Non-linear phenomena and dynamics of flame propagation

THEORETICAL ASPECTS AND IMPLEMENTATIONS

25 - 29 of September 2022

Borovoe (Burabay) National Nature Park Kazakhstan

Institute of Combustion Problems, Kazakhstan

Scientific committee:

- Z. Mansurov *(Institute of Combustion Problems, Kazakhstan)*
- V. Babushok *(KTC Consulting, USA)*
- U. Maas *(Karlsruhe Institute of Technology, Germany)*
- H. Im *(KAUST, Saudi Arabia)*
- V. Kourdioumov *(CIEMAT, Spain)*
- Z. Chen *(Peking University, China)*
- A. Kasimov *(Skoltech, Russia)*
- V. Azyazov *(Samara branch of the Lebedev Physical Institute, Russia)*
- N. Smirnov *(Moscow State University, Russia)*

Organizing committee:

- V. Bykov
- R. Schießl,
- S. Minaev,
- V. Gubernov,
- R. Fursenko

Conference secretary:

- A. Ponomareva

Local organising committee/organiser:

- Akad. Z. Mansurov
- Prof. A. Naimanova

Supported by

- Institute of Combustion Problems (Kazakhstan)
- Institute of Mathematics and Mathematical Modeling (Kazakhstan)
- Combustion Institute (Russian Section)
- Institute of Thermodynamics, Karlsruhe Institute of Technology (Germany)
- P.N. Lebedev Physical Institute (Russia)

Email: npdfp@bk.ru

WWW: http://www.npdfp.org/

Conference Schedule

25 September, Registration and Welcome Party
29 September, Farewell

26		27		28		29	
09:00	Z. Mansurov	**09:00**	D. Knyazkov	**09:00**	V. Azyazov	**10:00**	A. Ponomareva
09:30	V. Bykov	**09:30**	R. Schießl	**09:30**	A. Kirdyashkin	**10:20**	T. Soloveva
10:00	V. Gubernov	**10:00**	E. Fernández-Tarrazo	**10:00**	A. Maznoy	**10:40**	V. Mislavskii
						11:00	A. Moroshkina
10:30	*break*	**10:30**	*break*	**10:30**	*break*	**11:20**	*break*
11:00	N. Smirnov	**11:00**	I. Yakovlev	**11:00**	S. Sharipkhanov	**11:40**	Presentation of a new Journal on combustion
11:30	A. Beketaeyeva	**11:30**	E. Skryleva	**11:30**	D. Sabitova		
12:00	I. Yakovenko	**12:00**	E. Mikhalchenko	**12:00**	A. Zhaulybayev		
12:30	*lunch*	**12:30**	*lunch*	**12:30**	*banquet*	**12:00**	*roundtables*
							Roundtable discussions K.Shtym, V.Gubernov, N.Smirnov, S.Minaev and all participants who interested in scientific collaboration
14:00	S. Minaev	**14:00**	D. Fernandez-Galisteo				
14:30	V. Volodin	**14:30**	I. Kirillov				
15:00	V. Kurdyumov	**15:00**	R. Fursenko				
15:30	*break*	**15:30**	*break*			**13:00**	*lunch*
15:45	B. Lesbayev	**15:45**	M. Atamanov				
16:15	E. Dats	**16:15**	E. Sereshchenko				
16:45	L. Stamov	**16:45**	A. Kasimov				
		17:15	M. Kuznetsov				

Recent Achievements and Future Challenges in Nanoscience and Nanotechnology

Zulkhair Mansurov
Institute of Combustion Problems, Kazakhstan
ZMansurov@kaznu.edu.kz

Smalley in his famous work noted 10 urgent problems associated with the development of mankind. Among them are clean air, clean water, energy, health. Fundamental and applied research is carried out in these areas at the Institute of Combustion Problems. This talk summarizes the results of the research obtained during the last 5 years. The main topics cover

- Energy intensive nanocarbon materials;
- Bio-waste-derived few-layered graphene/$SrTiO_3$/PAN;
- Carbon fibers based on coal tar pitches by the method of electrospinning; Biologically soluble membranes;
- Synthesis of nanocarbon sorbents for different applications.

The listed above topics were carried out under the projects of the Ministry of Education and Science of the Republic of Kazakhstan. We should note a wide international cooperation, invitation of foreign scientists as co-advisers as well as holding International Symposium on Combustion and Plasma Chemistry and Carbon Materials and Nanoengineering. The ultimate goal will be outlined, the development of technology for producing nanomaterials will be presented and their practical use will be demonstrated.

Problem oriented model reduction of mechanisms of chemical kinetics: theory and applications

Viatcheslav Bykov
Karlsruhe Institute of Technology, Germany
viatcheslav.bykov@kit.edu

Modelling of chemical kinetics of combustion processes has become complicated in terms of a number of variables and physical parameters involved leading to extensive CPU time and memory storage demanding computations. In order to perform computations in a reasonable CPU time, reduced kinetic models are needed and have been rapidly developed in recent years. The current talk is devoted to this challenging problem.

An approach to cope with this problem will be suggested. It is based on detailed study of a real system dimension in a system thermo-chemical state space. Two powerful approaches - singular perturbations and invariant manifolds methods are combined to meet the goal. Several applications - detailed mechanisms represented by methyl methacrylate (MMA) combustion system and ammonia oxidation will be presented to illustrate the approach.

Investigation of diffusive-thermal oscillations of the burner stabilized CH_4-H_2-air flames

Vladimir Gubernov
P.N. Lebedev Physical Institute, Russia
gubernov@lpi.ru

In this talk we present our recent results on the investigation of the onset and dynamics of the diffusive-thermal instabilities of laminar flames of the binary fuel mixtures stabilized over a flat porous burner. The mixture of methane and hydrogen (hythane) is used as a fuel, which is considered today as a promising intermediate step in the transition to the hydrogen energy. The emergence and characteristics of the flame oscillations are analyzed via the observation of the OH* chemiluminescence. The structure of the combustion wave is also investigated by using the LIF method allowing us to determine the time and space resolved profiles of OH* radicals. The experimental results are also compared to the data of numerical calculations obtained within the models with detailed reaction mechanisms. It is shown that the addition of hydrogen to the fuel mixture extends the regions of the existence of flat combustion fronts and the onset of flame pulsations in the parameter space.

Author acknowledges the financial support provided within the Project RSF 21-13-00434.

Transient Modes of Gaseous Detonation Onset and Decay

Nickolay Smirnov, Valeriy Nikitin, Elena Mikhalchenko, Vylen Azatyan
Scientific Research Institute for System Analysis RAS, Russia
N.N.Smirnov@niisi.ru

Detonation is a complex phenomenon due to a three-dimensional wave structure with an inhomogeneous dynamic wave front. The inhomogeneous front contains pressure triple points moving along it. If the triple points move in the vicinity of a soot-covered detonation tube surface, shear forces from them mark a fishnet-like pattern on the inner walls of the tube. This pattern is known as a detonation cell. As the leading shock front propagates downstream, the triple points alternate. Simultaneously, the transverse waves oscillate perpendicular to the direction of propagation. Sizes of these detonation cells have been found to be one of the most important parameters in detonation research.

The chemical reaction of hydrogen with air is a classic example of a branching chain reaction. In chain reactions, radicals play an important role as intermediate products of elementary stