Numerical data were compared with experimental one. We got a good correspondence between melting temperature vs particles radius dependences. Then new physical and mathematical phenomenological models were proposed to describe the process of melting of metal nanoparticles. It took into account the experimentally observed fact of reduction of the melting temperature with decreasing particle radius. Two-front modes of melting were found for the first time for thermal fields of plane, cylindrical, and spherical particles. The melting times for different types of symmetry were found to be ordered, and the corresponding approximation dependences of this parameter on the particle size were derived.

The second part of the paper was devoted to mathematical modeling of the burning of micro- and nano- particles from the point of view of MRHM. The hierarchy of the models for describing the ignition, burning of these physical objects was presented. This allowed us to describe the time of ignition and combustion of the particles of different sizes at different temperatures and pressures of the environment. Comparison with some of the available experimental data has shown the adequacy of the models.

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Continuous-detonation combustion of hydrogen: results of wind tunnel tests

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D.A. Vnuchkov², D.G. Nalivaichenko², A.A. Berlin¹, V.M. Fomin²*

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Use of detonation combustion of fuel–air mixture in ramjets is regarded as one of challenging directions in the development of advanced aerospace engines. Energy efficiency of detonation engines was first discussed theoretically by Zel'dovich in 1940 and has recently been demonstrated in three-dimensional numerical simulations and experimentally. The most promising schemes of arranging detonation combustion in the airflow include schemes with continuous spin detonation and with pulsed detonation.

The purpose of this work was an experimental study of detonation combustion of hydrogen in an axisymmetric 1-meter long, 300-millimeter diameter ramjet demonstrator with an air intake, annular combustor and nozzle in a pulse wind tunnel of ITAM SB RAS "Transit-M" at approach stream Mach numbers M ranging from 4 to 8 (Fig. 1).

The possibility of self-sustained detonation combustion of hydrogen in supersonic airflow in the ramjet combustor was demonstrated experimentally for the first time. Two modes of detonation combustion were registered at approach stream Mach numbers from 4 to 8, namely, continuous spin detonation with a single detonation wave rotating in the combustor annulus with a velocity of ~ 1600 m/s and pulsed detonation with repeatable detonation reinitiation at the combustor exit and detonation wave propagation upstream towards distributed hydrogen injectors with a velocity of ~ 1600 m/s. Detonation combustion was accompanied with a considerable pressure rise (Fig. 2).

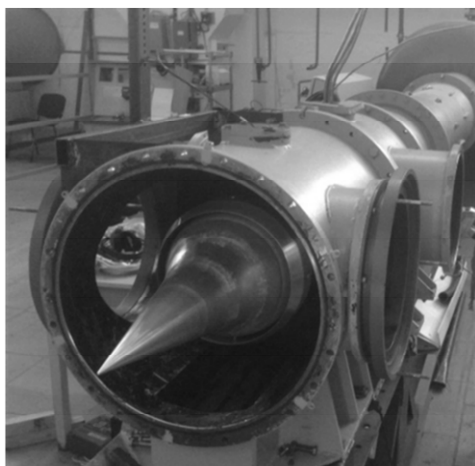


Fig. 1: Ramjet demonstrator in a wind tunnel

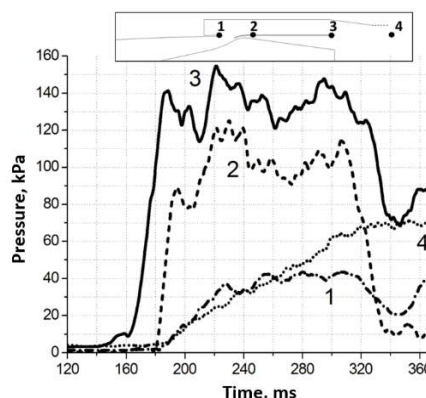


Fig. 2: Example of total and static pressure records by sensors 1–4 at $M = 5$

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Combustion of oxygenated biofuels in flames*P.A. Glaude*

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More than 90% of the liquid fuels consumed in the world for transportation are derived from petroleum. Possible scarcity of the resource in the long term and the need to reduce greenhouse gas emissions have led to growing interest in fuels produced from renewable vegetal matter. The first generation of biofuels, such as ethanol or methyl esters of fatty acids suffer from the limitation of resources and of the competition with food crops. Second-generation biofuels, derived from ligno-cellulosic biomass, i.e. derived from non-edible raw materials, are preferable for the reduction of greenhouse gases since the whole plant would be used, and for the reliability of the feedstock. According to the chemical process, these fuels can be alkanes, alcohols or ethers, which are produced via synthesis gas, or saturated or unsaturated cyclic ethers, such as derivatives of furan and tetrahydrofuran. Another interest in the addition of oxygen-containing compounds to fuels lies in their ability to reduce soot formation in diesel engines, but in some cases offset by increased emissions of toxics or irritants, such as aldehydes.

The study of the structure of premixed laminar flames of hydrocarbons and oxygenates makes it possible to know the reactivity of these compounds and to follow the formation of intermediates and reaction products in the flame front. Flames of several saturated and unsaturated cyclic ethers, tetrahydrofuran, methyltetrahydrofuran, tetrahydropyran, furan, methylfuran dimethylfuran, valerolactone were investigated under low pressure under stoichiometric and rich conditions using argon as a diluent. The reaction products were sampled by a microprobe and analyzed on-line by different chromatographs, which made it possible to quantify a large number of stable species. In the case of furan derivatives, the same experiments were carried out in parallel with the University of Bielefeld with mass spectrometry (EI-MBMS) analysis which allowed the quantification of free radicals.

Besides the structure, the flame velocity is a key parameter for the design of burners and combustion chambers. A heat flux burner was developed and used to measure the adiabatic laminar flame velocities of liquid hydrocarbons and oxygenates as a function of the richness and temperature of the fresh gases. Kinetic models have been developed to simulate the different experimental results and to compare the reactivity and pollutant production of each type of fuel. For example, the surprisingly surprising ability of DMF to form soot precursors with respect to less substituted furans has been observed experimentally and is well explained in the model.

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New developments in fire retardants– Inorganic-organic hybrid fire retardants*Yuan Hu*

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Inorganic–organic hybrids have attracted great attention of scholars worldwide because they combine the advantages of both inorganic and organic components, and provide a versatile route for controlling the structure and properties of materials on the molecular level. To develop new inorganic–organic hybrid fire retardants, layered inorganic nanomaterials based hybrid fire retardants has been described and investigated. For instance, functionalized reduced graphene oxide (FRGO) wrapped with a phosphorus and nitrogen-containing flame retardant (FR) was successfully prepared *via* a simple one-pot method, then FRGO was covalently incorporated into epoxy resin (EP) to prepare flame retardant nanocomposites. Also, another novel strategy of using supramolecular self-assembly for preparing sandwich-like melamine cyanurate/MoS₂ sheets as the hybrid flame retardants for polyamide 6 (PA6). The introduction of MoS₂ sheets function not only as a template to induce the formation of two-dimensional melamine cyanurate capping layers but also as a synergist to generate integrated flame-retarding effect of hybrid sheets, as well as a high-performance smoke suppressant to reduce fire hazards of PA6 materials. The inorganic-organic hybrid fire retardants will provide a new solution to highly efficient flame retardant polymeric materials.

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Species identification for the development of chemical kinetic schemes

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Combustion technology needs to adapt to new challenges. New fuels from biogenic sources are slowly replacing part of the fossil fuel mix. New motor concepts, such as HCCI engines, operate in different combustion regimes than current technology. New energy storage and transport schemes, such as GTL or BTL, associated with the efficient use of solar, wind or geothermal power often make use of partial oxidation of fuels to synthesis gas. All of these changes require a more detailed understanding of the chemical kinetics than has been needed before, to anticipate the formation of unwanted pollutants from new fuels, control ignition in HCCI engines and select the most efficient conversions schemes to store energy in chemicals. In addition, flame synthesis is very promising process for scalable production of new materials, e.g. inorganic nanoparticles.

The first step in the development of chemical kinetic schemes is to identify the species involved in the chemical conversions. From an analytical point of view, species identification is a challenging task because of the large number of species with highly variable concentrations involved in the combustions reactions. Mass spectrometry is a very suited analytical technique for the task of species identification because it allows detection of stable, radical and ionic flame species without prior knowledge about their molecular properties, it has a large dynamic range, and typically high sensitivity. Stable molecules and radicals have to be ionized before detection. The ionization process is based on molecular properties and can be used to obtain additional information about the species, e.g. ionization energies, ionization efficiency curves or photoelectron spectra. Photoionization photoelectron coincidence spectroscopy was used in experiments performed with VUV-photoionization in experiments at the Swiss Light Source to identify the fuel radicals and key intermediates in soot formation processes in flames of hydrocarbon fuels. Selected data will be presented here to highlight the value of this analytical technique for species identification in combustion processes.

Material synthesis processes lead to the production of comparatively large molecules and a detailed identification of individual molecular products is usually not required. Instead, common properties of the products, such as their oxidation states and average size, are of greater interest. However, the flame conditions and the interaction of the precursor molecules with flame species determine the formation pathways of larger molecules. Similar to fuel destruction processes they can be studied by mass spectrometry. The data can be used in the validation of detailed models describing the destruction of precursors and the formation of small clusters. Mass spectrometry has the disadvantage that a sample needs to be extracted from the flame. The introduction of a sampling probe reduces the flame temperature and changes species concentrations. In addition, the sampling probe may clog when particles are formed leading to a reduced sensitivity of the measurements. Our experiments show that less clogging is observed when naturally occurring ions are sampled from a synthesis flame for iron oxide particles and that the ions can be detected with excellent sensitivity. Selected results are presented using flame ions as diagnostic tools and strategies for data reduction, simulation of processes including flame ions and comparison of simulation and experiment are discussed.

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Modeling of flame spread over solid fuels*A. Kumar*

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Flame spread over solid fuels in concurrent and opposed configurations are two canonical problems studied to gain insight into interaction between spreading flame and solid condensed phase. Here we look at evolution of flame spread modelling on solid fuels in opposed flow configuration over the years. Since early model proposed by de Ris models of spreading flame have evolved in their complexity to include more detailed physics which enable them to predict more detailed features of the flame spread phenomena. The current state of art numerical models and direction for further improvement in them is also presented.

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Intermittent flame at combustion of hydrogen - oxygen mixture containing SO₂*A.A. Mantashyan*

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Study rarefied low-temperature flame of hydrogen-oxygen mixtures containing additives SO₂ at $P < 200$ Torr and $T = 450-500^\circ\text{C}$ (with parameters that characterize the region of autoignition), have shown that at certain speeds of the reacting mixture flow in reactor the flame passes to new, previously unknown mode of combustion - in intermittent mode. In this mode, the combustion is characterized by continuous flashes of light of a certain frequency and intensity. Specially developed technique allowed to recording these characteristics in a continuous mode in time, then transform and transmit them for continuous recording on a computer. In this unit a signal to the computer records can be increased in size, and the coordinates represented in expanded form as well. The time from onset of the signal to achieve maximum light emission, obviously, can be taken as a time for flame development.

The frequency and intensity of flashes of light depends on the composition of the reacting gas mixture, pressure, temperature and gas flow rate at which the process is carried out. The chemical feature of the process is that the SO₂ is converted to form elemental sulfur, which is deposited from a flow of reacting gases at the outlet of the reactor in special traps as an amorphous fine powder.

Importantly, under these conditions, if the oxygen in the reaction mixture is replaced by an inert gas - nitrogen, then the sulfur formation was not observed. Under these conditions, in the absence of oxygen, hydrogen does not recover sulfur from its dioxide. In other words, SO₂ conversion takes place only under the influence of the hydrogen oxidation chain reaction.

Kinetic analysis of the mechanism of self-ignition of hydrogen-oxygen mixtures in the presence and absence of SO₂, which was done by solving the kinetic equations in a quasi-stationary approximation, leads to the same differential equation for the leading active center - the hydrogen atom, if it reacts with SO₂ forming less active radicals and does not inhibit the process and reacts with the hydrogen atoms realizing chain propagation reaction.

Experimentally flash unit registered in static conditions for implementation of the mixtures showed that in the presence of SO₂ $\Delta\tau$ autoignition time is reduced. For example, the data obtained at $T=470^\circ\text{C}$ and $P=2-3$ Torr for the mixture composition of H₂:O₂:SO₂:N₂=10:1:1:0.5, shows that the $\Delta\tau = 0.023$ sec. But if SO₂ is completely replaced with N₂, now $\Delta\tau = 0,04$ sec. So SO₂ additives accelerate the development of the conjugated radical-chain process.

Detailed kinetic analysis, also by numerical methods for the all possible chemical reactions of conversion of sulfur dioxide under the effect of a chain reaction of hydrogen oxidation involving the reactions of atoms and free radicals, showed that in this conjugated process sulfur atoms which are formed can react with oxygen, resulting in efficient increasing of active particles together with the main chain branching reaction - the reaction of hydrogen atoms with oxygen. These kinetic results clearly reflect the accelerating effect of the SO₂ addition on chain process of self-ignition of hydrogen-oxygen mixtures.

The results obtained allow doing some conclusions about the nature of the phenomenon of "intermittent flames".

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Coherent structures in turbulent swirling flames

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Flow swirl is commonly used to stabilize flames in combustors. Breakdown of the vortex core of the swirling flow, occurring for high swirl rates, intensifies local mixing. Besides, formation of the central recirculation zone provides heat transfer from the combustion products to the reactants. Another feature of swirling flows is the phenomenon of vortex core precession. Moreover, flow precession in high-swirl jets becomes much more intensive after formation of the central recirculation zone. It is considered to be due to rotation of a coherent structure of spiral vortices formed due to global flow instability mode, which usually remains after the flame ignition.

The present research reports on the results of the experimental study of coherent structures in turbulent swirling flames by using planar optical techniques, viz. PIV, PLIF and Rayleigh scattering. Fully premixed and partially premixed flames (of propane or methane) at atmospheric pressure have been studied. Proper orthogonal decomposition has been used to extract coherent structures in the instantaneous distributions of the velocity and density. For analysis of flame front deformations and mixing PLIF data have been processed. The results of 3D PIV experiments are also reported. In general, except for conditions close to lean flame extinction, dynamics of high-swirl flows, heat and mass transfer, as well as the flame front deformations, are influenced by movement of a pair of helical/spiral large-scale vortex structures.

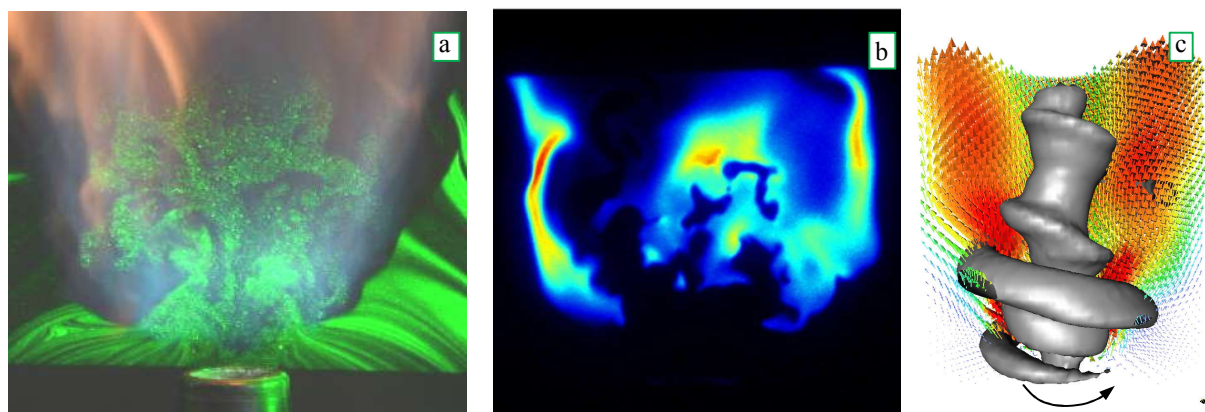


Figure 1. Planar measurements of (a) velocity and (b) flame shape by PIV and PLIF (OH*) techniques. The snapshots are taken separately. (c) Coherent flow structure consisting of large-scale vortices, namely, precessing spiral vortex core and helical secondary vortex, providing mixing of the fuel jet with ambient air.

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Recent progress of combustion research by a micro flow reactor with a controlled temperature profile

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Our recent progress of combustion research using a micro flow reactor with a controlled temperature profile (hereafter MFR) will be introduced. As our first report on MFR [1] indicated, three types of flame responses were observed in a meso-scale quartz tube heated by an external heat source. Among the three types of flames, so-called “weak flames” observed at low inlet mixture velocity condition have been utilized to examine the ignition-related properties of given fuels to date. For instance, low-temperature oxidation, partial oxidation and full oxidation of *n*-heptane/air mixture at ignition-relevant condition were observed successfully as multiple weak flames which are steady-state, weakly reacting separated three-stage reaction zones [2]. Based on it, Research Octane Number of PRF (*n*-heptane and *iso*-octane) was found to be indicated by the appearances of the multiple weak flames [3]. This technique have been applied for various fuels, e.g., each component of natural gas, ethanol and others up to carbon number 16. Lately, soot and PAH formation in comparatively low temperature conditions up to 1300 K have been also addressed [4].

Recently, optical measurement and speciation of flames in MFR have been applied for fundamental low carbon-number fuels, such as methane, DME, etc. and performances of extensively utilized chemical kinetics were examined. Since MFR has advantages in examining chemical reactions at low temperature conditions up to, say, 1000 -1200 K with comparatively longer residence time, existing kinetics exhibited unexpected significant quantitative discrepancies for predicting weak flames of the above-mentioned fuels. Some discussion for possible improvements in the kinetics will be presented.

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Multichannel model of filtrational gas combustion in porous media*S.S. Minaev¹, R.V. Fursenko²*¹Far-Eastern Federal University, Vladivostok, Russia²Institute of Theoretical and Applied Mechanics SB RAS, Novosibirsk, Russia

Fundamental investigations of filtrational gas combustion in porous media are of the interest for advanced combustion technologies based on conversion of combustion heat into infrared radiation. The radiative burners offer high power density, high power dynamic range and very low NO_x and CO emissions, owing to the high levels of heat capacity, conductivity and emissivity of the solid matrix, compared to a gas. Development of the advanced combustion systems requires adequate mathematical modeling of the systems based on coupled solution of the heat transfer and the chemical kinetics equations. In the recent past, models assuming existence of two interpenetrating continuous solid and gas media have been developed with varying degrees of sophistication. These so-called two-medium or two-temperature continuum models, have frequently been applied in the literature. There is a good qualitative agreement between flame speeds, concentration and temperatures which are predicted by continuum models and those obtained experimentally. However, explanation of some combustion wave characteristics in porous media still remains problematic or even impossible within continuous models framework. In particular, experimental observations show that the filtrational gas combustion is can be accomplished with the local oscillations of the flame front in the space between solid matrix elements and flame fronts scattering. The latter can lead to a disintegration of the combustion wave onto separate fragments and significant widening of the preheating zone. The proposed multichannel model of filtration gas combustion in inert porous media describes a collective propagation of the separate flames in micro channels of different width. If all channels have the same width, then the model reproduces results of conventional continuum two-temperature model. The model explains the distortion of the flame front as a consequence of porous media inhomogeneity which looks like a finger-like structures and hot spots. The obtained numerical results imply that existence of even a small irregularity in the channel's width can lead to a significant widening of the preheating zone.

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Advances in Hydrogen Safety Research*V.V. Molkov*

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This plenary lecture presents the advances in hydrogen safety research achieved at HySAFER Centre of Ulster University during last years. Thermal hazards from cryogenic release of hydrogen were studied numerically and compared to experiments carried out at Sandia National Laboratories.

The dependence of hazard distance on the release axis angle has been investigated for hydrogen unignited releases and jet fires from high-pressure storage vessel through thermally-activated pressure relief device (TPRD).

The phenomena of under-expanded jet flame liftoff and blowoff for TPRD of different diameter were reproduced in collaborative work with Toyota Technological Institute (Japan).

The novel theory of blast wave decay after high-pressure hydrogen storage tank rupture in a fire is presented and applied to calculate hazards distances for human and buildings. Contrary to currently used in hydrogen safety engineering methods to calculate blast wave decay without taking into account contribution of combustion, the strong effect of combustion on the blast wave strength is demonstrated. Experimentally measured blast wave pressures at different distances in tests performed in USA for stand-alone and under-vehicle were reproduced by this theory. The theory is able to reproduce even the “plateau” in the blast overpressure with distance observed in the experiment with 350 bar hydrogen tank located under a vehicle.

The catastrophic rupture of high-pressure hydrogen tank in a fire is accompanied by devastating blast wave, fireball, and projectiles. Exclusion of such events is the main safety challenge for emerging hydrogen-powered vehicles and infrastructure. The conjugate heat transfer three-dimensional (3D) computational fluid dynamics (CFD) model to simulate heat transfer from a fire through a composite tank wall, which undergoes degradation, and liner to real gas inside the cylinder is applied to reproduce unique experiments performed in USA and Germany. This study allowed to spot a weakness in high-pressure composite tank design to withstand fire, suggest innovative engineering solutions to drastically increase fire resistance rating of hydrogen onboard storage beyond the duration of longest vehicle fire of about 2 hours, and develop proposal for update of fire test in the Global Technical Regulations #13 for hydrogen-powered vehicles.

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Combustion of fire whirl*Liu Naian, Lei Jiao*

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Fire whirl is a type of special swirling flame induced by the interaction between general buoyant fire and surrounding rotating flow field. Fire whirl is characterized by the fact that in a swirling ambient air atmosphere, a general free burning pool fire can suddenly undergo a rapid enhancement in its burning rate, flame temperature, radiation output as well as flame height. Fire whirls are often reported to occur in large-scale wildland and urban fires, and they are usually a key mechanism for the increase or acceleration of the fire intensity and fire spread rate. Since the pioneering experimental work by Emmons and Ying (Emmons, H.W. and S.-J. Ying, The fire whirl. Proceedings of the Combustion Institute 1967, 11(1): 475-488), many laboratory studies on fire whirl have been conducted in the past half century. However, quantitative experimental works and reliable theoretical models are still very limited.

Since 2004, a series of new facilities on both medium- and small-scale fire whirls have been established at the State Key Laboratory of Fire Science (SKLFS), and new theoretical models have been developed based on the experimental data and theoretical analyses. This speech summarizes the researches on fire whirl at SKLFS, consisting of three parts: 1) quasi-steady combustion characteristics of fire whirl; 2) formation and evolution of fire whirl; and 3) challenges for further research on fire whirl.

1. Quasi-steady combustion characteristics of fire whirl

A fixed-frame facility, consisting of a square enclosure made of tempered glasses, with dimension of 2m x 2m x 15m, was used to investigate the combustion characteristics of quasi-steady fire whirls, by using liquid fuel of n-heptane or gas fuel of propane. The pool diameter ranged from 10 to 55 cm for heptane fire whirl, while for propane fire whirl, the largest burning rate was 300 kW. It was found that the burning rate of heptane fire whirl depends on pool size, and as the pool size increases, the transition to turbulent burning for fire whirl occurs sooner than a general pool fire with the same pool size. We found that the increase of burning rate in fire whirl results from the enhanced convective heat and mass transfer in the inflow boundary layer above the liquid fuel surface. A semi-empirical correlation $\dot{m}=HI^{-1/(1+m)}$ couples the mass loss rate to ambient circulation and pool size. The correlation agrees well with the data from different sources.

Flame height correlations in literature were mainly developed for small-scale fire whirls and the flame height was shown to be proportional to the fuel burning rate. In our work, a theoretical correlation

$H^* = K(\dot{Q}^* \Gamma^{*2})^m$ was proposed to couple the flame height of turbulent fire whirls to the fire release rate and imposed circulation. It correlates well the data of fire whirls with different types of fuels. The turbulence suppression is suggested to be the dominant mechanism which controls the flame elongation in turbulent fire whirls compared to free turbulent pool fires of equal fire size.

Experimental data showed that fire whirls maintain a higher ratio of continuous flame height to the overall flame height, and also higher maximum centerline excess temperature in continuous flame region, as compared to general pool fires. Radial temperature profiles in the continuous region of the fire whirl were confirmed to be hump-type, implying the existence of fuel-rich inner core. The radial profile of excess temperature varies consistently with the continuous flame shape and the radial decay rate of excess temperature decreases in the intermittent flame and plume.

In the continuous flame region, the increasing rate of the centerline axial velocity with height is lower in fire whirls as compared to buoyant flame. The mean axial velocity radius is confirmed to be greater than the mean excess temperature radius in the continuous flame. The ambient imposed circulation is

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relatively steady within the continuous flame. The radial profile of tangential velocity varies steadily with height, and is little affected by heat release rate.

It is found that the air entrainment is strong at the bottom inflow boundary layer, while the mass flow rate increases slowly with height as compared to buoyant pool fires. The suppression of air entrainment was attributable to the radial force balance and stable stratification in the centrifugal acceleration field. The entrainment coefficient in the continuous flame is about one to two orders of magnitude lower than that in a buoyant pool fire, and it generally increases with height in the plume of fire whirl, approaching the value for pure buoyant plume.

The vertical radiative heat flux firstly increases and then decreases slowly, and finally collapses with the vertical distance normalized by the flame height, with a maximum value at $z/H \approx 0.4$. The radiative heat flux in the radial direction was correlated by $\dot{q}''(r) \cdot r^{-m}$ with the exponent being approximately 1.1 for both heptane fire whirls and general heptane pool fires. It is also found that the radiative fraction of fire whirls is nearly 42 %, 1.4 times as large as that for general pool fires.

2. Formation and evolution of fire whirl

The formation and revolution of fire whirl were usually studied in a wind tunnel with controlled wind speed or a rotating screen facility with independently controlled heat release rate (\dot{Q}) and imposed circulation (Γ). It was found that fire whirl forms under certain critical wind speed or imposed circulation in wind tunnel and rotating screen facility. The fire whirl may move upwind or downwind over line fire under different wind speed. The linear hydrodynamic instability analyses demonstrated that laminar and turbulent fire whirls form at certain critical values of the governing parameters $Re/B^{1/4}$ and $Re/B^{1/3}$ respectively, where Re and B are respectively the dimensionless imposed circulation and the dimensionless buoyancy flux. In a large range of imposed circulation, nine flame patterns were identified, including free buoyant flame, inclined flame, weak fire whirl, conical fire whirl, cylindrical fire whirl, transitional fire whirl (between conical and cylindrical fire whirls), curved cylindrical fire whirl, flame extinction and irregular flame. When the imposed circulation was very low, the original vertical buoyant flame inclined with a certain angle and revolved around the facility central axis steadily. For a given burning rate, the inclined flame was observed to be converted into fire whirl at a certain critical imposed circulation, while at another lower critical circulation the fire whirl would decay back to inclined flame. Only when $\dot{Q} \geq 1.20$ kW, the conical fire whirl could be converted to a cylindrical fire whirl. Otherwise, flame extinction of conical fire whirl occurred at a critical imposed circulation. For $\dot{Q} \geq 6.25$ kW, the cylindrical fire whirl would be transformed into irregular flame with no flame extinction. The variations of flame height and flame diameter with imposed circulation differed greatly in different regimes of flame patterns.

3. Challenges for further research on fire whirl

Future research should pay more attention to the formation and evolution of fire whirls in real open space environment and the transitions between fire whirls and other extreme fire behaviors.

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A gas burner emulator for condensed-phase burning

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The use of a gas burner to emulate the burning of condensed-phase (CP) fuels has many advantages: (1) ease of studying flames, (2) immediate establishment of steady burning, (3) precise identification of ignition and extinction. The accuracy of a gas burner to replicate the flame of a CP fuel is based on the hypothesis that the low uniform flow velocity of the burner has a negligible effect on the resulting flame structure. The mass flow rate of the burner, equal to the burning rate of a CP fuel, gives an almost identical flame. This results provided the properties of the CP fuel match those of the burner mixture; namely, the heat of combustion, the smoke point, the vaporization surface temperature, and the heat of gasification. The heat of gasification is derived from the mass flow rate of the burner, its surface temperature, and the average flame heat flux to the surface. Two techniques will be discussed for measuring the average heat flux: (1) two discrete measurements along with an averaging-technique, and (2) the use of the burner top as a calorimeter.

Experimental and theoretical results are discussed for a wide range of applications for the burning rate emulator (BRE). Early work demonstrated that burner experiments could reproduce the burning of laminar ceiling and wall fires. The results for burning rate were correlated with B number and match theories for corresponding CP fuels. Over the past several years we have studied the use of BRE burners for small vertical wall and pool fire configurations. The flame structure was shown to match the CP burning conditions for flat surfaces burning at various orientations over 180°. For 50 mm diameter pool fires, the BRE is shown to match the burning of methanol, heptane, PMMA and POM in terms of properties, flame structure and color. Ignition and extinction have been studied for pool fire diameters of 25, 50 and 100 mm. The BRE results give precision values for the critical burning rates at these limits, and compare favorable to data more difficult to obtain for corresponding CP fuels. Critical flame temperature theory is used to correlate and explain these results.

All of this work with BRE burners has been motivated by the desire to establish the burning conditions in microgravity for a quiescent atmosphere in terms of CP material properties. Up to now most microgravity studies of CP fuels rely on ambient flow or flame spread to assist the burning, or have alternately examined quiescent burning of a candle flame or small droplets. The candle flame persisted for a relatively long time, but the droplet burning appears to lead to radiative extinction or cool flames. Upcoming BRE experiments on the International Space Station will examine the dynamics of long duration microgravity burning related to CP fuels. Up to now, many experiments have been conducted with BRE burners of 25 and 50 mm diameter in a NASA 5-s microgravity facility. The fuel mixture, pressure, ambient oxygen and a wide range of mass flow rates were studied. These experimental results will be presented, and steady state theories are shown to correlate the 5-s end state. However, full steady state is not achieved. These aspects will be discussed.

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Recent Advances of Combustion Study with Synchrotron-based VUV Photoionization Mass Spectrometry

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We will report recent advances of synchrotron-based vacuum ultraviolet photoionization mass spectrometry (SVUV-PIMS) in various research topics of combustion chemistry including premixed flame, oxidation in jet-stirred reactor, pyrolysis in flow reactor, coflow diffusion flames, and analysis of polycyclic aromatic hydrocarbons (PAHs) and soot. We will provide some new results using the upgraded instruments located at Hefei Light Source (HLS) [1-2]. Benefiting from the new design with short distance between the sampling position and the ionization region, a lot of “new” reactive species can be unambiguously detected, i.e., H, O, OH (in Fig. 1), and hydroperoxides (in Fig. 2). Furthermore, the techniques can be applied in the detection of gas-phase products of heterogeneous reactions including catalysis reaction, biomass pyrolysis etc.

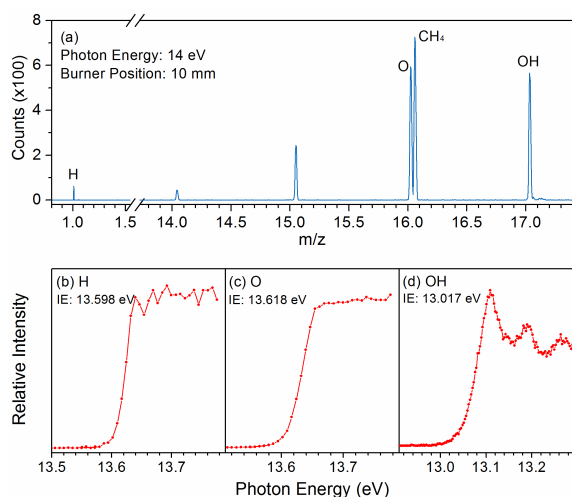


Figure 1 (a) Partial mass spectrum of C₂H₄/O₂/Ar flame ($\phi=0.5$) showing the detection of H, O and OH at the burner position of 10 mm with 14 eV VUV light, (b-d) Photoionization efficiency spectra of H, O and OH, respectively.

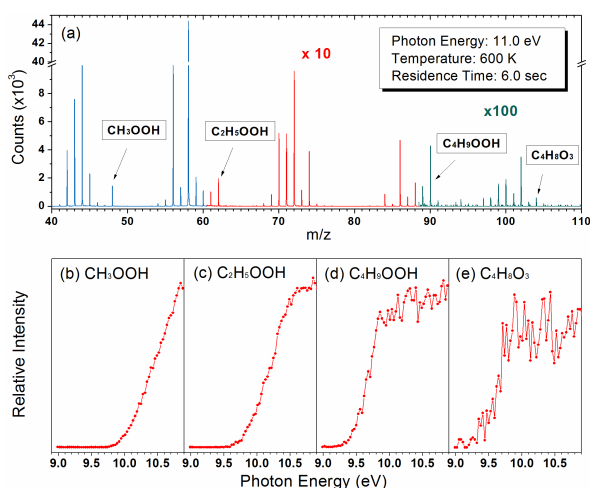


Figure 2 (a) The mass spectrum obtained for the oxidation of n-butane. (b-e) Photoionization efficiency spectra of CH₃OOH, C₂H₅OOH, C₄H₉OOH and C₄H₈O₃, the temperature inside the reactor is kept at 600 K.

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Modernization of air-blown entrained-flow two-stage bituminous coal IGCC gasifier

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Integrated gasification combined cycle (IGCC) is advanced solution to improve the efficiency and environmental friendliness of coal power engineering. A key element of this plant is the gasifier of solid fuels (coal, petcoke, biomass, etc.). According to gasifying agent the gasifiers are divided into oxygen-blown and air-blown units. The advantage of the first is high cold gas efficiency, and the second - low capital and operating costs. In this paper we consider the issue of modernization (improving) of air-blown entrained-flow two-stage bituminous coal IGCC gasifier.

The only commercial air-blown entrained-flow gasifier is a two-stage MHI 1700 t/d unit. Therefore, it was chosen as the initial design of further modernization. The modernization purpose is increasing of the gasifier efficiency and syngas H₂/CO ratio control to improve the environmental performance of the syngas burning in the combustion chamber of the IGCC gas turbine.

The modernization consisted in an additional air blast heating to 900°C by high temperature air heater and steam (900°C) supplying in the gasifier second stage. Determination of the influence of the proposed modernization on the gasifier characteristics and the optimization of its operating parameters were performed by carrying out multivariate calculations by zero-dimensional, one-dimensional and three-dimensional (computational fluid dynamics, CFD) models. Using zero-dimensional equilibrium thermodynamic model the parameters range is investigated in the widest intervals. From the plurality of "coal-blowing" system states selected the most efficient ones according to the criterion of cold gas efficiency with the minimum temperature limitations. Achievability of these states was investigated by a one-dimensional kinetic-thermodynamic model, which takes into account the kinetics of the fuel conversion in the gasifier. Using this approach it was possible to determine the optimal operation gasifier regimes by varying the proportion of primary and secondary fuel flows. The parameters (founded by the previous models) received as input data to CFD-model, which allowed carry out a more refined analysis of the problem: the flame formation and the recirculation zone location in the gasifier, a choice of fuel supply and flow control ways, etc.

The gasifier modernization has improved the synthesis gas thermal capacity and cold gas efficiency from 77.2% to 84.9%, and increases the H₂/CO from 0.344 to 0.602. The IGCC efficiency was increased from 48 to 50-52%.

This work was carried out at the Ural Federal University and financially supported by the Russian Science Foundation (project no. 14-19-00524).

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Associated Website: [https://science.urfu.ru/portal/en/persons/--\(f55217dd-1863-4ee1-b0a4-445681da75de\).html](https://science.urfu.ru/portal/en/persons/--(f55217dd-1863-4ee1-b0a4-445681da75de).html)
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Diffusion combustion of hydrocarbon under the conditions of jet source instability

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Control of mixing and combustion processes in the jet flows is an actual and important problem. This paper presents the experimental results on instability of diffusion combustion of a hydrocarbon jet in still air. The feature of this study was investigation of the jet flame at instability development both in the jet flame and inside the source of jet formation. It is well known that the initial conditions affect significantly dynamics of the jet flow. However, the method of combustion process control due to the laminar-turbulent transition in the jet source (a cylindrical tube) has been hardly studied. The principal advantage of mixing and combustion control in the unstable regime is the use of jets with low Reynolds numbers ($Re < 4000$), which meets the objectives of energy saving and energy efficiency.

In this work, we studied successively the jet without burning (“cold jet”) and then the jet at combustion (“hot jet”). The measurements in the jet and visualization of the flow were made for propane-butane mixture flowing out of a quartz tube with diameter $d = 3.2$ mm at Reynolds numbers $Re = 300 - 8000$. The longitudinal velocity and velocity fluctuations were measured for the “cold jet”. It is shown that the initial conditions (jet flow from the nozzle or tube) affect significantly dynamics of the jet flow [1]. For the flow from the profiled nozzle, the laminar-turbulent transition occurs in the layer of jet mixing, where the velocity gradients are high. For the flow from a long tube, the transition to turbulence can occur inside the tube. As a result, we have a system of two-cascade hydrodynamic amplifier. The first cascade is instability inside the jet source (tube) and the second one is unstable mechanism of the jet, which always has the inflection point in the transverse velocity profile. Instability of the diffusion flame can be caused by various factors, including an external acoustic action [2]. The changes in the shape of the attached flame, accompanied by low-frequency oscillations of the flame tip position, are visually registered under the considered conditions in a narrow range of Reynolds numbers. Presumably, such instability can be associated with the laminar-turbulent transition inside the jet source.

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Mathematical modeling of wildland fire initiation and spread*V.M. Agranat*¹, *V.A. Perminov*²¹ACFDA, Thornhill, Ontario, Canada²Department of Ecology and Basic Safety, Tomsk Polytechnic University, Tomsk, Russia

The aim of this paper is to create a user-friendly computational tool for analyses of wildland fire propagation and its effects on urban interfaces by students, researchers and fire management consultants. A physics-based multiphase Computational Fluid Dynamics (CFD) model of wildfire initiation and spread has been developed and incorporated into the multi-purpose CFD software, PHOENICS. The forest is considered in this paper as a chemically reactive multiphase medium containing gas phase with a volume fraction of ϕ_g and condensed phase with a volume fraction of ϕ_s (liquid water, dry organic matter, solid pyrolysis products and mineral part of fuel). The interaction between phases is modeled by two sets of phase governing equations linked with proper source terms expressing the gas flow resistance, multiphase heat transfer and chemical reactions. Model takes into accounts for all the important physicochemical processes: drying, pyrolysis, char combustion, turbulent combustion of gaseous products of pyrolysis, exchange of mass, momentum and energy between gas and solid phase, turbulent wind flow and convective, conductive and radiative heat transfer. Turbulence is modeled by using a RNG $k-\varepsilon$ model and the radiative heat transfer is approached with a model similar to P-1 radiation model. The Arrhenius-type kinetics is used for heterogeneous reactions (drying, pyrolysis and char combustion) and the eddy-breakup approach is applied for gaseous combustion. The model has been validated using the experimental literature data of Mendes-Lopes and co-workers on ground fire propagation in a bed of *Pinus pinaster* needles, located in a wind tunnel. The predicted rate of spread (ROS) is well agreed with experimental values obtained at various wind speeds (from 1 to 3 m/s). The distributions of gas temperature and velocity predicted at small wind speed shows that a large clockwise eddy is formed ahead of strong buoyant plume and the plume is oscillating with time. As wind speed increases a transition from buoyancy-dominated regime to wind-driven regime is observed and the plume becomes more stable. These flow patterns were also reported by other authors. The CFD model is being further validated using the data on large forest fires including crown fires.

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Wave instabilities arising during centrifugal SHS surfacing of Ti: Numerical model and experiment

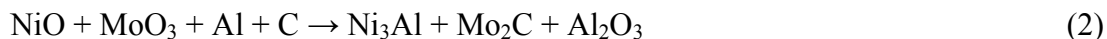
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In fabrication of layerwise materials, including SHS-assisted surfacing, of key importance is a structure of the transition zone between a substrate and deposited coating, a property that defines the strength and other parameters of joining. In this context, it seemed interesting to investigate instabilities that could be expected to arise during transversal wave propagation in the field of centrifugal forces by using a specially designed mathematical model and appropriate experimental setup.

We explored the possibility of centrifugal SHS surfacing in a mode of transversal deposition both experimentally and also by theoretical modeling for a laterally ignited double-layer system used as a model. Overall reaction schemes used in our experiments are given below.



Experiments on SHS surfacing of Ti were conducted in graphite cartridges placed in a centrifugal machine as described elsewhere [1], with the only difference that ignition was done at the side sample surface within the zone of contact between Ti substrate and green mixture.

The coatings deposited through reaction (1) showed better results as concerning both their practical implementation and perspectives for subsequent more detailed investigation. The front instability arising during combustion was found to result in formation of the wavy structure within the transition zone, which is known to facilitate strong joining between the coating and substrate material, just as it happens during explosive welding of dissimilar metals [2].

This work was supported by the Russian Foundation for Basic Research (project no. 15-03-01986).

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Thermography of flame during liquid hydrocarbons combustion with superheated steam

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At the Institute of Thermophysics SB RAS a new method for fuel combustion with the use of steam when the gasification of carbon-containing particles during the incomplete combustion of liquid hydrocarbons occurs is proposed [Pat. RF No. 2219435, 2003]. It was shown that the supply of overheated steam to the liquid hydrocarbon combustion zone sharply intensifies combustion [Alekseenko S.V. et al. // Combustion, Explosion, and Shock Waves, Vol.52, No.3, 2016]. This combustion method provides stable ignition, high completeness of fuel combustion and a low levels of toxic components in combustion products. This method is promising for utilization of low-grade liquid hydrocarbon fuels and combustible industrial wastes with producing of heat energy. To study the influence of steam parameters on the main characteristics of the liquid hydrocarbons combustion process (the composition of combustion products and the specific heat release capacity) it is necessary to obtain the data for different combustion regimes.

In analogy with the procedure applied in previous work [Anufriev I.S., Kopyev E.P., Loboda E.L. // Proc.SPIE 9292, 929226, 2014], the thermal imaging measurements were conducted for the outer flame during combustion of liquid hydrocarbon fuel (diesel fuel) in a perspective burner device with the controlled forced supply of overheated steam into the combustion zone. A thermal imaging camera (FLIR, JADE J530SB) was used in the experiments. This device has a high temporal resolution: the frame rate up to 177 Hz with a maximum resolution of 320x240 pixels and up to 18 kHz with a resolution of 320x4 pixels. The minimum time of frame exposure is 6 μ s. The operating range of the thermal imager is in the middle infrared range of 2.5-5.0 microns. Temperature measurement range is determined by the thermal imager calibration and equals 583-1773 K (for the selected narrowband F0616 dispersion optical filter with a bandwidth of 2.5-2.7 microns).

The studies were conducted at the firing stand equipped with a new burner device (power up to 10 kW), an electric steam generator (average consumed power 1.5 kW), a plunger metering pump (flow rate up to 1.6 l/h), an automatic steam generator control system, a fuel supply system, an electronic scales to control the flow of water and fuel and necessary control and measuring equipment. In the experiments the direct-flow evaporative type burner device was used. Measurements were carried out in a wide range of regime parameters (fuel consumption at a constant 0.8 kg/h): steam flow rate 0.25-1.0 kg/h, superheated steam temperature 150-550°C at a pressure of 8 atm.). The dependence of effective emissivity coefficient of the flame from the steam flow rate has been obtained. The steam parameters have been found to influence the temperature in the outer flame of the burner device.

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Effect of KOH-activated rice husk on thermal decomposition of hydroxylamine nitrate monopropellant

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HAN - is a high-energy substance that has the prospect of becoming a substitute for hydrazine, so it becomes very popular in the field of propellants. This material is less toxic, has a high density and performance superior to most energy-intensive materials used and is regarded as the primary oxidant for hybrid rockets.

The thermal decomposition of hydroxylamine nitrate (HAN), a "green" alternative of fuel/oxidizer formulation to hydrazine nitrate as a rocket propellant in the presence of the high SSA (up to 3000 m²/g) activated carbon obtained via activation of rice husk at 850 °C (RH) KOH AC was investigated. RH is a large scale vegetable unique material, e.g.: it is a renewable, green material with low commercial value. Decomposition of the mixture (HAN spiked with RH-derived KOH-activated AC by 1 mass %) was monitored by electron ionization mass spectrometry (EI MS) at different heating rates (from 16 to 128 K/ min).

EI MS analysis of AC influence of HAN decomposition showed two different pictures, i.e.: intensity of the formation of major gas products (NO, NO₂ and H₂O) was varied. Also, presented the products distribution at decomposition of monopropellant at low and high heating rates where was shown decreasing of NO gas value. A possible mechanism of reaction pathways of HAN decomposition with the AC is proposed.

Decomposition kinetics of mixture (HAN spiked with the 1 AC mass %) was assessed by DTA – TG thermal analysis at different heating rates. The study was conducted at a heating temperature of system ranging from 297 K to 723 K under nitrogen atmosphere at a flow rate around 100 ml/min in aluminium pans. DTA-TG analysis results showed that the initial temperature of HAN decomposition in the presence of the obtained RH-based AC is comparable to Iridium catalytic effect, e.g.: the effect of 1% AC on initial temperature from 185/86°C vs 1% Ir 185/75 °C.

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Classification of the dynamic problems of the theory of combustion and explosion*V.S. Babkin¹, P.K. Senachin²*¹Institute of Kinetics and Combustion SB RAS, Russia²Altay State Technical University, Barnaul, Russia

Modern state of the theory and practice of combustion processes and explosions of gases and fuel-air mixtures in confined volumes and internal-combustion engine is characterized increased complexity of solving scientific and technical problems and considered at that dynamic problems. At considering concrete problem it is important to attribute to any class of dynamic problems of the combustion theory. This is necessary for analysis and use of previous scientific experience at solving analogous tasks with the point of view of the combustion theory. Unfortunately this classification is absent now.

Another important problem is adequate description very complicated hydrodynamic, thermodynamic, chemical and physical processes and (including energy, pulse and mass transfer processes) that occurs at gas explosion in confined volumes and at combustion of fuel-air mixtures in internal-combustion engines of various types. At that it is important to describe the considered processes not only quality but also quantity.

1) This communication is an attempt to classify dynamic problems of the combustion and explosion theory the most well-known of those are the problems of classical theory of thermal explosion (TE).

2) The classification has been carried out on the base of analysis of the ratios of 6 characteristic times of physical-chemical processes in the problems of combustion theory.

3) The theoretical analysis of dynamic problems shows in the combustion theory there are not less than 6 similarity criterion that characterizes concurrent of characteristic times of different physical-chemical processes and the group of criterions of composite type (in which there is not less than 3 characteristic times and not less than 2 of dynamic similarity criterions, accordingly).

4) The analysis of the problems of combustion and explosion theory shows that at the limit (i.e. at the critical values of the dynamic variables: pressure, temperature and other) the problem solution is a criterion equation (composite dynamic similarity criterion) consist of the characteristic times at the beginning of the process and dynamic variables of the problem at the limit.

5) The dynamic similarity criterion that obtained as the result of solving a problem or corresponding composite criterion at the limit is closed to 1 on the order of magnitude.

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Modeling of condensed combustion products in combustion chamber

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Usage of aluminum fuel leads to formation of condensed combustion products (CCP) that significantly affect on propulsion system operation. Properties of CCP determine the implementation of slag accumulation, specific impulse losses, thermo-chemical interaction of CCP with construction elements, operation stability.

The tools providing determination of CCP characteristics depending on propellant composition and chamber properties were developed. The tools consist on the decision-making system about CCP properties at burning propellant surface and the model of CCP evolution in combustion chamber.

The decision-making system is based on ideology of expert systems. The system includes a set of formalized and unformalized procedures that respectively based on mathematical models and experimental regularities. The system provide determination (or estimation) of sizes, chemical composition and internal structure of CCP particles depending on propellant formulation and chamber pressure. Herewith the propellant formulation factors such as active or inert binder, various types and sizes of oxidizer, micron- or nano-sized aluminum are taken into account.

The evolution of CCP is understood as a complex of physical and chemical transformations of CCP within the flow of combustion products. The evolution of CCP is related to presence in the multiphase flow of agglomerates (enlarged particles of CCP). The developed model describes the following phenomena at agglomerate evolution: (1) combustion of aluminum with formation of smoke oxide particles; (2) chemical interaction of condensed aluminum and its oxide with formation of gaseous products; (3) changes in structure of agglomerate; (4) coagulation of agglomerates and smoke oxide particles; (5) agglomerates spatial moving.

The developed model takes into account size distribution of CCP, influence of agglomerates combustion on chemical composition and temperature of gas flow as well as spatial multiphase flow nature. The model provides determination of CCP properties at various sections of combustion chamber.

Parametric analysis of the model was performed. The results allowed to establish the regularities of influence of CCP properties that ejected from propellant surface and the geometrical sizes of the combustion chamber on characteristics of multiphase flow.

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Study of relations between kinetics of methane-air mixture combustion and modeling of flame parameters using ANSYS CFX software

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The results of numerical modeling of methane-air fuel combustion by ANSYS CFX are given for various chemical kinetics models, e.g. WD1, C1, C2, LCSR, C1C4 and GRI-Mech 3.0. The data were compared to the ones of ASTRA Multipurpose Software Package and experimental results (turbulent flames by Sandia Flame D). It was shown that selection of chemical kinetics model in flamelet library generation is of great importance for correct determination of contents of such intermediate components, as OH, CO and H₂. The values that are the closest to experimental results are achieved by using of GRI-Mech 3.0 Mechanism, and also C1C4 and LCSR Mechanisms integrated in ANSYS CFX software.

The present article is concerned with the study of relations between the kinetic pattern of methane-air combustion and simulation of flame parameters by ANSYS CFX. *WD1, C1, C2, LCSR, C1C4 Kinetic Models* and *GRI-Mech 3.0 Mechanism* [3] provided with ANSYS CFX [1, 2] were selected for the study.

Given that the information about kinetic model is stored in ANSYS CFX in such a format that is unavailable for users, ANSYS CFX Kinetic Models can be tested by means of the methods, as follows:

- comparison to combustion product equilibrium temperature;
- comparison of components contents to the temperatures of the Sandia Flame D, a turbulent flame pattern well-studied in experiments.

The calculation of combustion product equilibrium temperature indicated that the key differences between the mechanisms can be observed in case of excess fuel in the mixture (“fuel-rich mixture”) and in stoichiometric relationship. The comparison to the data resulted from *ASTRA Multipurpose Software Package* [4] indicated as follows:

- if excess air presents in the mixture $\alpha > 1.0$, then each mechanism provides the correct equilibrium temperature, i.e. $\Delta T \leq 2$ K.
- *WD1 Global Mechanism* overpredicts temperature values both in “fuel-rich combustion” range for $\alpha = 0.5$ and in stoichiometry for $\alpha = 1.0$ by 460 K and 95 K, respectively.
- *C1* and *C2 Mechanisms* overpredict temperature values in “fuel-rich combustion” range by 335 K and 297 K, respectively for $\alpha = 0.5$, for $\alpha = 1.0$ the deviation is $\Delta T \leq 5$ K.
- *LCSR, C1C4* and *GRI-Mech 3.0 Mechanisms* overpredicts temperature values by 110 K, 94 K and 126 K, respectively, for $\alpha = 0.5$, for $\alpha = 1$ the deviation is $\Delta T \leq 15$ K.

The comparison of computed results to the experimental data resulted from *Sandia Flame D Turbulent Flame Model* [5] indicated as follows:

- each mechanism provides the temperature in the flame axis to an accuracy of 130 K, the lowest deviations ΔT_{max} predicted by *LCSR, GRI-Mech 3.0* and *C1C4 Mechanisms* are 72, 84 and 90 K, respectively;
- the greater difference between the mechanisms is observed in determination of the contents of intermediate substances, i.e. *CO* and *OH*. *GRI-Mech 3.0* and *C1C4 Mechanisms* predicted the values that are the closest to experimental data.

LCSR, C1C4 или *GRI-Mech 3.0 Mechanisms* are recommended to be used in the calculations associated with “fuel-rich combustion”.

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Numerical simulation of the thermal impact from forest fires on the coniferous tree trunk

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Every year forest fires in various regions of Russia destroy the State Forest Fund, pollute the atmosphere and lead to loss of life and damage to rural areas [1].

Fires can be attributed to global phenomena on the scale of the impact of forest. Wildfires – important environmental factor in the dynamics of the forest cover. They greatly affect the biodiversity, the age structure of the stands, the ratio of species, and biogeochemical cycles in forest ecosystems.

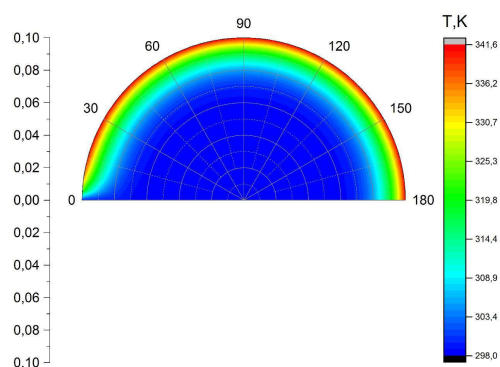
The impact of fire on woody plants often manifested in the formation of thermal damage. Trees got various injuries which occurs as a result of heat exposure from forest fire line [1]:

1. trunk burns;
2. burns and burn the roots;
3. crown burns.

Paper objective is numerical modeling of heat transfer processes in a layered structure of pine tree trunk when exposed to radiant heat flux from the front of a forest fire.

Heating of the trunk material thermally decomposes to release gaseous combustible pyrolysis products as a result of impact of forest fire. Under certain temperature occur thermal injuries of tree trunk [1].

Mathematically wood heating process under the influence of thermal radiation described by the system of non-stationary nonlinear heat conduction differential equations in polar coordinates with appropriate initial and boundary conditions.



Exposure to high temperatures leads to different effects on different species of conifers. This aspect depends on many factors such as the diameter of the trunk of pine tree, height up to the beginning of the live crown, where the cambium is most vulnerable, the depth of the root system and the age of the tree. As a rule, young trees are more susceptible to the effects of heat from a forest fire front. Temperature distribution is obtained in a layered structure of a coniferous tree trunk for different types of forest fires (Fig.1).

Fig. 1. Temperature distribution in the layered structure of the trunk of a pine ordinary subject to ground fire and the exposure time of 500 seconds.

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Mathematical simulation of deciduous tree ignition by the cloud-to-ground lightning discharge using WWLL Network data

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In recent decades, the problem of evaluation, monitoring and forecasting of forest fire danger has become more relevant [1]. This is largely due to the growth of anthropogenic load on forested areas, especially near urban territories. However, significant proportion of fire accidents and the area covered by the fire on remote territories is characteristic of the forest fires that have occurred as a result of storm activity. All modern methods and systems of forecasting of forest fires from thunderstorms are based on an analysis of statistical or factual information about the fire incident. All these methods have poor physical basis.

The purpose of research is numerical analysis of processes of deciduous tree ignition by the cloud-to-ground lightning discharge taking into account the data of WWLL Network (World Wide Lightning Location Network).

The passage of current in the deciduous and coniferous trees of various difference and explains the internal structure of a tree trunk. Moisture transport in the trunk of deciduous carried in large moisture transport ways - vessels, which will be the conductors of the resistor type. Heat production within the vessel is calculated according to the law of Joule. We consider the conductive heat transfer in a deciduous tree trunk. Moisture evaporates and the material is thermally decomposed as a result of heating to release the gaseous combustible pyrolysis products. These components are diffused into the gas phase region, where they are mixed with an oxidant (oxygen from the air). Tree trunk gas phase ignition takes place under certain temperature and concentration of the reacting gas phase components.

Mathematically the process of deciduous tree ignition describes by the system of nonlinear non-stationary heat conduction and diffusion equations with appropriate initial and boundary conditions. Numerical implementation is made using the finite difference method. Locally one-dimensional method is used to solve the two-dimensional equations of mathematical physics.

Energetic parameters of cloud-to-ground lightning discharge specified in accordance with the relevant information from the WWLL Network. Gorno-Altaysk State University is part of the global network and has station.

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**Mathematical modeling of the thermal impact from forest fires
on the coniferous tree roots**

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The purpose of work is numerical simulation of heat transfer processes in layered structure of coniferous tree root when exposed to damaging factors of forest fire. It should be noted the differences in the systems of the root system of coniferous and deciduous trees. The depth of the roots is small (root of the branch are in the topmost layer of soil, sometimes coming to the surface).

The following is the mechanism of thermal damage to the root system. Root branch heats and thermally decomposes with release of gaseous combustible pyrolysis products as a result of the heating of the material. At certain temperatures there is a thermal trauma of the wood in the area of influence of a forest fire (radiant heat flux, convective flow).

Mathematically the process of root wood heating under thermal effects is described by a system of non-stationary nonlinear differential equations of heat conduction in polar coordinates direction with the appropriate initial and boundary conditions.

The high temperatures great for different species even of the same species of coniferous trees. It depends on various characteristics: diameter of trunk and root branches of the coniferous tree, depth of root system, presence of open areas, where the root tissue is most vulnerable, and the age of the tree. Characteristically, the undergrowth of coniferous trees more susceptible to thermal influence of the damaging factors of forest fire. Numerical research of heat transfer processes in layered structure of the root branches of the coniferous tree under thermal influence from the forest fire front. Temperature distribution in the system "air-forest combustible material-topsoil-clay-root" for different points of time obtained. Note that the structure of the stem of coniferous and deciduous trees in the root zone is different. In the structure of the trunk of a coniferous tree it is possible to allocate a protective cortical layer, narrow subcortical area, which is the transport of moisture and resinous core. In consequence, this will also be taken into account in the mathematical model. In addition, the distributions of volume fractions of the phases, dry the organic matter and gas components in the surface layer of the root branch. Thus, the developed framework is physically reasonable theory of thermal damage to the forest stand when exposed to radiation from forest fires.

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Direct modelling of the shock and detonation waves interaction with micro-particles*I.A. Bedarev¹, A.V. Fedorov^{1,2}*¹Khristianovich Institute of theoretical and applied mechanics SB RAS, Novosibirsk, Russia²Novosibirsk State Technical University, Novosibirsk, Russia

The work is devoted to the mechanics of reacting heterogeneous media, coupled with the development of methods for studying the shock wave, explosion and detonation phenomena in reactive gas mixtures and microparticles. The problem is caused by explosion and fire safety issues, in particular with the development of methods for suppressing gas detonation by inert particles. This is interesting when study the suppression of detonation waves phenomena at the micro scale, as well as initiation and detonation reinitiation at the interaction of shock waves propagating in a combustible mixture with particles.

The purpose of this work was numerical study of quantitative characteristics of transient shock and detonation waves interaction which propagating in a combustible mixture with the microparticles system to determine the effect of flow regime on the resistance coefficient, thermal and velocity relaxation times of the particles, as well as the dynamics of the mixture ignition. The used mathematical model was averaged by Favre unsteady Navier-Stokes equations, supplemented by modification of SST $k-\omega$ turbulence model and the ideal gas equation of state. To describe the process of fuel and oxidizer mixture combustion involved the reduced kinetic mechanism. To take into account the particles collision it is used the model of elastic interaction of particles.

The modeling of transition of plane detonation wave through the grid of motionless isothermal particles was made. This formulation of the problem is valid for particles with a high heat capacity (Al_2O_3 , SiO_2) and the diameter of about 100 microns. Analysis of the shock wave configuration showed that the depending on the transverse distance between the particles, resulting in the forming discontinuities in the flow before the particles, in flow behind the detonation wave may occur the different regimes of shock waves interaction. At small distances - collective configuration of shock waves is realized, which at increasing the distance becomes first in Mach and then in regular interaction. Furthermore, at wave passage the detonation failure with the decay of its front into shock wave and combustion wave is observed. For large longitudinal distances between particles (low volume concentrations) further combustion wave can catch up the shock wave and detonation reinitiation happen. With the increasing of the volume concentration, as expected, it is possible complete failure of detonation without the reinitiation.

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Experimental measurements and numerical simulation of stretch rate for methane-air flame

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Improvement of quality of modeling results for turbulent burning and development of optical methods for diagnostics of burning processes are noted by scientific council on burning and explosion of the Russian Academy of Sciences among paramount actual problems of scientific and applied researches. The most important sign of quality of modeling is accuracy of a prediction of burning velocities depending on aerodynamic conditions of flame propagation. When burning a turbulent flame, at least to $Re=65000$, the important role is played by the theory of distribution laminar micro flames in the conditions of the combined deformation of a flame front: divergence of speed gas mixture flow and divergence of the direction of movement of flame front. In the presented work measurements of dependence of distribution speed for conical methane-air flame in a range of a stoichiometry ratio from 0,9 to 1,2 from local values of strain rate and curvature of the flame front by means of an optical method of visualization of streams PIV, and also numerical 3D calculation with application of global kinetics according to Westbrook – Dryer scheme are presented. The PIV method allows to study in details dynamic structure of a flame with the high precision defined by resolution of the camera. Interpretation of results of measurements has resulted in need to formulate a principle of stabilization of the flame front, called us Landau-Markshtein's effect. Comparison of experimental and calculated data has carried out verification of Markstein's law about linear dependence and establishment of the mechanism of the phenomenon of dependence of speed free flame distribution from a divergence of speed of gas mixture flow and a divergence of the direction of movement of flame front in a wide range of values of stretch rate (up to 2000 1/s). At small curvatures the flame front (up to 8 1/cm) the thermal mechanism of interaction of molecular transfer and the chemical reactions, responsible for Markshtein's law is revealed. At high stretch rates results of calculation with use of 3 reactions cannot qualitatively and quantitatively reproduce dependence of velocity of flame propagation from stretch rate.

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**Pulsating combustion of acetylene in micro-channel
with controlled temperature gradient**

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Experiments were performed with acetylene/mixtures over a wide range of equivalence ratios to investigate its combustion behavior in micro-reactors. C₂H₂/air mixtures were supplied in a quartz tube with an inner diameter of 0.7 mm at atmospheric pressure. The channel was heated externally by three H₂/O₂ flames (Spirig blowtorches) to ensure a stationary temperature profile from ambient temperature to about 1600 K. The temperature along the outer side of the channel was continuously measured by a FLIR A655sc thermal camera. A Princeton Instrument spectroscopy EMCCD camera, equipped with an optical band-pass filter (20BPF10-430), was used to collect the CH* chemiluminescence indicating the flame position. The acquisition frequency was set at 4260 Hz and pixel binning was performed. The signal was amplified (high EM gain) and the spatial resolution was 62 pixels/mm. In order to track the unstable flames propagation, a high-speed camera Phantom V1611, equipped with a teleconverter Teleplus MC7, was employed. A sample rate of 12000 fps and an exposure time of 82 μs were adopted to simultaneously optimize picture brightness and temporal resolution. Flame regimes typical from micro-combustion (Stable Flames, Flames with Repetitive Extinction and Ignition, and Weak Flames) were observed, but their regions of existence were found to be strongly depend on the operating conditions. Moreover, oscillating regimes were identified at the transition between the three main regimes.

For acetylene/air mixtures, the FREI region and the oscillating FREI regime are spread over a wide range of inlet velocities. However, in the FREI region, the frequencies recorded are particularly low: the mixtures auto-ignite at lower temperatures than that of methane and ethylene, and the flame is also quenched at very low temperature. As observed previously for methane and ethylene, the FREI frequencies increase with the inlet velocity. This dependence is clearer for fuel-rich and fuel-lean mixtures. Indeed, under these extreme equivalence ratio conditions, the flames run shorter distances and the wall temperatures are higher: high temperatures enhance flame speeds reducing the time available for the flames to propagate. Therefore, the smallest frequencies are obtained for $1.0 \leq \phi \leq 1.3$. In the oscillating regimes, two different tendencies are observed with respect to the nature of the oscillating behavior. The frequencies drop down if periodic fluctuations before extinction are present ($0.7 \leq \phi \leq 1.3$) while frequencies increase if the flames are characterized by thermo-diffusive instabilities ($\phi \leq 0.5$, $\phi = 1.7$). A flame splitting was also observed soon after the flame ignition, and a peculiar distribution of the CH* signal with multiple peaks was noticed at $\phi = 1.7$. In the oscillating flame region, diffusive-thermal oscillations were observed for very lean and very rich mixtures, while for the other equivalence ratios oscillations before extinction were detected.

The high flame chemiluminescence enabled the investigation of ultra-lean conditions, down $\phi = 0.1$. In such conditions, only weak and oscillating weak flames were observed. These results confirm the capability of micro-combustion to achieve combustion under very lean conditions and thus to extend the flammability limits of a given fuel. Combustion under lean and very lean conditions is nowadays seen as a very promising technology for clean and high efficiency combustion: indeed, NO_x emissions are reduced because of the low flame temperature. Furthermore, it ensures complete oxidation, reducing hydrocarbon and CO emissions.

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Fuel and waste combustion in a fluidized bed of catalyst

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Nowadays, there are many ways of thermal processing of energy-intensive materials, including fuels and waste. Most of them are based on direct high-temperature oxidation in furnaces of various types. A common drawback of all traditional fuel combustion methods is the high process temperature - from 1000 to 2000 °C. The inevitable consequence of high temperatures is atmospheric pollution by toxic combustion products (nitrogen and sulfur oxides, CO, soot, benzpyrene).

Moreover, there are a great interest in inclusion of not previously considered low-quality fuels, including technogenic waste and renewable biomass in the fuel resources. The use of such materials is very difficult or impossible because of their properties (low calorific value, high humidity) and high environmental risk of processing.

In the Boreskov institute of catalysis was developed an unconventional method for liquid, gaseous and solid fuels combustion in the presence of catalysts, which allows eliminating many disadvantages of high-temperature combustion of fuels. The method is based on a combination of four principles: the use of deep oxidation catalysts; combustion of fuels in the fluidized bed of catalyst particles; combustion of fuel and air mixtures in a ratio close to the stoichiometric; the combination of heat release and heat removal in a single fluidized bed.

The work shows that the presence of deep oxidation catalyst in the reaction system reduces the temperature of organic fuel combustion from 1000-1500 ° C to 600-800 °C, while maintaining high combustion rates and ensuring complete combustion of fuel-air mixtures without significant air excess. At the same time, the technology provides high environmental safety of the combustion process.

The study described an efficiency of catalytic combustion in the fluidized bed for such materials as coal, sulfur oil, oil shales and tar sands, oil sludge and sewage sludge.

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Heterogeneous detonation wave propagation in a channel with the gradual extension*A.V. Fedorov¹, T.A. Khmel¹ and S.A. Lavruk⁻¹*¹Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, Novosibirsk, Russia

Detonation propagation in technical devices channels is of interest to next problems: on the one hand developing of detonation engine and detonation technologies and on the other hand preventions of detonation during emergency situations. Fundamental problem here is to find out main mechanisms of detonation waves propagation in the channels with different geometry.

In this study the heterogeneous detonation wave propagation in channels with the gradual extension was investigated. Channel was filled with stoichiometric mixture of aluminum particles and oxygen. Plane detonation wave (CJ type) was initiated at the left side of the calculation domain and regimes of further propagation was studied. Different detonation regimes were obtained by varying of channel width, angle of the extension and diameter of the aluminum particles. In this paper the diameter of the particles was varying in submicron range ($d_p=0.5\dots3.5\ \mu\text{m}$). Angle extension value was varied in the range from 30° to 60° .

The mathematical model is based on the concept of a two-velocity two-temperature continuum of the mechanics of heterogeneous media. Aluminum combustion is described as a reduced reaction initiated after the particle achieves a critical temperature (the ignition temperature) that accounts for incomplete particle combustion (due to the oxide film growth). The values of parameters (ignition temperature, activation energy, heat release, and chemical reaction velocities) were determined previously from the experimental data, including detonation velocity, ignition zone length and combustion delay. The transition from diffusion to kinetic regime of aluminum particle combustion was taken into account with burning time power dependence on particle diameter as $d^{0.3}$ in the interval $500\ \text{nm} < d < 3.5\ \mu\text{m}$.

During simulation different detonation regimes of propagation were determined. The supercritical (with a continuous propagation), the critical (with a partial failure) and the subcritical (with a complete detonation failure) regimes were defined. Flow pattern of the detonation was analyzed and comparison with similar flows of the shock waves and detonation waves in pure gas phase were done. Influence of the transverse waves on the leading front propagation and detonation failure was analyzed.

The effects of the main factors such as channel width, angle of extension and diameter of particles were investigated too. Parameters that influence on detonation propagation were planted on detonation regime map and plot of maximum pressures. A formula for critical channel width depending on the angle of gradual extension is presented. Detonation regime maps were presented in planes channel width – particles diameter for different extension angles.

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Combustion completeness of boron containing fuels in composite propellants

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The research object is the model composite propellant based on ammonium perchlorate, energetic binder and boron-containing fuel (pure boron, aluminum diboride or Al+B mechanical mixture). The aim of work is experimental assessment of the completeness of fuel combustion in composite propellant. First step involves the variation of “pure” boron content (12%, 18%, 24%, and 40%) in propellant formulation. Second step involves the replacement of boron with aluminum diboride or with “aluminum diboride simulator” – the mechanical mixture of aluminum and boron – in a propellant formulation with 40% fuel content. The firing tests are performed in nitrogen at pressures of 1.2 MPa or 2.5 MPa. The original sampling technique [1] (blow through bomb with extinguishing the particles in a co-current flow of nitrogen) and the original chemical analysis technique (cerimetric method [2] for quantitative determination of the combustion completeness of the combined fuel) are used. With particle’s extinguishing being performed near the burning surface, the oxidation of metal fuel on and close above the surface was actually investigated. It was found that the oxidation efficiency essentially depends on the burning rate and on the agglomeration process.

The following experimental results are reported in the present work: data on the burning rate at pressures of 1.2 MPa and 2.5 MPa; particle size distribution functions in the range of 0.5–1000 microns for condensed combustion product (CCP) particles; the CCP particles morphology (optical microscopy, SEM, EDS); mass fraction of the skeleton-layer remaining after burning; data on the combustion completeness of metal fuel, flame temperature at 0.1 MPa. Comparison of the combustion efficiency of boron, aluminum diboride and its simulator (Al + B) is also carried out for propellant formulation with 40% of metallic fuel.

It was found that CCPs of boron-containing propellants consist mainly of almost white particles of boron oxide and dark particles of the boron agglomerates. Particles of oxide have the micron and sub-micron sizes. Many boron agglomerates have the spherical and drop-shaped form that demonstrates the boron melting. The agglomerate size D_{43} equals 29 micron while D_{43} equals 3 micron for initial boron particles. Replacement of boron with aluminum diboride did not facilitate the fuel combustion completeness and the efficiency of energy release. Presence of aluminum as a part of the combined fuel has led to agglomeration strengthening that was revealed as increase in the size of CCP particles and in mass of the skeleton-layer combustion residues.

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Ignition of a metallized composite propellant by a hot particle

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In recent years, the prospects for the development of near and far space affect the development of the space industry in Russia, the USA, China, India, Japan and some other countries. One of the priorities of the successful implementation of this program is to develop new compositions of high-energy materials, which are used in rocket engines, booster accelerators, gas generators, catapults, etc. Also promising direction of space industry development is the creation of energy-efficient igniter of fuel charge. Principle of operation of such device can be based, for example, on the local conductive heat supply to a condensed substance by a small set of heat sources with limited heat content.

Experimental study of ignition process of high-energy materials is a difficult task. In many cases high-level metrological provision of experiments to study the interrelated physical and chemical processes in the condensed phase and gas area are not realizable in practice, for example, due to the relatively small values of ignition time.

A mathematical model is developed for predicting the characteristics of ignition process of a typical metallized composite propellant (butyl rubber + ammonium perchlorate + metal powder) by a hot particle within the mathematical apparatus of continuum mechanics. The mathematical model describes a set of interrelated processes: conductive heating of the near-surface layer of composite propellant, free-convective and radiant heat sink from the local heat source into the surrounding gaseous area, cooling of a particle, exothermic reaction of ammonium perchlorate and butyl rubber in the condensed phase.

As a result of the study the stability of ignition process is justified. Limit conditions and characteristics of the ignition of the metallized composite propellant is established. Analysis of influence of the group of significant factors (initial temperature, size, shape, thermal properties and quantity of local heat sources, their partial or complete immersion into the composite propellant, non-ideal thermal contact at the *hot particle – condensed matter* interface) on the characteristics of the induction period is executed. It is shown that analyzed factors influence more significant on the ignition characteristics in the conditions close to the limit ignition conditions in comparison with conditions of intensive physical and chemical processes. It is proved that taking into account explicitly the heterogeneous structure of condensed matter due to significant difference of thermophysical properties of dispersed components, as opposed to method based on the averaging thermophysical properties significantly increases the accuracy of the forecast of induction process characteristics, in particular, ignition delay time and minimum ignition temperature of a local heat source.

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Effect of organic coatings of nanoaluminum on the burning rate of mixed compositions

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Nowadays different methods for increasing the aluminum nanopowder (nAl) reactivity are known. One method is the modification of nAl particle by encapsulating with organic compounds. The study of the effect of encapsulated nanoaluminum powders on the combustion characteristics of mixed compositions is of particular interest.

The purpose of this work is to estimate the influence of different organic coatings of nano-sized aluminum powder on combustion characteristics and content of solid combustion product of mixed composition (MC).

Investigations were carried out with mixed compositions containing ammonium perchlorate and inert fuel-binder. Other conditions were being constant: excess oxidant ratio $\alpha=0.5$ and aluminum powder content 15 wt. %. The study of modified powders by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) as well as the study of oxidation of modified powders by heating in air using TGA and DTA were done. Determination of stationary burning rate at pressure $p>0.1$ MPa was carried out in constant pressure device and at subatmospheric pressures (the vacuum chamber was used). Determination of the condensed combustion products content (z) was carried out at atmospheric pressure by burning of samples outdoors. The chemical composition of condensed combustion products, crystalline structures and their volumetric content were determined by X-ray diffraction method.

Analysis of the results shows the influence of the nature of organic coating for Alex powder on the morphology and oxidation activity. The results of studies of the stationary burning rate in a pressure range of 0.04–6.0 MPa shows strong dependence of the burning rate vs pressure. The exponent v in the burning rate law takes values of 0.63–0.73 depending on the type of aluminum powder in the MC. Study of samples combustion at atmospheric pressure outdoors demonstrates the possibility to reduce the content of the condensed combustion products in MC. X-ray diffraction method gives chemical composition of the condensed combustion products, their crystalline structure and volumetric content. Qualitative and quantitative phase analysis allows determining the presence of carbon in the condensed combustion products in MC containing aluminum. This allows outlining possible methods to control condensed carbon content in the combustion products.

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Modeling of combustion waves in the solid shell-core energetic materials

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The properties and stability of combustion waves propagating in the composite solid energetic material of the shell-core type are numerically investigated within the one dimensional model with heat losses to the surroundings. The structure of such composite has inert core element, which is covered with the solid fuel annulus. The metal wire or carbon nanotubes can serve as inert central heat conducting element. It's main role is to provide heat recuperation from hot products to fresh combustible mixture. Similar excess enthalpy principle is also well known for combustion of gas mixtures in micro-channels. This allows to increase the burning rate and temperature of the solid fuel and stabilize the flame. Here we focus on the analysis of how the heat losses affect the enhancement of the burning rate and the limits of the stable combustion wave propagation in the model of solid shell-core composite energetic material.

It was shown that for optimal configuration the propagation of stable travelling combustion waves is possible for the parameter values, for which the flame fronts are unstable or do not exist for pure solid fuel, even in the case of significant heat losses. Thus the flammability limits of solid fuel combustion can be significantly extended by using the effective heat recuperation scheme via the inert heat conducting elements. Moreover in the case of the composite material the flame temperature is substantially superadiabatic and the flame speed can be several times higher as compared to the corresponding characteristics of the combustion of solid fuel only.

Two scenarios of the onset of pulsating instabilities are determined. Once the neutral stability boundary is crossed in the space of parameters of the problem either stable or unstable limit cycles are formed leading to the emergence of oscillations with finite constant amplitude or to the oscillations with growing amplitude causing flame quenching. The parameter values for the occurrence of these dynamical regimes are found. A new effect of the discontinuity of the Hopf frequency along the critical curve for the onset of instabilities is found and quantified. This can lead to interesting and complex dynamical behaviour due to the nonlinear interaction of instabilities with different frequencies near the singular point of the critical curve.

The effect of the different geometrical configuration of the composite material on the properties of the deflagration wave is discussed as well as possible experimental setup to investigate the process of flame propagation in solid composite.

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Facile preparation of organic nano-layered aluminum phosphonate for effectively reducing the flame hazards of polystyrene*Weizhao Hu, Lei Song, Zhou Gui*

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Heavy soot and toxic gases will be released during combustion of polystyrene (PS). These potential fire risks of PS can be decreased by effective combustion suppression. In this work, organic nano-layered aluminum phosphonate (OAHPi) was simply synthesized by one-step and firstly incorporated into PS to reduce flame hazards. The morphology and thermostability of OAHPi was characterized by various characterizations. Fire hazard assessment and flame retardancy of composites were also investigated. Results revealed that laminar OAHPi with nano scale was formed by a facile method. With relatively low additive amount, thermostability and char yield increased with increasing OAHPi content in PS, while total heat release, CO₂ output and smoke density decreased. Above results indicated that OAHPi had a significant effect on the flame retarding and heat endurance, which was beneficial to decrease fire potential risk of PS. The high efficiency was attributed to layered structure and phosphorus-containing. Meanwhile nanoscale size and organic fraction improved compatibility of OAHPi and PS. Theoretically, homogeneous dispersed lamellar sheets blocked the heat and energy transfer, and phosphorous compounds worked in condensed or gas phase. The possible flame-retardant mechanism was also proposed according to experiment results.

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Experimental study on pyrolysis of opaque non-charring polymers in reduced pressure environments

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In the recent years, polymers have been widely used in the industry and life for their characteristics of low-cost, light-weight. However, the huge amount of C, H atoms in the polymer make it high flammability and great danger to burn. Pyrolysis is the first step in polymers gasification and in other thermochemical conversion processes. Thus, the investigation of the influence of operating conditions on the pyrolysis behaviors is important for the study of the whole combustion process. This study investigated the pyrolysis behavior of opaque non-charring poly(Acrylonitrile Butadiene Styrene)(ABS) in a reduced low-pressure chamber under different heat fluxes of 18 and 36 kW/m². The volume fraction is controlled in the range of 4%-5% by a vacuum pump. The char residue has been observed, the mass loss rate, the temperature on the top surface and bottom surface temperature during the whole pyrolysis have been measured on real time, and the parameter of T_p , which describes the impact of pressure on the sample surface temperature has been introduced. Besides, the relationship of pyrolysis rate and pressure has been discussed.

The samples are black ABS sheets of 100mm*100mm*3mm. To assure the one-dimension pyrolysis process, all sides and the bottom surface of samples are covered by aluminized paper. And the paper are all 10mm higher than the samples' surfaces with the consideration of the thermal expansion of samples. The 0.5mm K-type thermal couples are fixed on and under the samples to measure the surface and bottom temperature respectively.

Pressure affects the heat convective transfer coefficient, consequently, affects the pyrolysis rate. And for lower heat flux, this effect is more significant. The results show under low-intensity heat flow, there is a loose layer of char residue left after the pyrolysis, and in addition, there are some bubbles in it thanks to the escape of the pyrolysis gas. While under the high-intensity heat flow, the char residue of ABS is thinner but denser, due to the higher pyrolysis rate and thermal hysteresis. And under the low-intensity heat flow, the sizes of pyrolysis bubbles go smaller and smaller with the decrease of the pressure. Under lower heat flow, T_p shows significant decrease as the pressures go up. While, under higher heat flow, the decreases of T_p is negligible. The pressure has a similar impact on the bottom temperature with that on the surface temperature. Under low-intensity heat flow, mass loss rate (MLR) shows a high sensitivity to the pressure, and the MLR decreases as the pressure goes up. While under high-intensity heat flow, the MLR shows a negligible sensitivity to the pressure. The pyrolysis rate \dot{m} is proportional to the a th power of the ambient pressure P . For 18kw/m² heat flow, $a = 1.3$ and for 36kw/m² heat flow, $a = 0.1$.

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**Numerical study of the polyethylene burning in counterflow:
Effect of pyrolysis kinetics and products composition**

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The polyethylene burning behavior in the counterflow of oxidizing air has been studied numerically by the coupled model describing feedback heat and mass transfer between gas-phase flame and polymeric solid fuel. A two-dimensional elliptic equation in axisymmetric formulation (revealing the polymer cylindrical sample used in experiment) is employed for the heat transfer in solid fuel and the set of one-dimensional hyperbolic equations – for solid-to-gas conversion degree of pyrolysis reaction. The gas-phase chemical kinetics and transport processes have been calculated by the Cantera open-source code. The heat flux from the flame zone to the solid fuel surface is assigned as a boundary condition for the prediction of heat transfer in the solid, while achieved surface temperature and mass burning rate appear as boundary conditions for the gas-phase conservation equations. Such an iteration procedure has been successively carried out until a convergent solution is obtained.

For the modeling of detailed chemical kinetics of gas-phase combustion, two mechanisms have been employed: 1) – 1997 reactions and 300 components for scheme involving lower hydrocarbons C₁–C₄ and 2) – 1411 reactions and 163 components for higher hydrocarbons up to C₁₂. The most crucial point of the present analysis refers to the composition of polyethylene pyrolysis gaseous products adjacent to solid fuel surface. This input parameter is generally regarded as uncertain since no reliable data have been reported on exact component fraction values of this composition. Thus, five sets of compositions are considered: 1) – pure ethylene C₂H₄, 2) – C₂H₄/C₂H₆/C₃H₆/C₃H₈/C₄H₆/C₄H₈/C₄H₁₀, 3) – C₃H₆/C₄H₆/C₆H₆, 4) – CH₄/C₆H₆, 5) – C₁₂H₂₆. Two modifications for kinetic parameters of solid fuel pyrolysis reaction have been considered.

The distributions of temperature and chemical components (oxygen, carbon monoxide, carbon dioxide, water vapor, propylene, butadiene and benzene) in the flame zone have been calculated and compared with the results of experimental study of the combustion of ultrahigh molecular weight polyethylene. As it has been found, higher hydrocarbon composition (C₁₂H₂₆) shows the best agreement of temperature and species profiles with the measurements, especially for low-level mass fractions of by-product components – namely, propylene, butadiene and benzene. In opposite, low hydrocarbons provide a slightly better agreement on the mass burning rate of solid fuel.

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Small-scale investigation of the fire hazard characteristics of wood samples due to the different type of thermal impact while forest fires

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The main factors influencing on the ignition of combustible constructional material and the propagation of wildland-urban interface fires are the radiative heat transfer (convective in the gas atmosphere) of flame, as well as the transfer of burning/smouldering particles [1].

The goal of this work is to study experimentally the fire-hazard characteristics of wood exposed to heat: 1) front of the model surface fire, 2) smouldering pine bark particles.

The arrangement of the experiment and the description of the setup are given in [2]. To measure the temperature of the wood surface in the range of 293 - 550 K and 500 - 850 K, the thermal imaging camera JADE J530SB was used with an optical filter (2.5 - 2.7 microns). The front of the model ground fire was simulated by the combustion of the pine needle layer. The samples of pine ($0.23 \times 0.095 \times 0.022 \text{ m}^3$), aspen ($0.17 \times 0.1 \times 0.02 \text{ m}^3$), and larch ($0.17 \times 0.1 \times 0.02 \text{ m}^3$) were used as the samples which simulate the wood applied in the construction industry. In some experiments, the wood samples treated with a fire retardant «FUKAM» were studied. In all experiments, pine bark with a typical linear size of 15; 20; 30 mm and a thickness of 4÷5 mm was used as smouldering particles. In the experiments, the number of smouldering particles was varied from 1 to 10 to simulate the ignition of wood, starting from a single particle and ending with a firebrand showers.

The conditions for the ignition of wood samples exposed to different thermal effects were studied under the laboratory conditions: 1) model ground wildland fire 2) smouldering pine bark particles. The results have shown that fire retardants influence on the fire-hazard characteristics of wood. The probability of ignition and the ignition delay of wood were determined depending on the size and number of firebrands, the presence of the air flow in the landing zone of particles, as well as on the initial temperature of wood. The experimental temperature distribution was obtained on the surface of wood exposed to the model ground fire using infrared thermography.

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Investigating the paired fire-tube furnace with a controllable flame flow path

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Increasing the capacity of existing boilers causes a number of problems: the volume thermal stress increment reduces the resource of the metal heating surfaces; a huge fuel-air mixture flow rate through the burner increases the flow velocity, and respectively the aerodynamic resistance of the furnace increases as the square of the velocity magnitude. Improvement of gas flows inside a combustion chamber could be the solution of problems described above. For this purpose new paired fire-tube furnace is proposed in the paper. Paired fire-tubes are connected by channels at both ends. Only one fire tube is equipped with a burner, which is located frontally and delivers the fuel-air mixture by straight-through (untwisted) flow. The transfer of the combustion products into the second pipe in a direction opposite to the fuel supply creates a vortex. Thus such layout makes possible vortex combustion for the straight-through burner.

Full-scale field tests of the combustion chamber with proposed design are expensive and very time-consuming, because they require multiple-factor experimental research of three-dimensional turbulent combusting dynamics. Therefore functional processes in the proposed combustion chamber with a controllable flame flow path were simulated by means of the proven computer-aided engineering software ANSYS CFD Multiphysics. For the computational research, a full geometrical model of the paired fire-tube furnace was implemented. For fuel supply the exact model of direct-flow burner Weishaupt WKGL70 version 3LN was used. The numerical computation results display the vortex combustion processes within the paired fire tube furnace with a bypass channel. Vortex is observed between the two coaxial counter flows. Entering the vortex fuel-air flow spins. That substantially accelerates its ignition and further burning, owing to considerable intensification of mixing fuel with air. This reduces the length of the flame and excludes its pouncing on the heating surface during all modes of boiler operation. The intensive heat transfer from the flame leads to a reduction of the flame core medium temperature. Low combustion temperatures are favorable for decreasing the emission of thermal nitrogen oxides, thereby moderating harmful effects on the environment. Uniform distribution of heat dissipation along the length of the paired fire tube furnace with a bypass channel becomes the reason for the relatively reduced levels of wall heat fluxes. It is conducive to use cheaper materials for the heating surfaces. Straight-through fuel supply, together with the vortex aerodynamics in paired fire tube furnace with a bypass channel create the most favorable conditions for the complete fuel combustion fuel burn with minimal flow resistance.

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Modelling of detonation processes in gas suspensions of micro and nanosized aluminum particles

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Study of the detonation regimes of combustion in aluminum dusts is relevant both in terms of prevention of explosions, and in relation to its potential applications as additives in working mixtures in the nozzles of the engines. Of particular interest are the nanoparticulate powders having high sensitivity to ignition. Problems of detonations in micro-sized aluminum suspensions have been widely studied earlier in the frame of semi-empirical models [1-3]. Some results on the initiation and propagation of cellular detonation in mono and polydisperse suspensions of aluminum particles on the base of the model [3] were presented in [4-5].

This paper presents a semi-empirical model of the detonation gas suspension of sub-micron and nano-sized aluminum particles in oxygen. The transition from the continual to the free-molecular regime of gas particle flow and the heat transport properties is taken into account when the particle size decreases. The model includes the pre-ignition reaction of particle surface oxidation and the particle melting. The ignition criterion is based on the melt-dispersion mechanism; the transition to the heterogeneous combustion reaction occurs when the particle is completely melted. Description of the combustion under reduced chemical kinetics based on the known experimental data presented in [6] and in other works on aluminum nanoparticle burning time dependences on the ambient gas pressure and temperature, oxidant concentration, and the particle size.

On the basis of the problem of stationary detonation structure solution the analysis of the main characteristic parameters is performed. It is shown that the Knudsen numbers in detonation flows in suspensions of particles of greater than 50 nm do not exceed 1, indicating the transition regime of aluminum particle combustion. For micro-sized particles the characteristic scaled of the zones of thermal and velocity relaxation of the phases and the combustion zone are comparable. For nanometer particles the scale of the combustion zone is substantially greater than the phase relaxation zones. On the base of numerical simulation of 2-D unsteady flows in the channel the scenarios of cellular detonation formation and propagation are studied. Data on the detonation cell size in suspensions of particles with different particle sizes are obtained. The dependencies of the detonation cell size on particle diameter for particles less than 1 μm and micron particles are sufficiently different.

The work was supported by the Russian Foundation for basic research (grant 16-08-0778).

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Theoretical model for quantitative estimation of the fundamental concentration limits for deflagration propagation in the hydrogen-air gas mixtures

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Report is aimed at clarification of a notion “fundamental flammability limits”.

History of the “flammability limits” concept is shortly introduced.

Practical deficiencies and inherent contradictions of the empirical (utilitarian) flammability limits are demonstrated.

Non-empirical, computationally-inexpensive method for quantitative estimation of the concentration limits for deflagration propagation in dry hydrogen-air gas mixtures is proposed.

Notion of the fundamental concentration limits (FCL) for plane deflagration propagation is discussed and compared with the available engineering and normative concepts.

Procedure for the quantitative estimations of the FCL is described.

Model is validated against the available empirical correlations for dependence of concentration limits upon initial temperature of the dry hydrogen-air gas mixtures.

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Features of inverted hydrogen-air diffusion flame*D.O. Kochergin¹, V.V. Lukashov²*¹Novosibirsk State Technical University, Novosibirsk, Russia²Kutateladze Institute of Thermophysics, SB RAS, Novosibirsk, Russia

Selective diffusion, expressed by a significant difference between the diffusion coefficients of individual gas mixture components and thermal diffusivity, leads to disruption of similarity between the diffusion and thermal processes in the reacting gas flow. Excluding violations of similarity, it is impossible to explain a number of observed phenomena.

For example, it is noted in the paper of D. Frank-Kamenetskii [1] concerning diffusion combustion that equality between the stationary temperature of the reaction front and theoretical adiabatic combustion temperature occurs only in a particular case of $Le=Pr/Sc=1$. The differences in the Lewis numbers of fuel Le_f and oxidizer Le_o can cause asymmetry of the density field under the symmetric boundary conditions [2]. We should note that violation of flame stability could be caused by other reasons. The loss of flame symmetries is observed, for example, in [3]. The authors explained this by the fact that under the combustion conditions, close to flashback, the uneven character of conditions at the inlet to the combustion zone becomes stronger.

Effects related to $Le \neq 1$ have a strong influence on combustion of mixtures of hydrogen diluted with inert gas in the inversed flame. The “normal” flame means fuel burning in the oxidant atmosphere. Inverse flame occurs, when the oxidant is fed to the fuel atmosphere. In present paper, we consider the reactive flow in a circular channel with the air jet supply into the co-current flow of the fuel mixture. The results of measurements of average temperature in different sections along the channel during combustion of H_2/CO_2 and H_2/He are analyzed. For the H_2/He mixture, effective number $Le_{eff} = (1+\phi)/(1/Le_f + \phi/Le_o)$ is close to one. The temperature distributions in this case are symmetric and the maximal temperatures T_f in the flame front are almost equal to adiabatic temperature T_{ad} of combustion of the considered fuel-air mixture. For the H_2/CO_2 system, $Le_{eff} \approx 2$. In this case, with an increase in the hydrogen mass fraction from 2 to 3% in the fuel mixture, violation of flow symmetry was observed. At that, the level of maximal temperatures reduced $T_f/T_{ad} \approx 1.3$ to 0.7. Under the above conditions, flow stability are influenced not only by Le_{eff} , but by the Re number and velocity ratio.

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Numerical simulation of flame spread over vertical and inclined combustible surfaces

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Coupled simulations of flame spread over the surface of a combustible material remain extremely challenging, particularly when performed in realistic fire scenarios. Indeed, while certain successful attempts to predict flame spread numerically can be found in literature, examples of using Fire Dynamics Simulator (FDS), one of the most popular open-source fire code, to predict flame spread are limited and struggle to replicate experimental data.

This paper explores the capability of FDS 6.4 to accurately predict upward flame spread over vertical and inclined surfaces of PMMA. Different configurations were considered, including large (5 m height) and bench-scale slabs (20 cm height), where the sample is exposed to the constant radiative heating or burns in self-sustained regime.

The simulations were performed in 3D LES mode, and the default FDS settings were retained wherever possible, except for those aimed at improving radiative heat flux calculations. For the large-scale scenario, computational grid in the gaseous domain was generated to obey the plume resolution index, $D^*/\delta x$, to be within the range normally accepted in engineering simulations, i.e. exceeding 10. It is found sufficient to replicate general flow patterns characteristic for flame spread over vertical and inclined surfaces, provided that the radiative heat flux dominates at the sample surface. Reasonable agreement with the measured heat release rates and heat flux spatial distributions has been obtained.

However, much finer grid resolution appeared to be necessary to resolve near-wall temperature gradients at smaller scales as the flame size is reduced down to the optically thin range and the convective heat flux dominates. The necessary grid requirement was elaborated by replicating heat flux measurements for flames attached to a vertical wall. To avoid excessive grid refinement in the near-wall region, modified boundary condition has been considered, which allows for the convective heat flux from the diffusion flamelet not resolved by the grid. These approaches have also been applied to predict the self-sustained burning of flammable material without flame spread.

It has been demonstrated that the flame propagation regime is very sensitive to how the material is ignited. Two qualitatively different flame spread regimes have been observed, depending on the ignitor power and size. In the axial regime, the flame concentrates and propagates rapidly around the centerline, leaving the periphery regions unburned. In the frontal regime flame propagates over the entire sample width.

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Implementation of low NO_x firing systems to fire coals of the Kansko-Achinsk coal basin on boiler P-59 of a 330 MW power unit

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A topical issue in design of firing systems for large-scale coal-fired boilers is the implementation of technical solutions based on the present-day scientific and technical achievements, ensuring the best possible combinations of reliability, efficiency and environmental safety criteria.

One of the ways to reduce nitrogen oxides (NO_x) when firing solid fuel in a boiler furnace is to arrange low-NO_x staged flame combustion.

The paper presents the key results of refurbishment of boiler P-59, unit No.2, at the Ryazanskaya GRES aimed at switching the boiler to firing off-design Kansko-Achinsk coals, increasing its capacity and reducing NO_x emissions.

When implementing a low NO_x firing system on boiler P-59, an important stage was a CFD-simulation of the firing processes in the boiler furnace at different loads and with various combinations of operating mills using ANSYS FLUENT software package. Based on the results of the CFD-simulation, the following technical solutions have been approved:

- Conversion of coal pulverizing systems from air to gas fuel drying;
- Arrangement of the main burners in 3 levels;
- Recirculation of flue gases to burners of the 2-nd and 3-d levels;
- Installation of OFA, bottom air supply and curtain air nozzles.

The paper compares CFD-simulation results with operational tuning data and estimates the efficiency of the applied methods of design and implementation of a low NO_x firing system.

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An experimental study of horizontal flame spread over PMMA

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The flame spread over the surface of horizontally placed slabs of four types of PMMA specimens in still air have been studied. Temperature distributions in the gas phase near the solid fuel surface and in the condensed phase were measured using microthermocouples. Spatial variation of the species concentration in the gas-phase flame near the solid fuel surface was measured using probing mass spectrometry. Also flame spread rate over the polymer surface was measured. The experiments revealed differences in the combustion character of the specimens investigated. At the flame spread over surface of 2 (out of the four) specimens boiling and formation of large bubbles were discovered. The main flame components including MMA, O₂, CO₂, H₂O, N₂, C₂H₄ (ethylene), C₃H₆ (propylene) have been first identified, and their concentration profiles at different distances from the flame front have been measured. The data on the chemical flame structure have been shown to be in good agreement with the data on its thermal flame structure. The size of the “dark zone” of the flame, in which the temperature near the polymer surface is minimal, correlates well with the size of the oxygen-free zone, which is adjacent to the burning surface. Conductive and radiative heat feedback from the flames to the condensed fuel surface was estimated on the basis of the experimental results. The conductive and radiative heat fluxes averaged over the burning surface were estimated to be approximately 7.8 and 11.1 kW/m², respectively. It has been established that, in contrast to the conductive heat flux, the radiative heat flux is minimal in the flame front and increases as the specimen burns out. The data obtained may be used for developing and validating a numerical model of flame spread over PMMA surface.

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Study of ignition and combustion of high-energy materials containing aluminum powder and metal additives

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Metal powders and catalytic combustion additives are widely used in high-energy materials (HEM) for their high heat of oxidation and specific impulse. While single metal particle oxidation mechanism is studied quite well and the oxidation in HEM is investigated much less because of huge numbers of possible combinations of metals and oxidizers.

The ignition and combustion study was conducted with HEM samples based on ammonium perchlorate and ammonium nitrate, active combustible binder MPVT-ASP and metal powders. We used aluminum powders (ASD-4, Alex) for base HEM compositions and powders of boron, iron, titanium, aluminium diboride and titanium diboride.

The ignition process of HEM samples was studied using the setup for radiant heating based on the CO₂-laser with a wavelength of 10.6 μm and power of 200 W. The combustion study of HEMs was carried out using a blow-through sampling bomb to determine the burning rate of samples and combustion condensed products characteristics.

Some experimental results of HEMs ignition are given in Fig. 1.

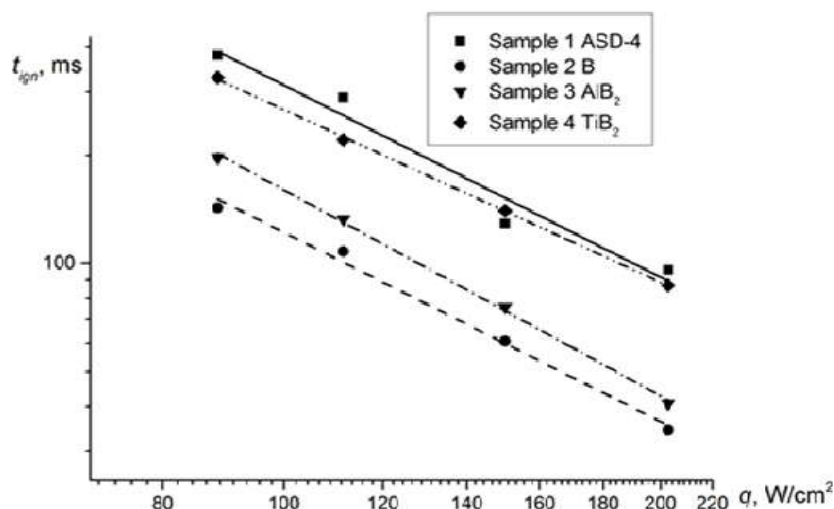


Fig. 1. The ignition time vs. the heat flux density for HEMs, containing metal powders: ASD-4 – $t_{ig}=9.90 \cdot 10^5 \cdot q^{-1.75}$; B – $t_{ig}=2.02 \cdot 10^5 \cdot q^{-1.61}$; AlB₂ – $t_{ig}=7.39 \cdot 10^5 \cdot q^{-1.83}$, TiB₂ – $t_{ig}=4.71 \cdot 10^5 \cdot q^{-1.62}$

Combustion study has shown that partial Alex replacement by iron in the HEM composition leads to 1.3–1.4 fold increase in the burning rate in the pressure range of 2.2–7.5 MPa.

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Ignition study of solid fuel samples by CO₂-laser

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Coal-fired power plants and metallurgical industry is the main source of greenhouse gas and other pollution like sulphur and nitrogen oxides. According to Zeldovich theory, supplying the lowest possible temperature in flame core is needed to decrease nitrogen oxide concentration in flue gases while supplying sustainable combustion. In this case, investigation of coal ignition characteristics is important.

In current study, coal ignition delay times were defined at different laser heat flux density in the range of 90–160 W/cm². Coal samples of T-grade bituminous coal and 2B-grade lignite of Kuzbass and Kansk-Achinsk deposits were studied. The scheme of experimental setup based on CO₂-laser for ignition study of solid fuel samples is given in Fig. 1.

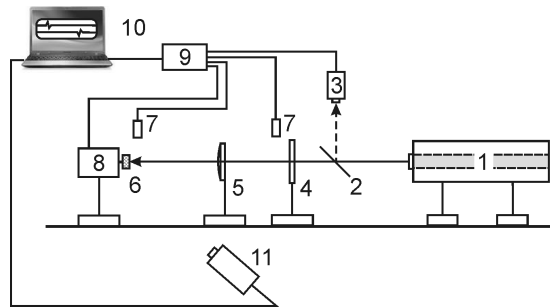


Fig. 1. CO₂-laser based experimental setup for ignition of solid fuel samples: 1 – CO₂-laser; 2 – semitransmitting mirror; 3 – thermoelectric sensor of radiation power; 4 – shutter; 5 – lens; 6 – coal sample; 7 – photodiode; 8 – sample holder; 9 – ADC; 10 – PC; 11 – thermal imager.

The experimental results for studied samples are given in Fig. 2.

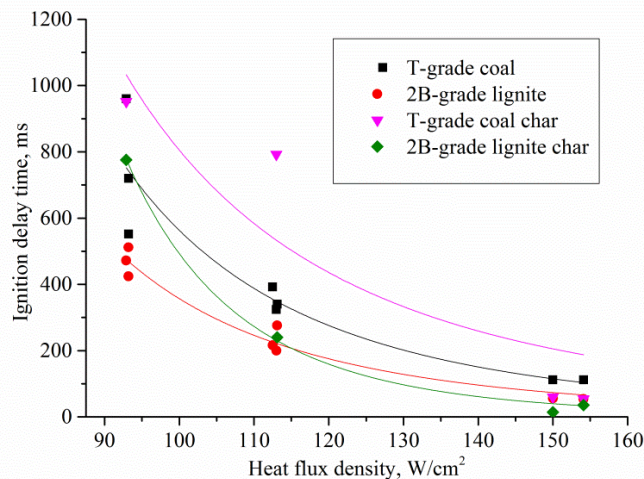


Fig. 2. Ignition delay times of solid fuel samples on heat flux density: T-grade coal – $t_{ig}=3.86 \cdot 10^{10} \cdot q^{-3.92}$; 2B-grade lignite – $t_{ig}=2.20 \cdot 10^{10} \cdot q^{-3.90}$; T-grade char – $t_{ig}=5.74 \cdot 10^8 \cdot q^{-2.95}$; 2B-grade char – $t_{ig}=3.94 \cdot 10^8 \cdot q^{-2.86}$.

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The kinetics of thermochemical conversion of lignite coke in the steam and carbon dioxide atmospheres

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An important aspect of the numerical description of the conversion process is the knowledge of quantitative laws of chemical processes occurring in the thermochemical conversion of fuels. The knowledge accuracy of the kinetic parameters of these processes depends on the accuracy of the estimates built deterministic models. The development of numerical modeling of gasification processes significantly inhibited as a deficiency judgment on its mechanisms (and as a consequence - high variability of kinetic parameters), and the lack of common methods of obtaining and recording these parameters. The process of conversion - a complex heterogeneous process of incomplete combustion, combines a large number of elementary reactions, the separation of which is difficult, so the construction of the exact mechanism of this process is a time consuming task. In this regard, most researchers fuels gasification kinetics approximate first order reaction flows in a one step process, excluding individual kinetics tar formation, devolatilization, the coke conversion, resulting in a significant deviation of the calculated velocity values of the process being studied experimentally obtained. Pressing question obtain reliable kinetic parameters in terms of fuel react with various types of individual oxidants: oxygen, water vapor, carbon dioxide. Development of recommendations for a unified approach to describe the kinetics of the heterophasic full-scale combustion of fuel is an important element towards the creation of a universal engineering model, which can be an effective tool for the purpose of designing energy processes and apparatus.

Experimental studies of the kinetics of the conversion of lignite coke conducted using simultaneous thermal analysis (STA 449 F1), produced by Netzsch. According to the results of thermal analysis to determine the true conversion of the kinetic constants of coke residues - activation energy of 186 and 143 kJ/mol, pre-exponential factors 6,1e-9 and 3,2e-9 m/s in the steam and carbon dioxide atmosphere, respectively. At the same time orders were determined reaction on fuel (0.8-1.3 - steam environment, 0.8-0.9 - carbon dioxide environment) and gas-reagent (0.8-0.9 - steam environment, 0.6 -0.8 - carbon dioxide environment). To determine the last parameter in the experiments varied reactant gas content in the reacting medium from 2% to 67%. Furthermore, in arrangements disclosed heterophase reactions taking place by reacting coke with steam and carbon dioxide. Some of these reactions were multistage competing routes.

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Dynamics of pressure and temperatures under flame propagation in a closed vessel with porous medium

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There are studied changes in pressure, temperatures in free space and porous medium during flame propagation in a vessel filled partially with porous medium (PM). Experiments were carried out in closed tube of quadratic cross section of $0.048 \times 0.048 \text{ m}^2$, 1.68 m of length filled with mixture of 4% propane with air. As a porous medium we use filling of Rashig rings with characteristic size of 0.006 m. Temperature measurements were carried out with W/Re thermocouples of $15 \cdot 10^{-6} \text{ m}$ in diameter.

Temperature measurements out of PM in fresh mixture show that in spite of heat loss into wall of the tube the compression of fresh mixture occurs in the process closed to adiabatic one. But compression of the gas in PM occurs in the process closed to isothermal one. In fig. 1 there is presented the dependencies of gas temperature in PM, current relative pressure $\pi = p/p_0$ and $d\pi/dt$ on elapsed time under flame propagation. Initial gas pressure is $p_0 = 0.11 \text{ MPa}$. PM was of 0.21 m height in down part of the tube and thermocouple was in a pore situated of 0.12 m from the interface between free space and PM.

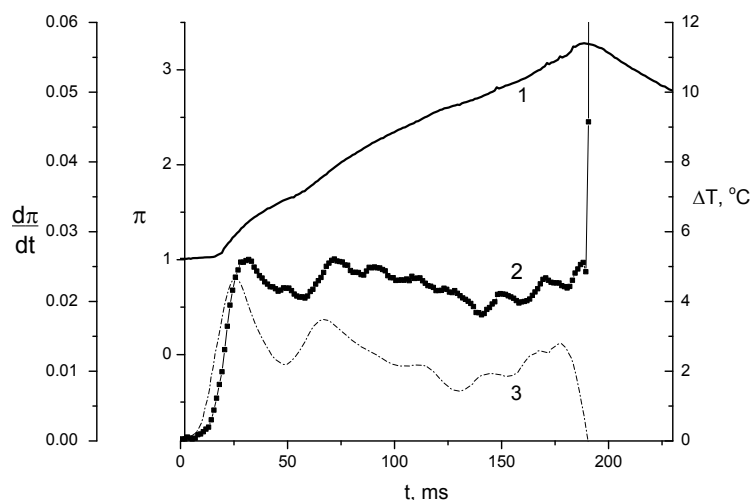


Fig.1. Dependencies of pressure (1), gas temperature in PM (2) and $(d\pi/dt)$ (3) on time.

One can see that gas is firstly heated on $\Delta T \approx 4^\circ\text{C}$ and then temperature rise is ceased. At flame penetration in PM in 0.12 m (Fig.1, $t=190 \text{ ms}$) one can see pressure drop during further flame propagation in PM. It is seen that both temperature rise and correlation of temperature with $d\pi/dt$ point to the dependence of gas temperature on pressure changing rate.

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Modeling study of Al nanoparticle oxidation in CO₂/H₂O environment

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In this work the modeling study of Al nanoparticle oxidation in CO₂/H₂O environment was carried out. It is known that aluminum nanoparticles are usually covered by alumina shell with 2-3 nm thickness. When such particles are injected into the hot oxidizer, the following processes take place: heating the particles to the melting temperature of aluminum core, melting of the liquid Al core, appearance of stresses in the oxide layer due to the expansion of Al core by 12% during melting, cracking of oxide shell and, at last, particle destruction. As a result Al_n clusters, composed of hundreds or even tens monomers ($n \leq 250$), can arise. In order to take into account the presence of Al_n clusters in the mixture, the gas phase chemistry of Al oxidation in CO₂ and H₂O [1] was supplemented by the block of reactions describing the evaporation of small Al_n clusters ($n=1 \dots 250$) on the basis of kinetic approach [2].

Numerical study of Al nanoparticle oxidation in CO₂/H₂O environment was conducted for adiabatic

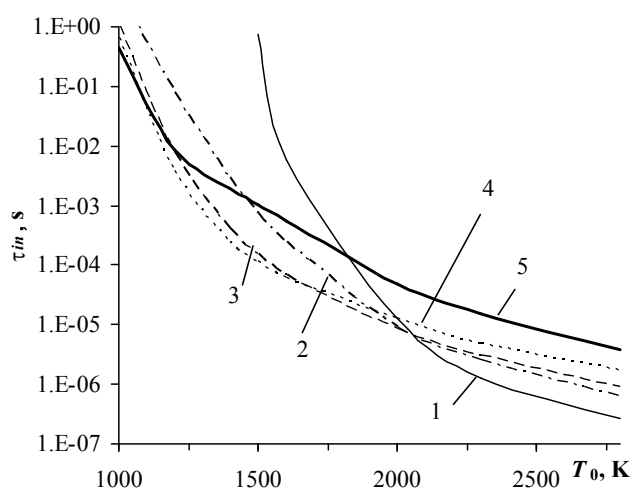


Fig. Induction time τ_{in} as a function of initial temperature T_0 in the stoichiometric Al₁₀₀-CO₂-H₂O mixture at $P_0=1$ atm:

- 1) 100%CO₂; 2) 70%CO₂+30%H₂O;
- 3) 50%CO₂+50%H₂O;
- 4) 30%CO₂+70%H₂O; 5) 100%H₂O.

constant volume reactor. It was investigated, how the size of Al clusters, that can form during dispersion of liquid aluminum upon the destruction of primary nanoparticles, influences the ignition characteristics of Al particles in CO₂/H₂O. The induction time and ignition temperature appeared to be strongly dependent on the size of Al_n clusters. It was revealed that the smaller are the Al clusters, the shorter is the ignition delay and the smaller is the ignition temperature of combustible mixture. The induction time also strongly depends on the composition of oxidizer CO₂/H₂O. At high initial temperature $T_0 > 2000$ K, the ignition delay is minimal in pure CO₂ and maximal in H₂O environment. At low T_0 the inverse tendency is realized. The mechanisms, responsible for the effects during the ignition in the Al-CO₂ mixture, were studied in detailed manner and principal reactions were indicated.

This work was supported by the Russian Science Foundation (grant no.14-19-01128) in the part of development of reaction mechanism for the description of evaporation and combustion of aluminum nanoparticles and numerical analysis of Al nanoparticle combustion in CO₂-H₂O environment and by the Russian Foundation for Basic Research (grant no. 17-01-00810-a).

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Ignition of the woody biomass wet particles

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The woody biomass has become more attractive as fuel for the thermal power plants in recent years in the several regions [1]. However, the physical and mathematical models describing the process of the particle ignition of the woody biomass have not been developed yet. Most of the known theoretical studies have been conducted in the framework of the simple mathematical models [2]. For this reason, the purpose of this work is to conduct the experimental studies of the particle ignition of the woody biomass and the development of the mathematical model of the ignition process.

The complex of the experimental researches on the setup that simulates accurately the conditions of heat transfer in the furnace chambers of the boilers. The equipment of recording has allowed to determine the main characteristics of the ignition process (the ignition delay time t_{ign}) with a sufficiently high accuracy. The dependences of the ignition delay times from the temperature of the external environment (T_e) have been determined according to the experimental results. The effect of humidity on the dynamics of fuel ignition has been analyzed. The mathematical model of the ignition process has been formulated in the form of systems of differential equations. Fig.1 shows the theoretical and experimental dependences of the ignition delay times of the wood particle from the ambient temperature. The dependency analysis shows that in the entire interval of the investigated temperatures the differences of the theoretical values of t_{ign} from the experimental do not exceed 14%.

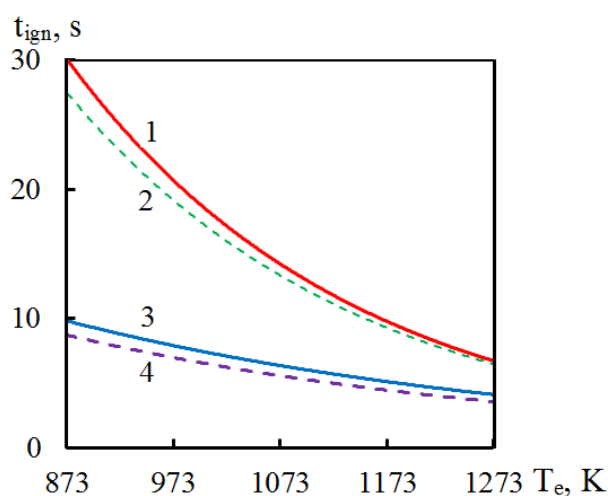


Fig.1. The dependence of the time delay ignition of the wood particle from the ambient temperature. 1,2 – particle diameter $3,0 \cdot 10^{-3}$ m; 3,4 – $1,5 \cdot 10^{-3}$ m; 1,3 – experiment; 2,4 – numerical solution.

The results of the research show that the developed mathematical model allows to conduct successfully a predictive simulation the processes of the particles ignition of the woody biomass in the conditions corresponding to the combustion spaces of the boilers.

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Experimental investigation of deformations of a premixed methane/air flame in a turbulent swirling jet

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The present paper reports on the investigation of turbulent combustion in a high-swirl jet by planar laser-induced fluorescence of formaldehyde (HCHO PLIF). The jet was organized by an axisymmetric contraction nozzle with the exit diameter of $d = 15$ mm. The jet swirl was provided by a vane swirler mounted inside the nozzle. The Reynolds number was 5 000. The equivalence ratio Φ of methane/air mixture issued from the nozzle was 0.7, 1.4 and 2.5. Despite differences in the combustion regimes (and also in case of the non-reacting jet), the swirling flow dynamics was driven by a global instability mode, associated flow precession [1]. The third harmonic (355 nm) of the Nd:YAG laser (Quantel Brilliant B, energy per each pulse was 45 mJ) radiation was used for the excitation of HCHO fluorescence. The fluorescence was collected by a 16-bit intensified CCD camera (Princeton instruments PI-MAX-4) equipped with a Sigma AF #50 lens. Figures 1 shows the direct flame image ($\Phi = 0.7$) and the examples of the HCHO PLIF data, providing information about regions of local heat release [2]. The flame front has a shape of inverted cone and is subjected to sufficient deformations. The full paper will provide detailed literature survey, description of the experimental setup, calibration and data processing routines. The analysis focus will be placed on spatial decomposition of the PLIF data. Namely, Fourier decomposition for the images, captured in the planes perpendicular to the jet axis, and proper orthogonal decomposition [3].

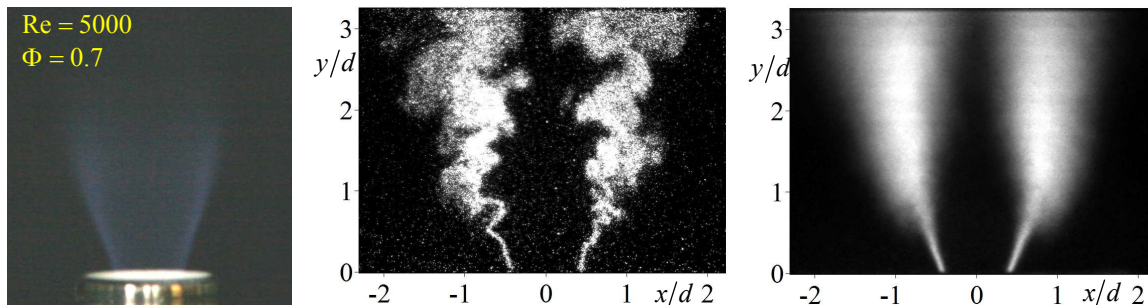


Figure 2. Flame image (left) and examples of the instantaneous (middle) and averaged (right) HCHO PLIF data.

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Excitation of the unique set of holograms of the energetic materials reactionary zones and manipulating by self-organizing of the micro- and nano-scale structures

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Fundamental understanding of the micro-scale combustion mechanisms is very essential to the development of the state-of-the-art technology for extreme control of propellant thrust for Divert and Attitude Control System utilizing electrically controlled solid propellants. The capability to significantly reduce the size of small engines and thrusters on commercial spacecraft and satellites can lead to increased payload capacity and simplification of the propulsion system. In the combustion chambers of such propulsion systems the scale factor has the significant influence. In this connection, the micro- and nano-scale structures arising in the energetic materials reactionary zones has a large influence on physical and chemical processes and on controllability of ignition and combustion processes.

The aim of this research is development of the new concept of application of the unique set of holograms of the energetic materials reactionary zones for manipulating by the resonance spectrum of the micro/nano-scale structures of the energetic materials reactionary zones. According to our hypothesis each energetic material has a unique set of holograms of the reactionary zones in available specific frequency bands. Our hypothesis is supported by the recent data, obtained in the various model experimental systems. In the energetic materials reactionary zones can be observed a unique set of holograms: image hologram, acoustic hologram, electro-magnetic hologram, thermal hologram. The analysis of available experimental data show that micro/nano-scale structures forms both the fractal and micro-cymatic patterns in the reactionary zones and can be considered as a fingerprints of the set of holograms of the reactionary zone. For instance, the condensed particles in the combustion products allows to make physically visible the sound wave patterns. Different frequencies can arrange the micro/nano-scale structures into the different geometrical patterns. For practical applications in the aerospace propulsion area we suggest new technology of scanning of the multi-component unique resonance spectrum of all molecules in the reactionary zones and programmed transfer of the quantum information into the reactionary zones for excitation of the resonance spectrums of the predetermined set of molecules by means of resonance laser radiation or by use of the system of resonance electro-magnetic and acoustic fields. Such excitation along with re-programming of the resonance spectrum of the micro/nano-scale structures of the reactionary zones gives the possibility for control by the scale and 3-D localization of the induction and energy-releasing areas and, accordingly, allows control inter-scale interaction in the aerospace propulsion systems.

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Laboratory studies of the smoke emission chemical composition and its transformation under UV irradiation upon smoldering combustion of forest fuels

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Wild forest fires and prescribed burning are known as a significant source of environmental pollution. Smoke emission, evolved by biomass burning, can affect on the chemical, optical, and radioactive properties of atmosphere, forest ecosystems, and various biological media (soil, water, plants, etc.). It is difficult to determine a reliable relation between the initial composition of forest combustible materials and the chemical composition of the resulting emission upon biomass burning when herbage, vegetative and soil cover burn. Since the capacity and composition of burning products depend on the type of combustible material, burning phase (flaming or smoldering), weather conditions, etc., the laboratory experiments on the combustion of individual plant material are necessary.

The aim of this work is the laboratory studies of the chemical composition of the primary smoke emission (particulate matter and gaseous products), and investigation of the secondary aerosols formation under UV irradiation of the gaseous compounds upon the smoldering combustion of various plant materials. Aerosols were collected on glass fiber filters and one portion of gaseous products fed the tubular flow reactor, where they were subjected to UV irradiation, and the other one was frozen in quartz tubes placed in a Dewar flask at -50°C. Chemical composition of the primary smoke emission and secondary organic aerosol, formed as a result of photolysis of gaseous products, was analyzed by HP 6890N/5973N GC-MS spectrometer (Agilent Technologies, USA). Number concentration and distribution size were measured using an aerosol diffusion spectrometer. Emission of carbon dioxide, carbon monoxide, methane and other gases was not measured.

It is experimentally demonstrated that during the smoldering combustion of the various types of forest biomass (larch, pine wood, Labrador tea, and lichen), 1-2% of the burnt plant materials transform into particulate matter and almost the same quantity evolves as gaseous products which are possible the precursors of secondary aerosol. The phenolic compounds are shown to be found in the composition of primary emissions as lignin thermal degradation products and furan derivatives are cellulose thermal decomposition products. Acyclic and cyclic compounds with a carbonyl group ($-C=O$) have been defined in the composition of photolysis gaseous products. It is shown that as a result of UV irradiation of gaseous products of oak sawdust smoldering combustion, were formed secondary particles with a mass median diameter about 70 nm with a concentration about 10^6 particles/cm³.

These results can be used to estimate the gas-aerosol emission during forest fires on the basis of the data on the resources of forest combustible materials and the degree of their combustion, to predict the feasible ways of photochemical transformation in the atmosphere and to determine the effect on the environment and human health.

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Flame synthesis of superhydrophobic carbon surfaces*Z.A. Mansurov^{1,2}, M. Nazhipkyzy^{1,2}*¹Institute of Combustion Problems, Almaty, Kazakhstan²Al-Farabi Kazakh National University, Faculty of Chemistry and Chemical Technology, Almaty, Kazakhstan

This paper presents the study of soot formation process having superhydrophobic properties by burning gaseous hydrocarbons and oil waste.

The flame synthesis to deposit soot particles on silicon and nickel substrates at various flame locations was made. The resulting variation in hydrophobicity and surface topology to determine an optimum synthesis location that produces maximum surface hydrophobicity was investigated. Whereas nanostructured soot particles are deposited upon a surface, they create a superhydrophobic topology that facilitates a water droplet to sit on the asperities of the roughness. Creating highly reliable waterproofing materials with nanostructures will help solve the problem of the negative impact of a moist environment and corrosive groundwater. As nanostructured material may be soot with superhydrophobic properties obtained under certain conditions the combustion of hydrocarbon fuels and combustion of waste oils.

In the modified combination burner was used for the synthesis of hydrophobic carbon black surface by burning propane - oxygen mixture, with application and without application of an electric field. It is found that the application of an electric field, regardless of the substrate material narrows the soot deposited on the substrate and a diameter of 2.5 - 3 cm from the center of soot formed superhydrophobic surface contact angle from above 170°.

The problem of recycling waste lubricating oil is acute throughout the world, as along with other hydrocarbons used lubricating oil significantly pollute the biosphere. Unlike oil and other petroleum products, waste oil when released into the environment is not rendered harmless by natural means (oxidation, photochemical reactions, biodegradation). In this regard, there is an actual problem of recycling waste oil.

A number of experimental studies to determine effective soot by burning waste oils were carried out. The raw materials used waste oil from service stations to replace oil cars. Used oil burned using a conventional wick, by impregnating carbon and glass fiber fabric. To check the resulting hydrophobic soot was soaked in an ethanol solution and after drying was tested for properties by the hydrophobic droplet reclining. The results showed that the surface of the soot produced by burning waste oil has a hydrophobic property to the wetting angle 145-150°. The experimental research on the production of soot by burning waste oils showed that the combustion of 100 grams of oil, depending on the combustion conditions can be obtained from 0.5 to 1.5 grams of soot. Extraction of the resulting soot shows a benzene soluble content of the small parts, which indicates non-toxicity of the product obtained.

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Investigation of influence of initial components on synthesis of cobalt oxides by solution combustion synthesis

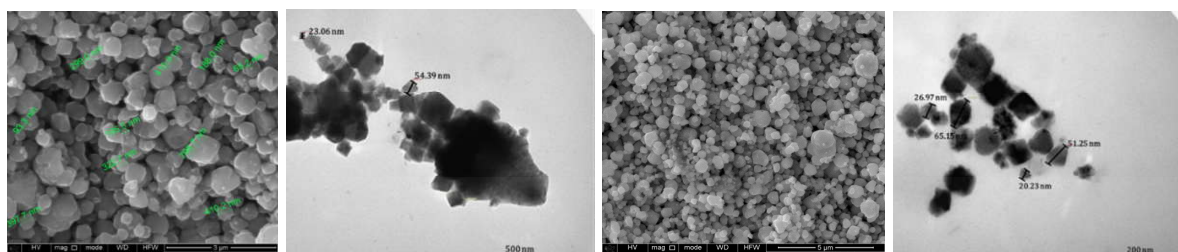
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For the synthesis of cobalt oxide nanoparticles, the method of solution combustion was used. The essence method is to prepare an aqueous solution containing glycine and cobalt or nickel nitrate, followed by evaporation of the solution to 5-7 ml, after which the temperature was increased to 230-240 °C at which self-ignition process take place to form ultrafine metal oxide powder.

X-ray analysis to establish the composition of the obtained cobalt oxide was carried out. The diffraction pattern shows of obtained cobalt oxide have the formula Co_3O_4 . To determine the effect of addition of nitric acid, experiments without the addition and with the addition of nitric acid in the initial mixture were carried out. Distribution of Co_3O_4 nanoparticles obtained without added nitric acid the bulk of particle has diameters 6-9 nm; there are also particles with diameters of 24-50 nm. Distribution of Co_3O_4 nanoparticles obtained with added nitric acid the bulk of particle has diameters 8-10 nm. In this example, all of the nanoparticles have a diameter of 16 nm and no particles of greater diameter. Obtained results showed that the addition of nitric acid allows obtaining more dispersed particles.

Cobalt oxide nanoparticles, obtained at various ratios of the fuel and oxidant were investigated by a scanning and transmission electron microscopy. On the figure 1 a, b is shown SEM and TEM images of Co_3O_4 at the stoichiometric ratio of fuel and oxidizer ($\varphi = 1$). On the figure 1 c, d is shown SEM and TEM images of Co_3O_4 at the stoichiometric ratio of fuel and oxidizer ($\varphi = 1.5$).



a) SEM image of Co_3O_4 nanoparticles ($\varphi = 1$); b) TEM image of Co_3O_4 nanoparticles ($\varphi = 1$); c) SEM image of Co_3O_4 nanoparticles ($\varphi = 1.5$); d) TEM image of Co_3O_4 nanoparticles ($\varphi = 1.5$)

Figure 1 – Microstructure of Co_3O_4 nanoparticles.

As seen from the obtained pictures of scanning and transmission electron microscopes for particles of cobalt oxide at a stoichiometric ratio of fuel and oxidizer $\varphi = 1$, the particle size range from 23 nm to 60 nm, also agglomerates with size more than 500 nm are present. For particles of cobalt oxide at a ratio $\varphi = 1.5$ particle size ranges from 20 to 65 nm, without big agglomerates. A comparison of the two samples on the basis of SEM and TEM images, illustrates the positive effect of the addition of fuel above the stoichiometric ratio. Reaction between fuel and oxidant results in decomposition of the starting components to form gaseous products that lead to further dispersion of the final product.

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Initiation of filtration gas combustion wave in an inert porous medium

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The process of initiation of filtration gas combustion wave (FGC) with heated area of an inert porous medium was studied numerically. This process is implemented in particular in the reverse process that is organized on the base of filtration gas combustion [1]. Under reversing gas flow there occurs new ignition of the FGS wave with the area of the porous medium that was heated in the previous half cycle.

There was simulated one-dimensional system, which is a tube of L in length filled with an inert porous medium. From one side the tube was fed with combustible gas mixture of a specified composition of velocity v . In initial moment there was specified rectangular temperature profile of the porous medium of l in length and T in temperature that simulated the heated area.

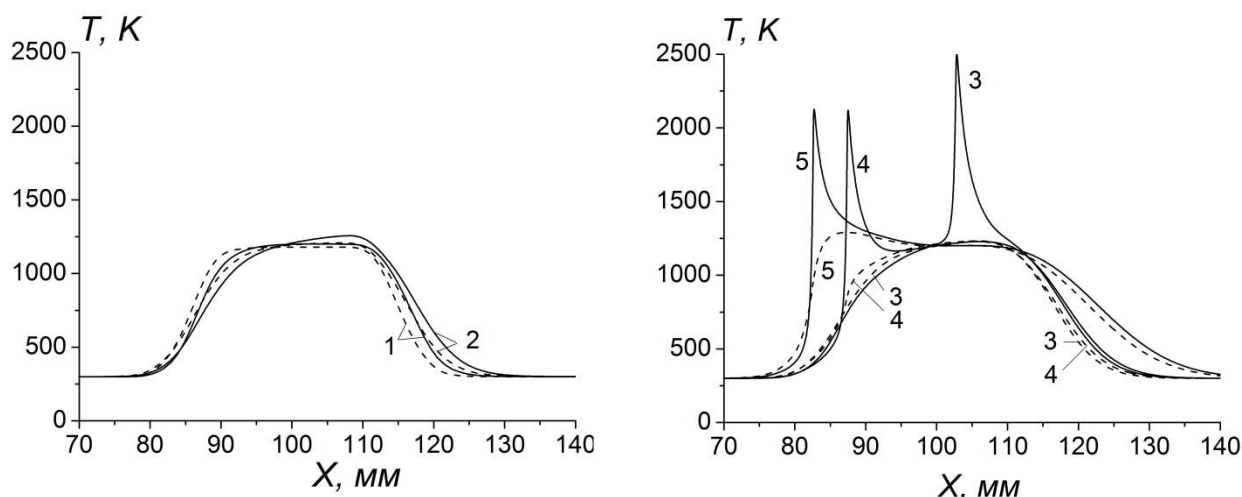


Fig. 1. Formation of the FGC wave. The temperature of the gas mixture (solid lines) and porous medium (dashed line). Time from the start of gas mixture feeding: 1 – 3 s; 2 – 12 s; 3 – 15 s; 4 – 18 s; 5 – 50 s.

Fig. 1 shows typical results of simulation of the process of formation of the FGS wave that allow one to select three stages of the process. In the first stage the gas is heated by the heated area of the porous medium (1) and there are activated slow chemical reactions (2). At the second stage there is ignition of the gas (3), as a rule, near the trailing edge of the temperature profile of the porous medium and fast flame propagation (flashback) through the heated area with further flame stabilization at the advance edge (4). At the third stage there begins intense heating of the porous medium with the flame and formation of steady-state wave of FGC (5). The simulation shows that at other factors being equal the decrease in the temperature of the heated area there exists the value of T_{ign} at which there is not ignition, i.e. one can say on the minimal temperature of ignition. It is determined that T_{ign} is raised with decrease in the length of the heated area and with rise of mean grain size of the porous medium. Decrease in thermal conductivity of the porous medium results in decrease in the ignition temperature.

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Low-NO_x firing systems with swirl burners for boilers PK-39-IIM and BKZ-420-140-5

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The paper presents main design solutions for the firing system and arrangement of burners for boilers PK-39-IIM and BKZ-420-140-5 when firing Ekibastuz coal. The developed low-NO_x firing systems ensure low nitrogen oxide emissions both at low furnace cross-section heat release rates and high furnace cross-section heat release rates.

Technical solutions developed for the firing systems are based on 3D multivariate CFD-simulation of the firing processes using ANSYS Fluent software. Dependence of combustion stability and NO_x emissions on swirling in air-coal ducts and secondary air ducts, velocity of air-coal mixture in the duct and installation of dedicated elements in burner air-fuel ports was studied in detail.

The main technical solutions for low-NO_x firing systems of the above mentioned boilers include the following:

- Vertically staged combustion due to OFA level;
- New design of low-NO_x direct-fired swirl burners with optimized flow rate and velocity characteristics of air-fuel mixture and secondary air, as well as dedicated elements in air-fuel ducts;
- Reduction of primary air portion in the main burners through installation of pulverized coal classifiers for boiler PK-39-IIM.

The CFD-simulation showed that it was possible to achieve the following NO_x concentrations: for boiler PK-39-IIM with high furnace cross-section heat release NO_x≤530 mg/Nm³ (under normal conditions and O₂=6%); for boiler BKZ-420-140-5 with low furnace cross-section heat release NO_x≤450 mg/Nm³ (under normal conditions and O₂=6%).

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Spectral and kinetic features of glow and gaseous products evolution from coals during irradiation with laser pulses

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The goal of the present work was to determine the spectral and kinetic features of the glow arising during influence of laser pulses on coal samples and to elucidate the products at these conditions of initiation.

The first harmonics of neodymium laser ($\lambda = 1064$ nm) operating in the free-oscillation mode with pulse duration 120 μ s. The maximum pulse energy of the laser was 0.8 J. The beam energy affecting the sample was varied with neutral light filter with previously determined transmittances. The focused laser beam diameter on the sample surface was 2.5 mm. The glow arising as a result of laser influence was detected with a streak-camera and a photoelectron multiplier.

The samples of lignite and sub-bituminous coal prepared as powders with bulk density 0.5 g/cm³ or pressed pellets with density 1 g/cm³.

The three temporal stages of the processes evolving during and after laser irradiation influence on the coal samples were distinguished: i) coal surface heating (during the laser pulse); ii) volatiles ignition (≥ 1 ms); iii) coke residue combustion (25 ÷ 150 ms). The stages evolution depends on the pulse energy density.

It was shown that there is sample surface glow arising during the pulse which was interpreted as a gray-body with temperature 3000 K glow. In the time range 1 – 10 ms the glow spectrum contain bands that we discuss as excited molecular glow of CO (in the blue part of the spectrum, the maximum at 470 nm), H₂ and H₂O (in the red part of the spectrum, the maximum at 650 nm). In the time range 20 – 150 ms the spectrum corresponds to the coke residue combustion with typical temperature 1700 – 1800 K.

The mass-spectrometry approached was applied for products analysis. We found out that the main molecular products of laser influence on coals are hydrogen H₂ and carbon dioxide CO₂.

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Determining the apparent kinetics of fast pyrolysis of lignocellulosic biomass using Py-FTIR and Py-GC/MS experiments*Deepak K. Ojha and R. Vinu*

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Fast pyrolysis is a promising thermochemical processing technique for resource and energy recovery from lignocellulosic biomass, which is projected as the one of the major sources of renewable carbon on earth. Fast pyrolysis involves rapid heating of the biomass at short timescales (few seconds at >1000 °C/s) to produce high yield of pyrolysis oil (or bio-oil), which can be catalytically upgraded to fine chemicals and fuel molecules. The existing kinetic models for fast pyrolysis of biomass are based on experimental data from thermogravimetric analyzer at slow heating rates (5-50 °C/min). This limits the applicability of the kinetic parameters to predict product yields under fast heating conditions. Moreover, understanding the time evolution of pyrolysis products at such short timescales is also essential to successfully model and predict the product distribution under different operating conditions. In this study, we demonstrate the use of micropyrolysis coupled with online Fourier transform infrared spectroscopy (FTIR) and gas chromatograph/mass spectrometry (GC/MS) to unravel the pyrolysate composition and isothermal mass loss profiles during fast pyrolysis.

The biomass samples tested include alkali lignin, Finnish pine wood (PW), empty palm fruit bunch (EFB) and Indian rice straw (RS). Experiments were performed in a Pyroprobe® pyrolyzer (CDS Analytical) coupled with GC/MS (Agilent 7890/5975) and FTIR (Agilent Cary 660). Typically, few milligrams of the samples were pyrolyzed at 20,000 °C/s from 400 to 800 °C at 50 °C intervals at various time periods (2-60 seconds). The sample mass was accurately determined using a microbalance. The FTIR profiles were collected every second and the pyrolysates were identified and quantified using GC/MS. The isothermal mass loss profiles were subjected to kinetic analysis using different decelerating models including first order and diffusion models to determine the apparent activation energy (E) and frequency factor (A).

The apparent activation energies for fast pyrolysis of alkali lignin, PW, EFB and RS were 23, 35, 44 and 27 kJ/mol, respectively. The frequency factors were low and varied in the range of 2-100 1/s. Kinetic compensation plots were constructed to validate the apparent rate parameters obtained in this study. Good correlation was observed between E and Ln(A) collected from various studies, which showed that the parameters obtained in this study were indeed valid. From FTIR analysis, the time corresponding to maximum evolution of vapor phase products was found to be 10-15 s. The GC/MS product distribution showed a strong relationship with the biomass composition. While guaiacols and syringols were the major pyrolysates from alkali lignin, low molecular weight oxygenates like furfural, acetone, acetic acid and acetol were the major products from other biomasses. More interesting results concerned with the pyrolysate evolution, and the extension of these experiments and kinetic analyses for combustion of biomasses will also be presented.

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The united mathematical model of ignition and combustion of aluminum diboride particles in a combustion chamber of rocket-ramjet engine

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Creation of aircraft with improved performance requires solving a few of problems. In particular, the development of fuel compositions with a high content of metallic components requires of the long, expensive experimental testing. It seems appropriate to complement the experimental testing of new fuels with a high content of metal compounds by numerical calculations on a computer.

The aim of this work is to develop a mathematical model to determine the rate of change of temperature, thickness of the oxide film and the particles radius, which are located in the flow of the oxidizing environment, and also to calculate the trajectory of burning particles in a given area. It is assumed that aluminum diboride particle it is boron and aluminum evenly mixed alloy, and the part of surface occupied by each of the elements is proportional to its mole fraction in the alloy. Parallel oxidation chemical reactions of Al and B occur on surface of the particle, proportional to the mole fraction of each element in the alloy. Radiative and convective heat transfer to the surrounding air from surface of particles is taken into account. The condition for ignition are accepted complete evaporation of film of the boron oxide or the achievement of melting temperature of aluminum oxide. The model is based on semi-empirical and experimental curves of the kinetics of reactions of oxidation and combustion of individual particles of boron and aluminum. We are found the dependence of time of ignition and combustion from the initial values of diameter of aluminum diboride particles and air temperature.

The numerical model of the ignition and combustion of single particles is used to determine the source terms in the calculation of the quasi-stationary two-phase flow of combustion products in the work area. To carry out such the calculations was created the computer program, based on a decision by the finite volumes method of the Navier-Stokes equations, which supplemented by the standard k- ϵ turbulence model. The developed program allows determining the velocity field, temperature, pressure, etc. inside the computational domain.

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The equilibrium equation of state of gas mixture with the detailed considering of the chemical composition*E.R. Prueel*

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The equation of state of rarefied gases for a wide range of temperatures and densities is important both for scientific and practical applications. In general, it is an unreasonably hard problem containing a complex relationship of the specific heat on the temperature, chemical reactions, and in some cases the formation of a gas suspension of the condensed phase. To solve an adequate approach being developed, and are a combination of the numerical calculations of quantum and classical mechanics of molecules, atoms and electrons; thermodynamic relations and experimental data.

In this paper we reviewed the rarefied gas of a mixture of components: molecules, radicals, ions, electrons, and the particles of the condensed phase. Assuming that the free energy of the thermodynamic potential of component does not depend on the environment and is determined only by the temperature, we can determine all the thermodynamics of the system. It is necessary numerically to find a minimum total free energy, taking into account all the possible components of the system at a given temperature and density (NVT ensemble). This approach allows us an uniform method to find thermodynamic equilibrium by varying the ratio between the components.

The developed package of libraries for C++ programming language and related programs, including the web interface (<http://ancient.hydro.nsc.ru/chem>) has the following features.

- Calculation of the equilibrium of the chemical composition of the gas mixture based on the elements H, He, C, N, O, Si, S, Ar in the temperature range of 200 - 20,000 K.
- The possibility of formation of condensed phases C, H₂O, S, SiO₂ and Si.
- Calculating the number of thermodynamic parameters: pressure, enthalpy, internal energy, heat capacity, adiabatic index equilibrium and frozen.
- Construction of equilibrium and frozen Hugoniot shock wave. Defining the parameters of stationary detonation waves. The adiabatic combustion at a constant volume.

The implemented approach has been used successfully for the quantitative prediction of energy and mechanical characteristics of high flows. To determine the fire and explosive hazard of gases and dust mixtures.

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Direct numerical simulation of iron oxide nanoparticle forming laminar flames: buoyancy and probe effects

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The formation of iron oxide nanoparticles from laminar, premixed, low-pressure flat flames doped with iron pentacarbonyl was investigated numerically in order to improve the interpretation of experiments. The burner operated at 30 mbar, burning either a hydrogen/oxygen mixture or a hydrogen/methane/oxygen mixture, diluted with argon. The burner fired in downward direction, causing strong buoyancy in the flow field. Together with the invasive probing applied, a complex flow field resulted, so that 2D simulations of the reacting, particle forming flow had to be conducted in order to interpret the measurements.

The simulations were performed using a finite volume method for the solution of the reacting flow. The combustion was described by finite rate chemistry and detailed transport models for diffusion and the mixture properties [1]. The particle formation, growth and possible combustion were solved using a method of moments. The reaction kinetics of the fuel/oxygen/precursor system was based on a reduced, skeletal version of the iron pentacarbonyl combustion mechanism proposed by Feroughi et al. [2] combined with a reduced version of the C1 mechanism by Li et al. [3] for the H₂/O₂ system or the DRM-19 mechanism [4] for the cases with CH₄.

The results revealed a strong impact of the reactor orientation on the velocity field. The buoyancy decelerates the flow on the centerline, causing a stagnation point below the burner. In presence of a probing nozzle, the overall shape of the flame changes dramatically, depending on the distance of the probe from the burner. The corresponding residence times are strongly affected by the probe – an effect previously observed for upward firing flames with a stagnation plate [5]. The results were in good agreement with experimental findings and allowed further investigation of the reaction and particle formation dynamics applying detailed reaction mechanisms in one-dimensional models using the previously determined flow field.

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Experimental and numerical investigation of flame dynamics in a multichannel system

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Organization of combustion processes in porous media provides several advantages compared to combustion in the free space, namely a higher burning velocities, superadiabatic temperature in the reaction zone, extension of the flammability limits, low pollutant emission and the possibility of low-calorific fuels combustion. Despite the large number of theoretical and numerical studies devoted to the investigation of combustion processes in the interior of porous media, the flame behavior in the vicinity of porous media / open space interface is less studied. In particular, the flame dynamics in the course of combustion wave penetration inside the porous media have not been investigated in details. At the same time, many practical burners operate in the regimes with the flame stabilized near the boundary of porous body. Some similarities between the filtration gas combustion and flame propagating in the narrow channels suggests that the study of the idealized system consist of a set of microchannels may provide relevant knowledge on flame behavior near the boundaries of porous medium. In such systems it is possible to exclude the probability factors associated with non-uniformity of the porous medium and investigate only the influence of heat and mass transfer on the flame behavior.

This work presents the results of experimental and numerical study of the flame penetration into the system, consisting of a set of planar quartz ducts of different channel sizes. The quartz plates of 6 cm width, 12 cm height and 0.1 cm thickness were used as the channel walls. The gap between the plates can be varied from 0.1 cm to 1 cm. The total number of the channels in the system depends on their transverse dimension and varied in the range from 1 to 20. Premixed methane-air mixture is supplied into the channels through a rectangular slot which size corresponds to the total size of a multi-channel system.

Experiments show that depending on channels configuration, equivalence ratio and mixture flow rate the different types of flame behavior including burner stabilized flames, upstream propagating flames and flames stabilized under the burner external surface are observed. For different channels configurations the regions of existence of different combustion regimes in equivalence ratio / mixture flow rate plate were experimentally found. In wide range of parameters such as equivalence ratio, mixture flow rate and channels transverse size the flame pulsations having the same nature and characteristic features as FREI phenomenon were observed. These pulsations are accompanied by noticeable sound and probably allow to explain the nature of noise often appearing in filtrational gas combustion. It was shown that at qualitative level the flames behavior in multi-channel system can be described in the frame of reduced thermal-diffusion model with prescribed flow field. Information about the topology and behavior of the flames stabilized inside the channels near their outlet may be useful for understanding of basic mechanisms of flame stabilization in the vicinity of external surface of porous burners.

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Structure of swirling turbulent flames. Investigation by PIV and spontaneous Raman scattering

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The study reports on the detailed experimental research of the flow structure, density distribution and concentration of the main gas components in a turbulent premixed swirling flame at atmospheric pressure. The flame was provided by burning propane/air mixture (with equivalence ratio 0.7) issued from a contraction nozzle with a vane swirler mounted inside. The nozzle exit diameter d was equal to 15 mm. The Reynolds number, based on the flowrate and viscosity of the air was 5000. The experimental study was performed by using PIV (particle image velocimetry) method in stereoscopic configuration and registration of the spontaneous Raman scattering (SRS) intensity by gas molecules.

The direct image of the flame, mean velocity field of the gas and distribution of the temperature and concentration of the gas species are shown in Fig. 1. The flow structure of the high-swirl turbulent jet (with and without combustion) was featured by breakdown of the jet's swirling core with a central recirculation zone present at the jet axis. From spatial distributions (shown for two cross-sections) it was concluded that the hot combustion products concentrated inside the central recirculation zone, whereas the fuel was in the annular jet around it. No evidences for sufficient CO presence (above 3%) in the combustion products was found. It was found (more details will be provided in full-paper) that the large-scale vortices formed in the inner mixing layer (around the central recirculation zone) promoted to the heat and mass transfer between the jet and combustion products in the central recirculation zone.

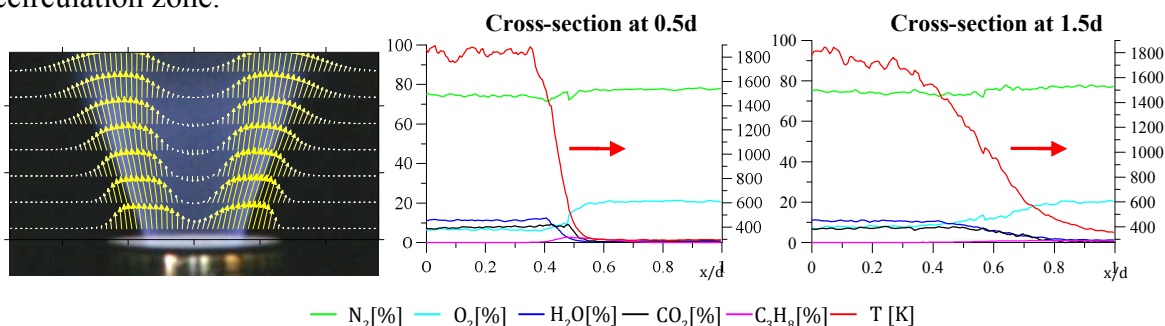


Figure 1. Left: Direct image of the flame and mean velocity field for the high-swirl lean propane/air flame. Middle and right: Distributions of temperature and concentration of the main gas species along cross-sections at two distances from the nozzle.

Modeling of the coal gasification process in a thermal reactor*P.A. Shchinnikov, A.A. Frantseva, D.S. Sinelnikov*

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Thermal treatment of fuel is pre-heated dust before its combustion in the boiler furnace to a high temperature (600-800 °C) in a special furnace extension. The whole process lasts for 0,5 ... 2 seconds, at that warming and volatile matter occurs almost instantaneously and in the rest of the time - partial gasification of coke. In general, a thermal treatment allows earlier ignition and deep enough burning of coal dust in the initial section of burners due to the content in the produced gas suspension flammable combustible volatile matter. The qualitative composition of the resulting two-phase product is largely dependent on the kinetics of physicochemical transformations undergone by solid fuel. However, the getting of universal, generalizing kinetic dependencies pyrolysis and gasification of coal is difficult and often only valid for the specific reaction conditions.

On the other hand, to obtain a mathematical model to an acceptable accuracy for engineering calculations may be sufficient to account defining a thermal treatment output of volatile reactions and partial gasification.

In addition, the proximity of the modeling process is due to the assumption that the initiation of fuel combustion takes place in a homogeneous medium without mixing with the stream of reactive coal working, dynamics of the combustion process is mainly determined by the reaction rate constant and the corresponding activation energy. In this case thermal resistance of carbon particles of coal can be neglected both laborer and initiation, as the criterion $Fo > 5$ and criterion $Bi < 0,5$, that is, the convective heat exchange from gas to coal particles is decisive in comparison with the transfer of heat inside the particles. Based on the foregoing, the concentration of the gas suspension components can be determined in accordance with the Arrhenius law as:

$$\frac{dc_j}{d\tau} = (c_j^0 - c_j) a_j = f_j$$

where – $a_j = k_j e^{-\frac{E_j}{RT_y}}$; k_j ; E_j – pre-exponential factor constant output speed components and the corresponding activation energy in the j-th thermochemical reaction (Table 1), T_y – particle temperature; R – universal gas constant; c_j^0 – the initial concentration of the components.

Table 1. Kinetic parameters of reactions.

Reaction	$ k_0, s^{-1} $	$ E, kJ / kmol $	
The output of the fuel CO	$ CO^{TOIII} \rightarrow CO $	$ 2 \cdot 10^{12} $	$ 186 \cdot 10^3 $
The output of the fuel CO ₂	$ CO_2^{TOIII} \rightarrow CO_2 $	$ 2 \cdot 10^{11} $	$ 137 \cdot 10^3 $
Out of fuel methane	$ CH_4^{TOIII} \rightarrow CH_4 $	$ 1,6 \cdot 10^{14} $	$ 216 \cdot 10^3 $
Steam gasification of coal char	$ C + H_2O \rightarrow CO + H_2 $	$ 2 \cdot 10^{11} $	$ 255 \cdot 10^3 $
Gas burning		$ 5,6 \cdot 10^{12} m/c $	$ 104 \cdot 10^3 $

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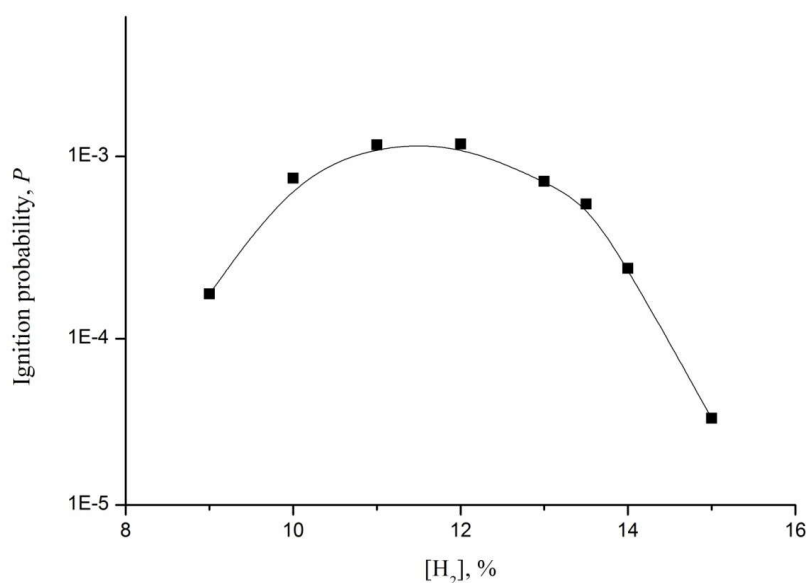
An experimental study of an ignition of flammable gaseous mixtures with mechanical sparks

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It is well known that particles formed as a result of a counteraction of moving surfaces can be heated to high temperatures depending on the sizes of these particles and the composition of the gaseous environment. These temperatures can be so high that they radiate in the visible part of spectrum. Such particles are called mechanical sparks and can be produced as a result of friction or the striking of moving bodies. Mechanical sparks are one of the most frequent ignition sources for flammable gaseous mixtures.

This paper describes a method for testing the safety of construction materials with respect to mechanical sparks (spark safety). This method was tested on examples of various materials and flammable gases. Hydrogen, acetylene, petrol, methane and LPG were used as the flammable gases. Various types of steel, aluminium, and copper and aluminium alloys were used as the construction materials. The typical experimental data on a dependence of a probability of an ignition on the hydrogen content in air are shown in the figure. A qualitative interpretation of the obtained results is given.



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Analysis of 2D distribution of the frequency spectra of the flame model fire whirl*M.V. Sherstobitov, R.Sh. Tsvyk, V.M. Sazanovich*

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Fire whirls (FW) occur sometimes during large-scale natural and technogenic fires. They are characterized by stovepipe elongation of swirling fire fed by the fire source, both its part and as a whole. The impact of a FW on the environment strongly increases as a high-power surface air radial inflow into the FW base. Real time studies of FW are expensive and dangerous; therefore, mathematical and physical simulations of this phenomenon are used. Today, there are many works on the physical simulation of FW. However, as far as we know, no studies were carried out on the use of thermal imaging for measurements of the flame rotation rate. The setup for physical simulation of FW by means of a fire torch formed during ethanol burning in a tank fixed on the axis of uprising swirl airflow.

This work devoted of experiment on the thermal imaging technique for getting the 2D distribution of the frequency spectra of torch. It is necessary to improve the method for determining the vortex speed [1].

The FLIR X6530SC IR camera is in 2.5–5 μm band, thermogram frame rates 514 Hz were used. It was recorded sequences from 7848 thermograms for combustion with or without swirling. In the flame image height 10 were selected (3 height of combustion without swirling). At each height evenly 5 points were chosen (averaged for flame width) to calculate the spectral function ($U(f) = f \cdot W(f)$; where $W(f)$ is FFT of temporary signal fluctuations). See Table 1.

Table 1. Frequency(Hz) of the main spectral maximum (a) with (14 Hz) or without swirling(b).

Height, mm	Width, mm	Point number (a)					Point number (b)					Width, mm
		1	2	3	4	5	1	2	3	4	5	
800	44	11,1	7,8	6,2	5,3	5,3						
700	59	9,9	9,1	8,5	5,3	5,3						
600	69	5,4	14,2	11,3	10,0	5,3						
500	69	14,1	14,1	15,4	14,2	14,2						
400	74	14,2	14,2	14,1	14,1	28,2						
300	77	14,2	14,2	14,2	14,1	28,2						
200	69	28,2	29,1	28,2	14,1	28,2						
150	69	28,2	28,2	28,2	14,1	14,2	4,3	4,3	4,3	4,3	4,3	90
100	64	28,2	28,2	28,2	14,2	14,2	4,3	4,3	4,3	4,3	3,8	133
50	61	28,2	28,2	28,3	28,2	14,2	4,3	4,3	4,3	4,3	4,3	120

Weak gray isolated dual frequency swirling, strong gray highlighted other frequencies and the fundamental frequency of the flame shows no separation. Thus flame detected "layers" basic, twice and other frequencies.

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**Combustion of porous media in conditions of artificial gravity:
Evolution of combustion front structure**

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Frontal high-temperature synthesis of target products in the field of centrifugal forces was analyzed by numerical modeling and appropriate experiments for the reaction $\text{NiO} + \text{Al} \rightarrow \text{Ni} + \text{Al}_2\text{O}_3$ taken as an example. A simplified reaction scheme used in calculations assumes the melting of starting reagents within the combustion wave to form a three-component reactive medium—comprising metal, ceramic, and gaseous products, each with its own temperature and subsonic velocity—whose mobility is described in terms of a 1D model [1]. The metal and ceramic phases are assumed incompressible, while the gaseous phase is regarded as an ideally compressible body. The processes of phase segregation are described in terms of 1D sedimentation of interpenetrating media. The system of differential equations involves the balances of mass, impulse, and energy.

Investigated was the onset of self-sustained combustion front in a cylindrical sample ignited from an open top, as well as its dynamics and structure. Typically, front structure was found to exhibit the zones with superadiabatic temperature of individual phases and the zones of thermal relaxation. The feasibility of true gasless combustion and a steady mode of quasi-periodic scintillating combustion will be discussed at presentation, as well as the effect of heavy centrifugal overloading [2].

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Kinetic study of the effect of ethanol addition on PAH and soot formation in ethylene flames

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The effects of ethanol (C_2H_5OH) addition to premixed laminar and diffusion flames of ethylene (C_2H_4) on polyaromatic hydrocarbon (PAH) and soot precursor formation is studied. The chemical kinetic mechanism, previously optimized using experimental data obtained in 30 different flames of methane, ethylene and ethane, was validated on mole fraction profiles recently measured in $C_2H_4/O_2/Ar$ and $C_2H_4/C_2H_5OH/O_2/Ar$ flames at low and atmospheric pressure, Fig.1. The simulations performed identify the kinetic effects of ethanol addition on the main precursor of benzene formation in premixed flames: reduction of the C_2H_3 production rate in ethylene/ethanol mixtures through a decrease of the H-atom abstraction reaction rate from C_2H_4 , and through an exchange of C and H-atoms between intermediates produced during ethanol and ethylene oxidation. That leads to a decrease in concentrations of the main PAH precursors, such as C_2H_2 , C_3H_x and C_4H_x . The computations performed for co-flow laminar flames show that the addition of ethanol has practically no influence on the concentration of the oxidizing species and therefore the oxidation of soot. The chemistry of the PAH production in diffusion flames cannot be explained only with chemical kinetic effects. The ethanol molecules may reduce active radical diffusion and increase the mixture viscosity. This leads to a decrease of the C/O ratio in the centerline of the ethanol-containing mixtures and consequently to an increase in PAH and soot production.

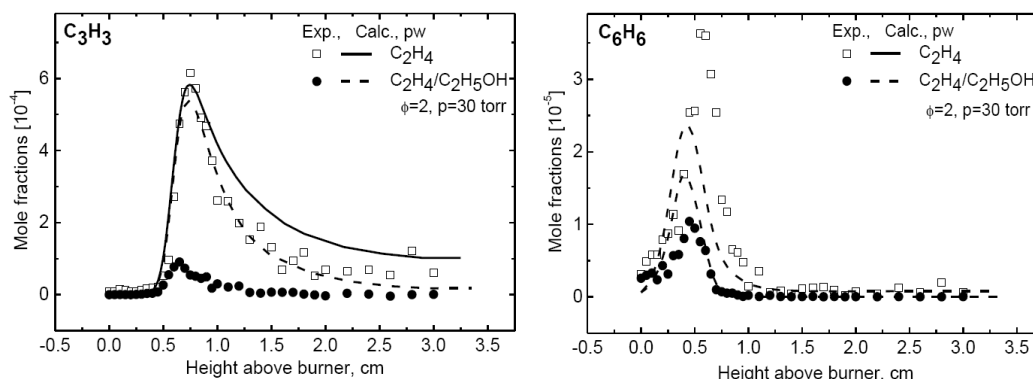


Figure 1. Mole fraction profiles of major C_3H_3 and benzene in pure ethylene and ethylene/ethanol flames at $p=30\text{torr}$, $\phi = 2$. Symbols: experiment Korobeinichev O.P. et al., 2012; lines: modelling using presented mechanism.

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Interaction of detonation waves in silane-air mixture with clouds of inert micro- and nanoparticles*D.A. Tropin- and A.V. Fedorov*

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The addition of inert particles in the reactive gas mixture is one of methods of modification and control of combustion and detonation in such mixtures. For example, the addition of chemically inert particles reduces the velocity of detonation, change the length of the chemical reaction zone of the detonation wave (DW). In this paper the interaction of DW in mixture of silane-air with clouds of inert micro- and nanoparticles are calculated.

In the paper the physical and mathematical models describing the processes of propagation, attenuation and suppression of the detonation process in the mixtures of silane-air by inert micro- and nanoparticles, based on the detailed chemical kinetics, were proposed. Based on this models the dependencies of detonation wave velocity deficit in the considered mixture on the size and concentration of inert micro- and nanoparticles were found.

It was revealed that the same types of detonation flows exist in the mixture of a gas and nanoparticles, as in gas suspensions with micro particles: 1. stationary propagation of attenuated DW at velocities less than Chapman-Jouget velocity; 2. the DW suppression. Furthermore, it is determined that the mechanisms of detonation suppression by micro- and nanoparticles are quite similar and lies in the decay of DW on frozen shock wave and attenuating front of ignition and combustion.

Concentration limits of detonation were calculated. It has been shown that detonation limits in are close for the particles with diameter ranging from 10 nm to 1 microns. It is determined that the tendency of increasing of detonation suppression efficiency with decreasing of the inert particles size during the transition from micro to nanosized particles is violated.

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Terahertz radiation as new technique for research of burning and detonation

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Any shared system of gas–dynamics and chemical–kinetics equations that describe wave propagation in chemically active media is unstable. The obtainable combustion and detonation waves and their structures are essentially not onedimensional. The spatial nonuniformity of the front considerably complicates studies of the kinetics of chemical reactions during combustion and detonation and hinders the search for an answer to the question, what is the contour of the reaction zone in such a structure? Knowledge of the detailed dynamics of chemical processes in combustion and detonation waves enables us to create better quality models for their description and to model (calculate) more accurately the nonstationary processes of transitioning from subsonic combustion to supersonic detonation.

This work attempts to overcome the existing difficulties in recording the detailed dynamics of reactions beyond a subsonic combustion front of gaseous mixtures using the Novosibirsk Free Electron Laser (FEL). Terahertz wavelengths from 115 to 200 μm contain many lines of the absorption of polar molecules of water and OH radicals. Most initial combustion components are nonpolar and transparent (e.g., O_2 , H_2). A free electron laser can be tuned to any radiation absorption line in this range, making it possible to study the kinetics of combustion and detonation waves in gaseous mixtures. The laser can thus help create unique measuring techniques in the terahertz band.

Schemes, experimental methods, and terahertz radiation records of a oxyhydrogen burning front are described. The selection of absorption lines of H_2O and OH for recording is discussed. The absorption distribution at a wavelength of 166.81 μm along the crosssection of a stationary oxyhydrogen burner flame is studied. The results obtained with optical detectors, pyroelectric detectors and Schottky barrier detectors in a dynamic experiment with the flame propagating along a pipe are presented.

On times about several milliseconds correlation between absorption of terahertz radiation, an optical signal and acceleration of the front of a flame with formation of a head shock wave is received. To see dynamics of complicated structure of the front, the line of fast Schottky barrier diode detectors is also necessary. This line doesn't exist yet and it needs to be created.

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An integral energy-release in divergent multifront detonation*A.A. Vasil'ev^{1,2}, V.A. Vasiliev¹*¹Lavrentyev Institute of Hydrodynamics, Novosibirsk, Russia²Novosibirsk State University, Novosibirsk, Russia

Excitation of combustion or detonation in a combustible mixture usually has a threshold character (yes/no) for any initiator. In an idealized model of a strong explosion propagating over an inert medium the governing parameter determining the blast wave properties is the explosion energy. By analogy, the minimum energy of the initiator that ensures 100% excitation of combustion or detonation is usually called the critical energy for combustible mixtures as well. The critical ignition energy (at least, in the case of spark ignition) is traditionally considered as the basic parameter of the fire hazard of mixtures. The critical energy of detonation initiation E^* by an ideal (in terms of spatial and temporal characteristics) initiator serves as a measure of the detonation hazard of mixtures: the smaller the value of E^* , the more hazardous the mixture.

The idea of formulating the initiation condition on the basis of only one parameter (critical energy) is extremely attractive. However, because of the multifront structure of a real detonation wave (instead of its idealized one-dimensional model with a smooth front), the problem of initiation of combustion and detonation waves cannot be considered as being completely solved: there are still poorly examined aspects of the influence of the spatial and temporal characteristics of the initiator on excitation of the combustible mixture and formation of self-sustained (combustion or detonation) waves in this mixture. The question about effective energy-release for multifront detonation practically not investigated experimentally.

In this paper, the “useful” energy of an arbitrary source is determined on the basis of the intensity of the blast wave generated by this source at the stage of a strong explosion. The theory of a strong explosion [1, 2] in an inert medium yield the following relationship between the instantaneously released explosive energy E_v , initial density ρ_0 , blast wave coordinate r , and time t : $r(t) = [E_v/(\alpha v \rho_0)]^{1/(v+2)} t^{2/(v+2)}$. In the coordinates $r^{(v+2)}-t^2$, which dependence should be a straight line. Based on its slope, it is possible to determine the energy E_v , which should be treated in our case as the “useful” energy of the source.

The theory of a strong explosion is used as a basis for the development of an experimental technique for determining the source energy that ensures initiation of the combustible mixture (initiation of blast wave in inert mixture and recalculation of blast wave trajectory from point of view of blast theory) and the energy, which became the basic energy for propagation of detonation wave at critical initiation regime (initiation of reactive mixture and recalculation of trajectory of wave at common influence of initiator energy and increasing energy of explosive mixture). From these data the effective energy-release of mixture was determined.

The data for stoichiometric mixture of acetylene-oxygen and hydrogen-oxygen at initiation with exploding wire are presented in this report.

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Ignition of slurry fuels based on coal processing waste and petroleum products

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Involvement of significant amounts of annually produced combustible wastes of coal processing and used petroleum products in the energy industry as components of composite liquid fuels is an approach, which allows to utilize unclaimed low-grade waste and to create an alternative fuel reserve. Despite the lower heat of combustion (in comparison with coal dust), coal-water slurries (CWS) and coal-water slurries containing petrochemicals (CWSP) allow reducing formation of anthropogenic emissions of carbon dioxide, sulfur and nitrogen oxides at combustion process. On the other hand, coal-water slurries are characterized by higher inertia and temperatures of stable ignition in comparison with coal dust due to the presence of relatively high proportion of inert fluid (40-50% water). For the industrial use of CWSP it is necessary to have experimental database and analysis of ignition characteristics and conditions of slurries based on coal processing waste and low-grade solid fuel with various energy additives (liquid combustible oils).

The aim of this work is to determine experimentally regularities, limit conditions and characteristics of stable ignition of slurries, prepared from coal processing waste with additive of waste liquid petroleum products.

In this study we used wet (40-50% of water) flotation wastes of coal processing (called filter-cakes) as the basic CWSP component. Used oils (turbine, transformer, motor, compressor, and others) and heavy oil were used as additive (5-15%). The experimental method was based on injection of single droplet of CWSP, which was fixed on the low-inertia thermocouple junction into the flow of heated air. The processes of heating, ignition and burning of single fuel droplets were investigated using means of high-speed video camera. Initial radiuses of droplets were varied in the range 0.5-1.5 mm; temperature and velocity of oxidizer flow were varied in the range 600-1000 K and 0.5-3 m/s.

The experiments have shown that heating of slurry fuel initiates the physical and chemical processes on surfaces and in deep layers of CWSP droplet. These processes correspond to certain stages that precede the ignition of CWSP droplet: inert heating, evaporation of water and liquid combustible component and thermal decomposition of coal organic part, gas-phase oxidation of volatiles and combustible liquid vapors in hot air, heating and heterogeneous ignition of carbon residue. We found that temperature range of stable ignition of CWSP droplets with different component composition is 650–900 K. The influence of significant factors (temperature and velocity of oxidizer flow, initial droplet size) on the ignition delay and time and minimum (limit) ignition temperatures were established. The received results illustrate the prospects of utilization of a large group of waste of coal, chemical, petrochemical, energy and transport industries by its combustion as components of composite liquid fuels.

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On the possibility of gaseous fuel self-ignition in a cylindrical or vortex detonation chambers*D.V. Voronin-*

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The problem of construction of engine based on detonation phenomenon is one of the widely studied in many research centers all over the world. There are many technological and scientific aspects here. Vortex or cylindrical chambers are one of the engine parts. The stability of the flow in the chamber is often interrupted by gas mixture self-ignition observed in experiments, although the value of mean gas temperature in the chamber (after the passage of initial pulse) is essentially lower than the value of self-ignition. The reasons of the effect are not quite clear. The recent paper is devoted to theoretical and experimental study of the problem.

The numerical calculations of the flow field in a planar vortex chamber and cylindrical detonation chamber have been performed. The model is based on conservation laws of mass, momentum and energy for non-steady two-dimensional compressible gas flow in case of swirl axial symmetry. The processes of viscosity, heat conductivity and turbulence have been taken into account. It was found that transition of kinetic energy of gas into heat due to processes of dissipation generates "hot spots" in boundary layers at the chamber walls. The gas temperature at the spots may exceed the temperature of gas ignition ($T = 1200$ K), while the surrounding regions remain still cold. It may be the reason of cold gas self-ignition observed in experiments.

For appreciation of the flow geometry on the appearance of the hot spots the three-dimensional approach has been used as well. Three-dimensional numerical simulations revealed the appearance of micro vortexes at the walls of the chamber that cannot be described within the two-dimensional approach. The existence of such a structure may play a decisive role in a flow self-ignition (as well as a generation of a mixing zone in case of separate inlet of a fuel and oxidizer within the chamber).

To appreciate the influence of turbulence on the gas self-ignition, the numerical simulations of laminar flow were performed on the base of Navier-Stokes equations at the same initial values of the problem parameters. For laminar flows the mixture self-ignition may occur as well. Although the maximum value of temperature in laminar hot spot $T = 1370$ K is significantly less than turbulent $T = 2110$ K at the same instant. So the flow turbulence may play decisive role in possibility of gas self-ignition.

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Two-dimensional inorganic nano-materials as high efficient flame retardants in polymer composites*X. Wang, L. Song and Y. Hu*

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Two-dimension (2D) inorganic nano-materials have aroused enormous research interests in developing multi-functional polymer nanocomposites over the past few decades. In our work, we mainly focused on the utilization of 2D inorganic nano-materials to improve the flame retardancy of polymeric materials. Several 2D inorganic nano-materials, including layered double hydroxides, layered zirconium phosphate, graphene, and their flame retardant behaviours in a variety of polymer matrices are summarized. These nano-materials have displayed high efficiency in reducing the heat release rate during combustion of polymeric materials: more than 30% reduction in PHRR has been observed usually at a relatively low loading of 2D nano-materials (≤ 2 wt%) [1-3]. However, in order to meet high industrial flame retardant classification (e.g., UL-94 V0 rating), modification for 2D nano-materials or combination with traditional flame retardants is required [4,5]. We also propose the flame retardant mechanisms of these layered inorganic compounds in polymer nanocomposites.

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Kinetics and structure of laminar, nanoparticle forming flames: silica and iron oxide

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Due to their presumed spatial one-dimensionality, laminar, premixed flat flames are popular to investigate nanoparticle formation from the gas phase. The flame is a steady, one-dimensional, generic flow problem which can easily be described by a set of ordinary differential equations. The measurement of laminar flame structure enables the development of reaction kinetics mechanisms, and reliable reaction mechanisms allow the prediction of the flame structure in turn. The latter is essential for process design and control, and for calculation of the thermochemical state in simulations of realistic, turbulent, reacting flows in synthesis reactors. The nanoparticle synthesis process is often assumed to be straight forward, beginning with a pure gas phase, in the premixed flat flame usually found in the small region close to the burner, followed by late particle formation and growth during cooling of the burned gases. The flame front and the zone of particle formation are therefore assumed to be spatially separated and distinguishable. Nevertheless, large concentrations of precursor species in the premixed gases may cause early particle formation with implications to the modeling of the process.

We discuss two popular systems in the gas phase synthesis of nanoparticles: iron oxide from iron pentacarbonyl doped flames and silica from flames doped with siloxanes.

In the case of iron oxide it has recently been shown, that premixed flames doped with iron pentacarbonyl, produce a notable amount of condensable matter, likely iron particles, in the pre-heating zone and in the flame itself (*Feroughi et al., Proc. Combust. Inst., 2015; Kluge et al. CrystEngComm, 2015*). These observations demonstrated the need for understanding the reaction kinetics in this particular system, as early formed clusters and nanoparticles strongly affect the product properties and of course the modeling of the system. Based on new experiments and complementary CFD simulations we could verify the hypothesis of early inorganic particle formation (and decay) in iron oxide particle forming flames, leading to an extended and improved view of the iron oxide synthesis process.

A similar observation could not be made directly for silica particle forming flames, but recent measurements (*Feroughi et al., Proc. Combust. Inst., 2017*) allowed development of simplified reaction mechanisms for a consistent prediction of silica particle growth in the late flame. However, at high nanoparticle precursor concentrations, the existing models were not able to predict distinct features of the measured SiO concentration profiles in the flame. Based on the available literature data and with reaction mechanism optimization techniques we developed an improved model for the formation and consumption of the SiO in siloxane doped flame, able to reproduce the measurements for a wider range of parameters.

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Flame propagation in aerosuspension aluminum boride nano-particles

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The aim of this work is the study of condensed and gaseous products of combustion aerosuspension nano-dispersed particles of aluminum borides (BA) using electron microscopy and recording the emission spectrum in the visible wavelength range.

Nano-particles obtained by the developed RSI CTOC technology, plasma synthesis, followed by condensation under an inert atmosphere (high purity argon). The particles (representing the color dark grey) specific surface is $S_{sp} = 19.1 \text{ m}^2/\text{g}$, a bulk density of about $150 \text{ kg} / \text{m}^3$. Despite the fact that the powder is the formation of conglomerates and structured BA nano-dispersed particles retained autohesive interaction forces, nevertheless it is loose and allows to arrange over the work area by known methods, including the displacement of the piston from the cylindrical container.

The condensed combustion products are formed and collected after the flame propagation process aerosuspension aluminum boride particles to set a constant volume. The working section length of 1500 mm is equipped with a flat transparent front wall of the PMMA, which allows you to register using a prism spectrograph ISP-51 and electronic consoles SIDS-1 spectrum BA flue gas emission in the air.

Transparent elements allowed to register during the propagation of flame intense green color, indicating the presence BO_2 molecule in products of combustion. On account of the radiation spectrum of molecular bands in the wavelength range of 547 nm.

Due to the gravity of the combustion products and unburned particles BA clung to the bottom cover of the working area. Selected samples were analyzed on a Philips electron microscope with the highest 100 nm scale. Particle images indicate that in the process of flame propagation and chemical reactions on the surface of BA formation of spherical particles is the particle diameter below 100 nm, which may indicate the formation of a new phase, for example, aluminum or boron compounds. This is confirmed by the results of the elemental analysis performed using a microprobe Edax-32 showing the content of free aluminum and boron in the different samples.

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Experimental and numerical study of premixed flame propagation in narrow gaps

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Propagation of premixed flames in narrow gaps between parallel glass plates is studied experimentally and numerically for methane-air mixtures. Such problems are of interest from the fundamental point of view because they reveal development of flame instability due to thermal losses to the walls of the gap. Also, studies of combustion in narrow gaps are important from the applied point of view in connection with development of micro combustors and engines.

Experiments were carried out on a facility consisting of two parallel glass plates of 0.5 m diameter, the space between the plates was filled with a premixed methane-air mixture with various composition, ranging from lean to stoichiometric fuel concentration. The gap between the plates was variable in the range of 2-8 mm. Initially, the mixture was quiescent, spark ignition was performed near the plate center, flame propagation was recorded by a high-speed video camera. It was obtained that for larger plate spacing, nearly cylindrical laminar flame was propagating through the mixture, whereas when the gap width was smaller, flame instability developed. In this case, the flame front was curved, exhibiting distinct long and short wavelength perturbations. The average flame propagation velocity depended on the gap width.

Numerical simulations of unstable flames propagating in narrow gaps were performed by a three-dimensional numerical model based on Navier-Stokes equations for multicomponent reactive gas in small Mach number approximation. Methane-air combustion was described by a detailed chemical mechanism. The parallel solver was implemented with adaptive mesh refinement in order to resolve sharp temperature and concentration gradients near the flame front. Results of numerical simulations are presented and compared with the experimental data, revealing development of flame instability and specific features of gas flow and combustion in such a configuration.

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Recognition of wildfires inducing flashovers of high-voltage transmission lines

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There are prevailing flashover accidents of high-voltage transmission lines caused by wildfires during fire seasons in Southern China. Substantial electric outages cause obvious property losses and bad social reputations.

By fire investigation analyses of existent flashover accidents and field surveys of typical burned, original and on-fire forest areas with overhead high-voltage transmission lines, the progresses of wildfire developments and their interactions with transmissions were deduced, the temporal properties (occurrence segment, duration and sequence) of wildfires were abstracted, the detailed features of fire environments surrounding the right-of-ways (transmission line corridors) were described including climate conditions (temperature, humidity, wind speed, direction and strength), geographical conditions (micro-terrain, micro-topography, hill side intersection angle, gradient, exposure, ridge strike, top altitude), forest stand conditions (type, structure, composition, tree species, item moisture content), fire propagation (fireline front, length, strike), apparent flame appearances (flame height, contour, structure, brightness, inclination, interface with smoke plume) and apparent smoke appearances (height, contour, structure, obscuration). Also the features of exposed transmission lines and towers were recorded including power type (AC or DC), phase allocation and gap, operation type, construction configuration, tower type and wave recorded ranging. Most importantly, the flashover processes were characterized by addressing the clearance between conductors and ground, discharge distance, type, temporal sequence, involved phases, attribution, severity and discharge tracking.

Based on above first-hand and rich information, the wildfires that can easily pose a flashover of transmission lines were recognized. The wildfire type, ground fireline and crowning fire intensity, propagation direction, spread rate were explored and figured out. A comprehensive indice system was required and proposed to cover the bilateral interaction of wildfires and transmission lines resulting in flashovers.

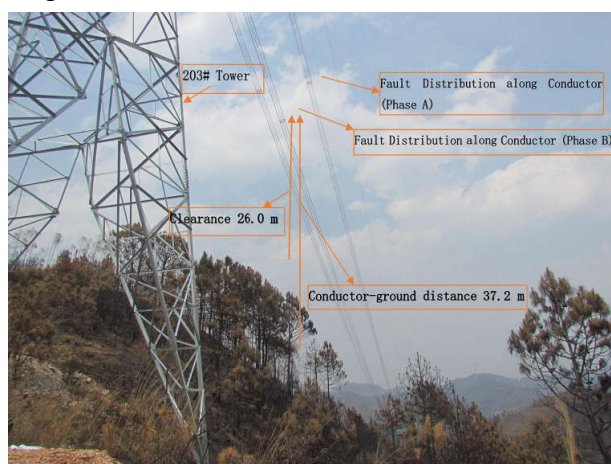


Figure 1. Exposed Discharge (Fault) Spot of Certain Transmission Line and Tower at Burned Area

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About the flame propagation limit*V.V. Zamashchikov¹, I.A. Zolotarskii²*¹Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia²Boreskov Institute of Catalysis, Novosibirsk, Russia

According to the thermal theory [1], the cause of the concentration limits of flame propagation is heat losses. Thus, the limit is reached when heat losses exceed the heat release in the flame front. Following the thermal theory, reduction of heat losses leads to expansion of concentration limits. However, it is difficult to eliminate heat losses completely because of the radiation flux from the flame front to the environment. When initiating ignition in the center of the vessel (at a distance from its walls) the contact of hot products with walls is excluded, but concentration limits are determined not only by radiation heat losses in this case. When approaching the limits, the burning laminar velocity decreases resulting in rising of flame seat up due to Archimedes forces. That leads to complexification of mass and heat transfer processes. The purpose of the present work is an experimental study of the upper limit of flame propagation.

Experiments were carried out with a closed 10-liter spherical vessel. Ethane and oxygen were used as components of a gas mixture. Ignition of the mixture was initiated either by the electric spark or by the impulsively heated nichrome coil in the vessel center. The evolution of the ignition seat was recorded using a high-speed Schlieren photography, while the pressure variation was recorded by the inductive sensor DD -10.

At relatively high laminar burning velocity the flame is almost spherically symmetric in case of spark ignition. The flame has the more complex shape, when the coil is used. But a spherical symmetry remains to some extent. The flame seat starts to rise up to the top of the vessel and then propagates downwards when the laminar burning velocity is decreasing. Top-down flame propagation becomes less intensive with further approaching to the limit. Finally, the flame rises up and is extinguishing. Pressure increase is detected when the flame goes down. And pressure increase is not detected if the flame is extinguishing at the vessel top. Thus, pressure recording allows detecting approaching to the limit.

It was shown experimentally that the limit slightly depends on the source of ignition. The limit is reached earlier at spark ignition. Most likely, the reason is poor formation of the flame front due to the rapid expansion of gas heated by the spark. Thus, the limit determined by pressure recording with coil ignition is predetermined by flame quenching when it is lifting up. Estimates have shown that An acceleration with which the flame rises up significantly exceeds the estimated one of Archimedes forces. The possible reason is entrainment of cold gas by the lifting flame due to viscous forces. However, the entrained gas mass is much larger than mass of the gas located in the flame front. In this case the heat from the flame front is transferred to the cold mixture, which burns in the front further on. Thus, the presence of the entrained mass results in minimizing heat losses from the flame seat. And the flame propagation limit is determined rather by cooling the combustion product in the upper part of the vessel.

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Researches of methane-air mixtures combustion assisted by transverse pulse-periodic laser radiation in supersonic stream*V.N. Zudov, P.K. Tretyakov*

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In the present work, the results of numerical and experimental investigations of supersonic flows with a localized energy supply are considered. The main attention is paid to the unsteady effects the role of which is determining at the integral flow structure formation. A physical model of energy source is formulated. The numerical and experimental data on the structure of the flow around the source and the characteristics of a thermal wake arising behind the source are compared. The energy pulses frequency and capacity are shown to determine the wake properties: the formation and development of subsonic regions, vortex structures, and reverse flow regions. The eventual goal of this paper was to determine whether or not a plasma torch operating with hydrocarbon feedstocks would be a good ignitor and flameholder in a supersonic combustor. The flame speed of conventional fuels is too low to burn at supersonic velocities. By injecting combustion-enhancing radicals from a plasma torch, it should be possible to enhance the flame speed by increasing the combustion reaction rates. Atomic emission spectrometry was used to search for excited atoms and ions in methane, hydrogen plasma jets to determine if these combustion-enhancing radicals were produced.

The purposes of the present study were directed on revealing of limits of ignition and the mechanism of stabilization of burning of a hydrocarbonic mix in a supersonic air stream at process initiation pulse - periodic laser radiation. As an energy source for initiation use, created in Institute of Laser physics (Novosibirsk), pulse-periodic CO₂ the laser (with average capacity of 0.5--2.5 kw) is offered. Experimental researches of influence of focused radiation pulse-periodic CO₂ the laser on formation and development of process of distribution of a flame in a stream of homogeneous fuel-air mixes and borders of steady burning are spent. Initiation and burning stabilization it was carried out by creation of a local zone in the centre plasma of the optical breakdown. It is established, that at formation of the optical category in a stream speed of burning increases and stability borders on speed and mix structure extend.

In the present work, the results of numerical and experimental investigations of supersonic flows with a localized energy supply are considered. The main attention is paid to the unsteady effects the role of which is determining at the integral flow structure formation. A physical model of energy source is formulated. The numerical and experimental data on the structure of the flow around the source and the characteristics of a thermal wake arising behind the source are compared. The energy pulses frequency and capacity are shown to determine the wake properties: the formation and development of subsonic regions, vortex structures, and reverse flow regions. The eventual goal of this paper was to determine whether or not a plasma torch operating with hydrocarbon feedstocks would be a good ignitor and flameholder in a supersonic combustor. The flame speed of conventional fuels is too low to burn at supersonic velocities. By injecting combustion-enhancing radicals from a plasma torch, it should be possible to enhance the flame speed by increasing the combustion reaction rates. Atomic emission spectrometry was used to search for excited atoms and ions in methane, hydrogen plasma jets to determine if these combustion-enhancing radicals were produced.

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Experimental investigation of ethanol evaporation and burning with cellular ceiling flame

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There are many theoretical and experimental studies of cellular flames of premixed gas mixtures. They deal with the stability, burning rate, with problems of heat transfer and so on. When components are not mixed preliminary, the cellular flame exists too. It is another phenomenon, and number of experimental investigations on this problem is significantly fewer.

In well-known studies [Orloff, De Ris, 1972] was found that cells exist in various fuel flows. Authors considered burning process "on ceiling", which was set as a result of arbitrarily blowing gaseous fuel. There are difficulties to correct measuring of heat fluxes at burner surface. In our current work the process has been self-sustaining, when the mass flux from the wall are set as result of the influence of reacting gas flow.

Experimental studies were carried out in the wind channel. In its rectangular test section the all horizontal surfaces were formed by porous plates, which are impregnated with ethanol. Speed of air flow of room temperature varied from 0.5 m/s up to 70 m/s. After ignition a self-sustaining burning mode took place when fuel consumption is determined by its interaction with the products of combustion in the boundary layer. Fuel system worked in experiments with burning "on the floor" and "on ceiling" to ensure of constant moistening of plates and measuring of evaporation rate. The data on velocity components were obtained by laser Doppler anemometry (LDA) and by PIV- method (particle image velocimetry). The local gas temperature was measured by thermocouple.

In experiments with burning of liquid ethanol "on ceiling" two main forms of flame were noted – the flame with a smooth surface and with longitudinal large-scale vortex structures. Besides, the cells were appeared in the flame, when air speed decreased to 0.6 m/s. Such kind of burning with a cellular flame is an extreme regime, since further reduction of air speed causes change of gas flow direction, and cells disappear.

When PIV equipment has been used, it was found that Rayleigh -Taylor instability manifested as alternation of ascending and descending mushroom structures in the diffusion cellular flame. It was shown the relationship between this three kinds of large-scale structures and the burning rate, they cause. The minimum of burning rate corresponds to laminar mass transfer during combustion of the flame front with smooth surface. With increasing of speed, when the longitudinal vortex structures are formed, the mass transfer is doubled. In a cellular diffusion flame, burning rate is near of the extreme mode; burning rate is three times its value in the laminar layer.

It is known, intensification of transport processes in turbulent non-reacting flow increases heat transfer up to 25-30%. It's evident, that control range of laminarized reacting flows is much wider.

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The specific features of burning of wood of long natural ageing

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The study of wood burning mechanism devoted quite a lot of work, both in our country and abroad. These results actually became the starting point for modeling the behavior of many carbonized polymeric materials under conditions of high heat or fire. Particular attention was paid to the influence of growth conditions, species, different processing methods and processing of wood on her fire hazard. Investigations to establish the impact of age-related changes that occur in the wood during its operation, the behavior of wooden structures (WC) in the event of fire are limited. In recent years, we have carried out extensive work on studying the features of the process of burning wood and WC long life. As objects of study have been used numerous fragments of buildings structures operation life up to 370 years old, located in different regions of Russia.

During all thermooxidative degradation temperature readings are reduced to an extended service life of wood: decomposition start temperature, the temperature of the maximum mass loss rate and others. For the samples studied, a shift in the start of the charring process to a region of lower temperatures was found, as well as a significant increase in the heat and rate of oxidation of the coal residue. An important feature revealed for a long service life of wood is highly exothermic oxidation process of coal residue. At this stage, the allocation of 70% of the heat produced by combustion of natural wood aging. It has been shown that increased oxidative capacity of coal layers and the high value of the thermal effect for WC long life due to more developed and open the inner surface of coal compared with a sample of modern construction. These changes are due to the occurrence of irreversible changes in the chemical composition and structure of the timber, primarily due to degradation of the carbohydrate portion and increasing influence of the aromatic components of wood composite. By increasing the lifetime of structures observed increase in hydrogen content (mean 1.5) and, consequently, increasing the lower calorific value. Despite the increase in calorific value, a decrease in such an important indicator of fire hazard as the smoke generation coefficient, as well as increased resistance to wood material flammability.

These behaviors are implemented fully and in a large-scale fire tests. According to tests set GOST 30403-2012 increase fire hazards WK long service life, which is caused by higher values of the thermal effect (the temperature rise above 50 ° C throughout the experiment) and substantial charring speed (1.7 times higher) in compared with current designs of timber.

The results obtained are necessary for modeling the dynamics of fire hazards in buildings and structures of various classes of functional fire hazard, as well as its estimated limit of fire resistance of structures made of wood.

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Effect of chemically active inhibitors on concentration flammability limits and flames speed of dimethyl ether/air mixtures

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The research presents an attempt of comprehensive investigation of effect of chemically active inhibitors on combustion of dimethyl ether/air mixtures. The effect of trimethylphosphate, CF₃Br and CF₃I on concentration flammability limits and laminar speed of dimethyl ether/air flames was studied experimental and by numerical modeling. The effect of the inhibitors on concentration flammability limits of flame was studied using a counterflow burner technique. Extrapolation of the dependence to zero value of the extinction strain rate provides the limits value in the absence of stretch effects and minimum heat losses. The measurement results obtained reveal that the inhibitors appreciably influence both lean and rich flammability limits but the inhibition effectiveness has been shown to be higher for the upper limit than for the lean one. The effect of inhibitors on the lower flammability limit of DME/air flames decreases in the trimethylphosphate > CF₃Br > CF₃I series. As to the rich limit CF₃I was found to be most effective inhibitor. The effectiveness of the other compounds decreased as follows: trimethylphosphate > CF₃Br.

The experimental and modeling results on the upper and lower flammability limits for the dimethyl ether/air mixtures with inhibitor additives are shown in Fig. 1.

The effect of trimethylphosphate on the speed of atmospheric-pressure dimethyl ether/air flames has been studied using PIV technique and numerical modeling (Fig. 2). Trimethylphosphate has been shown to be the effective inhibitor of dimethyl ether/air flames over the range of the equivalence ratio. The inhibition effectiveness was shown to slowly increase from $\phi=0.55$ up to $\phi=1.5$. At higher equivalence ratios the effectiveness rapidly decreases. It is noteworthy that similar dependences for the inhibition effectiveness were observed for methane- and propane/air flames inhibited by trimethylphosphate. The experimental results on flame speed were well predicted by numerical modeling.

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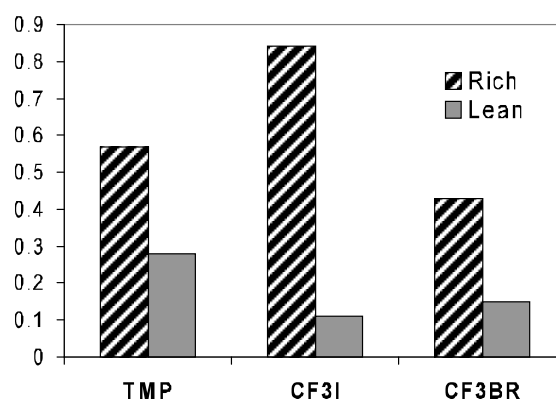


Fig. 1 Measured change (% by volume) of lean and rich concentration flammability limits in presence of the inhibitors; loadings 1500 ppm.

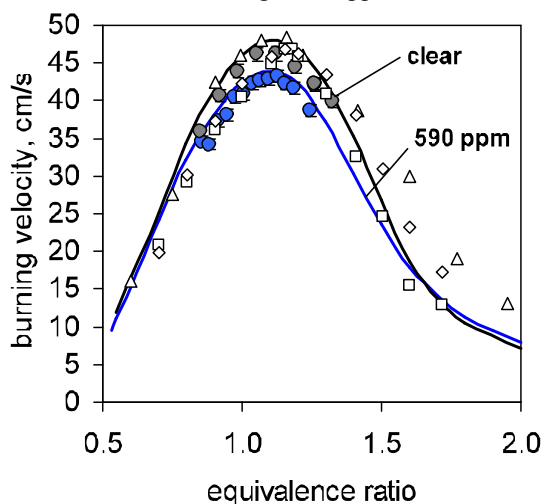


Fig. 2. The speed of dimethyl ether/air flames without additives ($T_0=298$ K, grey circles) and with 590 ppm of trimethylphosphate ($T_0=328$ K, blue circles); other symbols – literature data, curves – modeling.

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Investigation of influence of catalytic and inhibitory particles for burning rate of methane by using PIV method

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Inhibitory and catalytic particles in contact with the flame in front of his influence on the velocity of propagation. Using the PIV method were investigated the influence of solid particles on the flame propagation velocity methane-air flame of different compounds. Evaluation of the catalytic effect was conducted by measuring the velocity of propagation of a laminar methane-air flame with $\phi = 0,9$ using the recording and processing of stroboscopic images of the particles in the flow of the selected section using the PIV system POLIS. The system consisted of two pulsed Nd:YAG laser (wavelength 532 nm, pulse width of 5 ns, 50 mJ pulse energy, the beams are reduced to a single axis), a CCD camera (1360×1024 pixels, each pixel size $4,65'4,65 \mu\text{m}$) with two-frame record function, the optical lens Tamron SP AF 180mm (zoom ratio was 0.34, the number of apertures is maximized: $f \# = 32$), the CPU clock and the PC «ActualFlow» software. To calculate the displacement of particles in the range between the pair of laser flashes (100 ms) was used adaptive algorithm is an iterative cross-correlation calculation with the continuous displacement areas on the first and second frames. To analyze the degree of influence of the experiment was conducted comparing the results of numerical calculations using Chemkin program and mechanism of chemical reactions known GRI Mech 3.0 depending on the normal speed of the free distribution of a flame on the mass and specific surface area. According to the results of experiments and calculations of the flame propagation speed is changed only for nanoparticles with a specific area of $16 \text{ m}^2/\text{g}$.

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MBMS and numerical study of premixed flames fueled with two C₇H₁₄O₂ esters at 1 atm

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Biodiesel fuels based on ethyl esters are considered as more attractive and preferable than those based on methyl esters, because ethanol used for the esters production is also derived from biological raw materials, whereas methanol is mostly produced from syngas (coal). Therefore, the combustion chemistry of ethyl esters is now of interest, but combustion of fatty acid ethyl esters (FAEE) has not yet been studied sufficiently. The aim of this work was to obtain new experimental and numerical data on the combustion kinetics of ethyl pentanoate (EP) and methyl hexanoate (MH) at atmospheric pressure. These compounds are considered as model components of real ester-based biodiesel fuels.

The structures of stoichiometric EP/O₂/Ar and MH/O₂/Ar flames were studied using molecular-beam mass-spectrometry with soft ionization by electron impact. The flames were stabilized on a flat burner 16 mm in diameter at atmospheric pressure; the temperature of unburnt mixtures was 368 K. The flame sampling was carried out by a quartz nozzle with an orifice of 55 μm in diameter and an inner angle of 40°. The PREMIX code from CHEMKIN II package was used for kinetic modeling. Two mechanisms of esters oxidation were used: the first one contains 522 species involved in 2718 reactions [1], the second one contains 404 species involved in 2557 reactions [2]. All computations were performed using experimental temperature profiles.

The mole fraction profiles of reactants, major products and typical intermediates (including radicals H and OH) were measured in the flames. In the flame of EP pentanoic acid was also detected. The reaction pathway analysis has shown that, in the flame of EP, a monomolecular decomposition of parent fuels contributes significantly to the total consumption rate of these esters. In the MH flame, the fuel decomposition mostly proceeds via the reactions with H, OH, O radicals.

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Porous radiative burner - analytical solutions and stability analysis

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Mathematical models of the processes in porous radiating gas burners, which allow rather simple analytical solution, are considered. Unlike widely used in mathematical modeling the condition of temperature constancy on the entrance part of carcass equaling the ambient temperature, in this work the extent of heating of carcass on an entrance part of burner is determined in the course of the solution. For flat, cylindrical and spherical burners within the framework of one-dimensional and one-temperature model the analytical solution is obtained using assumption of a thin zone of chemical reaction and taking into account dependency of thermal conductivity coefficient on temperature. The effects of the size and shape of burner as well as of reradiation and combustion zone localization on the temperature distributions are investigated.

For two-temperature model of a flat burner without reradiation and with combustion zone localization at the burner exit the dependencies on the problem parameters are investigated of the radiant zone temperature, efficiency of transformation of gas mixture chemical energy to thermal radiation and the temperature profiles form. Stability of solution for flat two-temperature model without reradiation, but with a recuperator is explored.

The analytical solutions obtained will be useful when verifying numerical models and at assessment of a possibility of stationary solution existence for the parameters sets of the burner and gas mix.

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The parameters of the perturbation of the atmosphere during large forest fires*I.R. Khasanov*

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Major forest and peat fires are accompanied by intensive thermal disturbances in the atmosphere and the formation of extensive areas of smoke and gas combustion products.

Based on the analysis of major forest fires peculiarities of their development and impact on the environment. Air pollution a large amount of combustion products can lead to significant environmental and climate impacts. Among the environmental effects include the global trend of climate change and warming of the Earth (the greenhouse effect) related to the increase in atmospheric concentrations of carbon dioxide.

Suggested classification of forest fires depending on power, area, and their possible dissemination. Given the thermal characteristics and the heat dissipation capacity of forest fires.

Conducted complex experimental and theoretical studies to assess the quantitative and qualitative composition of the products of combustion of large fires. The results of experimental studies of the quantitative composition of combustion products for different types of fire load.

Assessment of the impact of forest fires on the environment is also associated with the development of the following areas of study: the study of nature of forest fires, taking into account regional peculiarities; pyrological study of the properties of combustible material to find means and ways of control of the combustion process and extinguish fires; development of remote sensing methods for the detection and sensing of fires; the development of tactics and organization of extinguishing large fires; a comprehensive study of the impact of the fires from the point of view of ecology, developing methods for more accurate accounting of damage from fires.

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How cold are the flame balls in the ultra-lean hydrogen-air gas mixtures?*I.A. Kirillov*

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Combustion of the hydrogen-air gas mixtures can pose the challenging risks for a safety of the nuclear power plants (as it was during the 11/11 Fukushima accident) and the hydrogen-powered vehicles.

Accurate and validated hazard estimations for different regimes of the hydrogen-air gaseous combustion – deflagration, detonation, etc. – is of vital importance for designers and safety experts in nuclear energy, rocketry and space engineering, system engineering for an emerging hydrogen energy infrastructure.

Now, the substantial empirical data, theoretical models and computational tools are available, mainly, for modeling and simulation of the self-expanding deflagration, sonic and detonation combustion waves, which exist in concentration range between 9.4 and 75 vol.% H₂.

Factual and verified quantitative information on the combustion characteristics of the ultra-lean (less than 9.4 vol.% H₂) hydrogen-air mixtures is scarce and incomplete. One of the question, which do not have a direct, quantitative answer is – how cold are the flame balls in the ultra-lean hydrogen-air mixtures?

According to the best knowledge of author, experimental measurements of the temperature profiles in the real, buoyant flame balls are absent. The available general-purpose reactive CFD codes do not have the suitable physico-chemical models for predicting of the buoyant flame balls characteristics in the Earth-gravity conditions.

Report is focused on a short historical (from 1914 up to date) excursion into hydrogen flame balls physics and chemistry, and on the theoretical arguments, based upon fundamental flammability limits theory (in accompanying paper), which defines the dependence of the maximal temperature in the buoyant flame balls upon concentration of hydrogen in the ultra-lean hydrogen-air mixtures. Principled distinction between the maximal temperature dependence in buoyant flame balls and the ones for the deflagration flames is explained.

Today, the proposed dependence has a status of theoretical hypothesis and should be verified in experiments. Requirements and limitations for the expected experiments are discussed.

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Experimental and modeling study of a premixed flame of dimethyl ether at atmospheric pressure

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Dimethyl ether (DME) is one of the most promising alternative transportation fuels among various clean, renewable, and low-carbon fuels, which are considered worldwide. DME can be derived from many sources (biomass, natural gas and coal). Fundamental studies of DME combustion chemical kinetics may therefore be useful in modeling optimizing and developing advanced clean combustion engines. The goal of this work is to provide new experimental data on the chemical structure of atmospheric-pressure premixed flame fueled by DME for validation of available detailed chemical kinetic mechanisms for DME combustion.

Laminar premixed burner-stabilized flame of stoichiometric dimethyl ether/oxygen/argon mixture (DME/O₂/AR= 0.0648/0.1852/0.75) at 1 atm is studied experimentally and numerically. Flame sampling molecular beam mass spectrometry is used to measure mole fraction profiles of stable flame species (DME, O₂, CO, CO₂, H₂O, H₂), and intermediates (methane, formaldehyde, acetylene, ethane, ethylene, ketene, hydrogen peroxide, propane) including flame radicals (OH, H, CH₃, HO₂). The experimental data are compared to the Premix simulation results obtained using two detailed chemical kinetic mechanisms for DME oxidation available in literature [Wang et al., *Combust. Flame* 2015, 162 (4), 1113-1125.] (mechanism 1), [Tran et al., *Proc. Combust. Inst.* 36, 2016] (mechanism 2).

Mechanism 1 was found to overpredict significantly acetaldehyde peak mole fraction. Moreover this mechanism does not involve the reactions of propane formation and oxidation, whereas its peak mole fraction in the flame was measured to be $\sim 3 \times 10^{-5}$. Methoxyethane (H₃CCH₂OCH₃) was identified in the flame, but this species is also not included in the mechanism 1. Mechanism 2 predicts adequately peak mole fractions of all species detected in the flames. According to both experiments and simulation, formaldehyde was found to be the most abundant intermediate in the flame. Its measured peak mole fraction is $\sim 8 \times 10^{-3}$, however both mechanisms underpredict this value. Kinetic analysis of the reaction pathways of DME oxidation was performed to reveal the deficiencies of the mechanisms in predicting peak mole fractions of intermediates.

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Structure of laminar premixed burner-stabilized H₂/CH₄/C₃H₈/O₂/Ar flames at 1-5 atm

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Liquid hydrocarbon fuels (gasoline, diesel, kerosene) are the leaders in a transportation sector. But recently a new tendency to their substitution by gaseous fuels like hydrogen, compressed natural gas, liquefied natural gas or dimethyl ether appeared. A promising idea is to add 20-30% of hydrogen to basic gaseous fuel. This is expected (1) to reduce CO₂ emission because of decreasing the C/H ratio in the fuel and (2) to allow burning much leaner fuel blends and therefore lowering combustion temperatures and NO_x emissions. In this respect, the chemical kinetic aspects of these combustion processes must be understood thoroughly.

A number of systematic studies of macrokinetic parameters and chemical reactions in binary mixtures of hydrogen and methane were performed earlier. Nevertheless, there are only few investigations of H₂+C₃H₈ and H₂+n-C₄H₁₀ mixtures. It is also an important fact that the studies of the chemical structure of the flames of multicomponent blends are scarce, in particular, for atmospheric and high-pressure conditions there are no works in the literature. Therefore, the aim of this work was to study chemical speciation in the premixed burner-stabilized flames of H₂/CH₄/C₃H₈/O₂/Ar mixtures in the pressure range from 1 to 5 atm in order to understand the effect of pressure on the species mole fractions in the flame.

The flames of stoichiometric mixtures H₂/CH₄/C₃H₈/O₂/Ar (0.019/0.019/0.019/0.143/0.8 in mole basis) stabilized on flat burners at pressures 1, 3 and 5 atm were examined using molecular beam mass spectrometry with soft ionization by electron impact. Sampling was performed at different heights above the burner using a quartz conic probe with the opening angle of 40 degrees and the orifice diameter of 30 microns. Mole fraction profiles of reactants, major products (CO₂, CO, H₂O) and intermediates (H, CH₃, OH, acetylene, ethylene, formaldehyde, ethane, propyne+allene, propene+ketene) were measured. Chemical kinetic simulation of the flames was carried out using PREMIX code and a detailed reaction mechanism for combustion of small hydrocarbons available in the literature (AramcoMech 1.3). The model was found to be, in general, adequate in predicting the mole fraction profiles of the species mole fractions in the flames. The observed changes in the flame structure with pressure were explained on the basis of a kinetic analysis of the model.

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Evaluation of fire retardant properties of polymeric membrane on base of polyethylene

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Authors study the methodology of testing building materials to determine fire safety properties in Russia. It is presented specific behavior of thermally thin materials. Including polymeric membranes, under heat exposure. Several comparison results of combustion heat, oxygen index, thermogravimetry to identify the material were presented for polymeric membrane Tyvek[®] FireCurb[™] Housewrap on the base of polyethylene with flame retardant coating on the base of phosphororganic compounds and standard products without flame retardant coating.

Received results confirm the effectiveness of flame retardant properties of membrane Tyvek[®] FireCurb[®] Housewrap, phosphorous containing agent promotes the formation of a 'char' layer at the surface when it is contacted by an ignition source, also no burning droplets appear during flame contact.

Additional large-scale experiment was made to prove flame retardant properties of the membrane.

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Thermographic studying the connection between the scale of turbulence in flame and temperature fluctuations

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Combustion with a diffusive oxidant flow is widely used and can be produced both in technological devices and wildland fires. Such combustion usually occurs during a turbulent flow of combustion products in flame. Turbulent combustion is a nonstationary process of mixing the gaseous combustion products with an initial mixture that is ignited due to the increase in temperature. This nonstationary process leads to the distortion of the flame shape, which increases the surface area and the combustion rate. The scale of turbulent fluctuations and the intensity of mixing significantly influence on the shape of flame and the combustion rate, as well as on the thermodynamic parameters of the process, the completeness and efficiency of combustion under turbulence conditions.

The paper represents the results of experimental studies concerning the combustion of certain liquid (alcohol, petrol, kerosene, diesel fuel) and solid fuels (wood of pine, birch, cedar, and other plant fuels). The results were obtained using the thermography techniques in the middle infrared narrow spectral ranges. The high-speed recording of infrared images showed the cyclical flame processes which caused the temperature fluctuations. These fluctuations were shown to be connected with the flow regime and the scale of turbulence in flame. The scale of turbulence is estimated by the two methods: direct measurement with the use of thermograms and a simplified mathematical model that allows the scale of turbulence to be estimated by the characteristic frequencies in the range of temperature changes in flame.

The different methods used to measure the scale of turbulence in flame showed a satisfactory agreement of the results. In addition, the experimental data were compared to the results of mathematical modeling for the combustion of diesel fuels, including the experimental and theoretical calculations for the scale of turbulent eddies.

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Combustion chemistry features of light isomeric fatty acids esters

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Depletion of petroleum sources makes search of alternative fuels very actual. Biodiesel is one of the most promising types of oxygenated fuels. It can be used separately or in blends with diesel fuels. Biodiesel contains both methyl and ethyl esters. Most studies focus on methyl esters oxidation and combustion. Fatty acids ethyl esters (FAEE) are considered as new generation biofuels, because bioethanol is used for their production. This makes FAEE environmentally safer.

The aim of this work was to obtain new experimental and numerical data on the combustion kinetics of biodiesel model components: ethyl acetate (EA) and methyl propanoate (MP). To better understand differences between methyl and ethyl esters combustion kinetics, the results for EA were compared with the experimental and numerical data for MP, which is an isomer of EA.

The mole fraction profiles of reactants, major products and intermediates were measured in the EA/O₂/Ar ($\varphi=1.14-1.73$), MP/O₂/Ar ($\varphi=1.14-1.73$) flames by use probing molecular-beam mass-spectrometry. Flames were stabilized on a flat burner at atmospheric pressure. Temperature profiles were obtained with micro thermocouples. The PREMIX code from CHEMKIN II package, two mechanisms of esters oxidation (by G. Dayma et. al. (2012) and by O. Korobeinichev et. al. (2015)) and measured temperature profiles were used for flame structure modeling. The comparison of numerical and experimental results shows that the kinetic mechanisms satisfactorily reproduce the experimental data.

The reaction pathway analysis shows that, in near-stoichiometric EA flame a monomolecular decomposition of parent fuel with ethylene and corresponding fatty acid formation contributes significantly (20-40%) to the total consumption. Increasing the equivalence ratio up to $\varphi=1.73$ enhances contribution of the monomolecular decomposition reaction in 2-3.5 times (up to 70-90%). However, in MP flames, the fuel decomposition proceeds via the reactions with H, OH, O radicals; moreover, the changes in equivalence ratio of unburnt mixture slightly influence on the contributions of these reaction pathways to the total consumption of MP.

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Kinetics of thermal decomposition of PMMA at different heating rates in a wide temperature range

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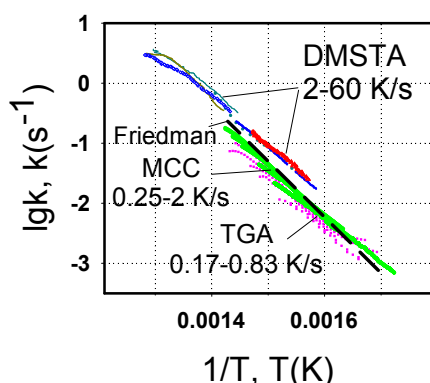
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Polymethylmethacrylate (PMMA, $[-\text{CH}_2\text{C}(\text{CH}_3)(\text{COOCH}_3)-]_n$) is largely produced in the world due to the advantages of its use in multifunctional structures. PMMA is known to be a combustible polymer that makes the study of the kinetics of its thermal decomposition, the characteristics of which determine PMMA ignition and combustion, relevant and important. PMMA is a convenient object for modeling polymer combustion, as a monomer is the main product of its thermal decomposition. The kinetics of PMMA thermal decomposition has been studied for a long time. Essential divergence in its kinetic characteristics is observed. This may be related to various methods of PMMA synthesis and different approaches to processing of the experimental data. The study of thermal decomposition of PMMA in inert atmosphere at various heating rates has been performed using thermogravimetry (TGA, 10÷50 K/min) and microscale combustion calorimetry (MCC, 15÷120 K/min, standard ASTM D7309-07) in the



temperature range 590÷700 K, and differential mass-spectrometric thermal analysis (DMSTA, 2÷150 K/s) at temperatures 630-780 K. A specimen 0.5÷2 mg was decomposed at a constant heating rate. In the present study, PMMA with molecular mass 350000 g/mol (Aldrich, CAS 9011-14-7) in the shape of spherical particles 30-300 microns in diameter or slabs 0.2-0.5 mm thick manufactured by hot pressing was investigated. The figure shows absolute values of the rate constants of PMMA decomposition in Arrhenius plots. Calculation was performed in the assumption of the first-order reaction in the range of the degree of

decomposition 0.1÷0.9. The values obtained by different methods in the temperature range 630÷700 K are in satisfactory agreement differing 1.3-2 times. Processing of MCC data using the Friedman method in the temperature range 590-710 K allowed us to determine the order of the reaction as equal to 1.2, the activation energy $E_a=178$ kJ/mol, $\lg(k_0, \text{s}^{-1})=12.6$. The results obtained can be used in the models of PMMA combustion.

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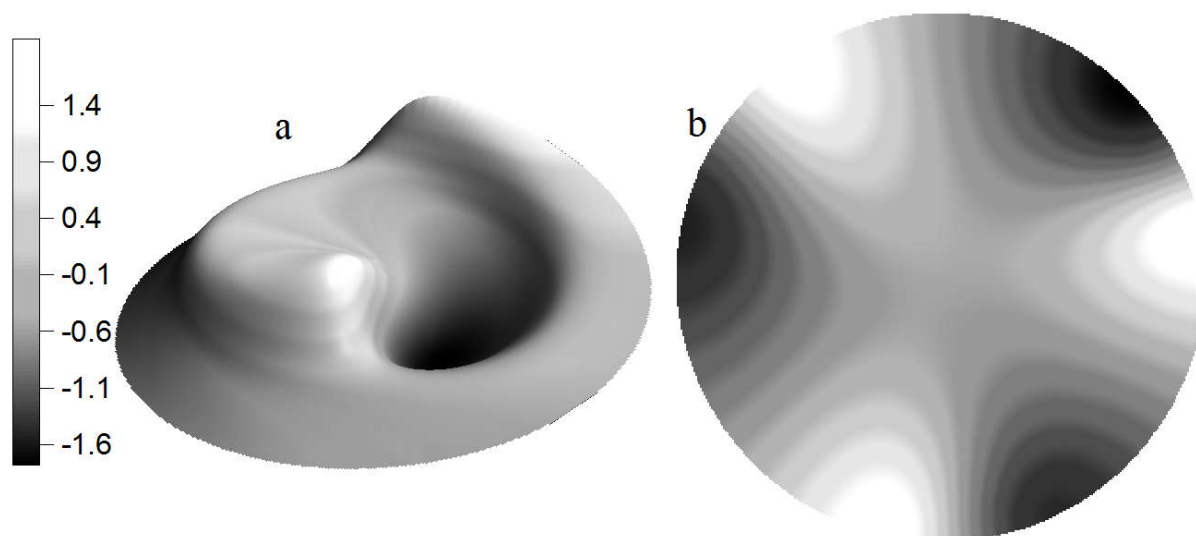
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Spinning regimes of gasless combustion*V.G. Prokof'ev¹, V.K. Smolyakov²*¹Tomsk State University, Tomsk, Russia²Department of Structural Macrokinetics, Tomsk Scientific Centre, Russia

Combustion gasless systems are accompanied by phase transitions: melting and eutectic components. The emergence and spreading of the melt in the pores leads to a change of the reaction surface, and in the case of large particles of fusible – additional (convective) heat transfer. The penetration of the melt in the starting mixture is shown as a "roughness" of the combustion front [1]. Modelling of the impact of the inert melting [2] and active [3] component of the mixture has been showed a significant effect of the phase transition to unsteady combustion modes, including a spin mode – spiral rotation of one or more hot spots. The simulation results are in qualitative agreement with the known experimental data [4]. It is investigated the influence of spreading and convective heat transfer filtering into the pores of the melt on the non-stationary modes of gasless combustion. The porous reactive mixture containing inert fusible component within multiphase media mechanics has been represented by three interpenetrating continua: a mixture of reactants, inert fusible component and the inert gas in the pores. In this paper we have considered capillary and thermocapillary flows. The results of direct three-dimensional calculations showing oscillatory and spinning propagation of the gasless combustion waves are presented. Symmetric and asymmetric combustion regimes can take place in the cylindrical sample, depending on the sample radius.

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Features of diffusion combustion of hydrogen in the round high-speed microjet*A.G. Shmakov^{1,2}, O.P. Korobeinichev¹, V.V. Kozlov^{2,3}, G.R. Grek³, Y.A. Litvinenko³*¹Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia²Novosibirsk State University, Novosibirsk, Russia³Khristianovich Institute of Theoretical and Applied Mechanics, Novosibirsk, Russia

Current combustion systems seek to use cleaner fuels and new technologies to reduce pollutant emissions. The increasing demand in energy brings hydrogen as a potential alternative for power generation fuel due to the large range of sources it may be produced from. A promising area of hydrogen energy is the use of microburners to produce energy. An important issue from the point of view of fire safety and from the point of view of optimizing the design of microburners is the study of the conditions and modes of stable combustion. The present experiments were performed to investigate the combustion of a round hydrogen microjet discharged into the air from thin-walled metal tubes with an inner diameter of 3 to 0.25 mm with a velocity of 100 to 1000 m/s, which corresponds to flow with high Reynolds numbers. The hydrogen flame structure was visualized using the schlieren technique. For nozzle diameters of 0.25, 0.5, 1, and 3 mm, the flame had a complex two-zone structure.

The first zone adjacent to the nozzle was a laminar diffusion flame of nearly spherical shape. The second zone was a turbulent flame of conical shape. The flame boundary between the first and second zones (so-called «bottleneck flame» region) had a characteristic restriction. When the hydrogen flow velocity exceeded a certain critical value, there was spatial separation between the first and second flame zones and combustion in the space between the two zones was absent. With further increase in the hydrogen flow velocity, combustion in the second zone ceased (turbulent flame blowout occurs), while combustion in the first flame zone continued until a critical velocity was reached. It was found that with increasing hydrogen jet velocity, the size of the first flame zone decreased monotonically to a critical value, after which flame extinction occurred. In a certain range of hydrogen flow velocity, combustion was possible only in the second zone (at ignition of hydrogen-air flow far away from nozzle), but this mode was unstable and a certain increase in the hydrogen flow velocity caused flame blowout. Thus, the laminar flame in the first zone generally stabilized the combustion of the hydrogen jet since it led to reignition in the second zone after flame blowout.

Using the microthermocouple technique, the dependence of the wall temperature of the nozzle (0.5 mm in diameter) on the rate of flow of hydrogen through it has been studied. The spatial distribution of temperature and concentration of H₂, O₂, H₂O, N₂ in the H₂ flame at a jet flow velocity of 500 m/s was also studied by microprobe sampling with subsequent mass spectrometric analysis of the combustion products composition. Comparison of the results of visualization of the flame by using the schlieren method and microprobe measurements showed satisfactory agreement.

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Non-stationary electric field effect on stability of a lifted diffusion gaseous hydrocarbon flame

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The relevance of the researches related to the study of hydrocarbon fuels combustion processes in a diffusion mode is undoubtedly because of the wide use of diffusion burners in technics, as well as the deficit of energy resources associated with their exhaustible and non-renewable.

From a practical point of view it's more favorably when combustion in open burner torch occurs steadily. Depending on the position of a zone of stable combustion diffusion flame can be stabilized both at the edge of the burner nozzle and at some height from it - lifted flame. The stability characteristics mean the conditions of detaching and attaching of the flame, its blowout, as well as liftoff height, amplitude and frequency of oscillations near the flame stabilization region.

The high concentration of charged particles (10^9 - 10^{12} cm⁻³) in gaseous hydrocarbon flames allows influencing on it by an external electric field (EF) in order to organize the most efficient and optimal combustion process.

The paper examines the impact of a weak non-stationary EF on a lifted diffusion flame of gaseous hydrocarbons (methane, commercial propane). Created the EF application scheme sets the rotation of the intensity vector (of constant magnitude) around an axis of a fuel jet, at Re numbers at the nozzle exit from 1100 to 3700.

A flame behavior was recorded by LaVision High Speed Star 3 and Imager intense CCD cameras. The interferential filters CH* (430 nm) and OH* (307 nm) are used together with Imager intense CCD to obtain spectrozonal images. Processing of obtained images is carried out using the DaVis program (LaVision).

Increasing of the fuel flow velocity leads to growth of the liftoff height of the diffusion flame over the nozzle edge. Subsequently it results in a flame blowout.

The EF application with the intensity vector rotation allows stabilizing lifted diffusion flame at the electrodes plane (or near it, Fig. 1), to decrease the amplitude of ignition points oscillation significantly, and intensify combustion in the torch stabilization region.

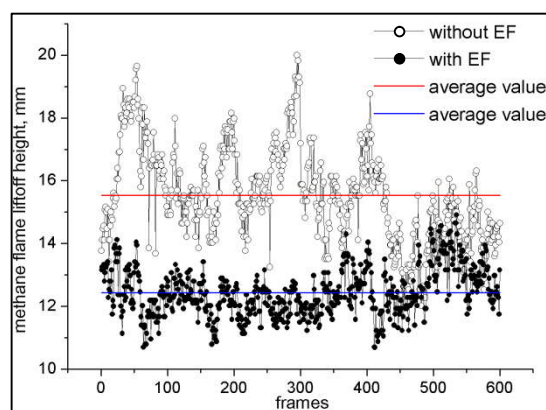


Fig.1 The dependence of CH₄ flame liftoff height on the time (t = 1.2 seconds).

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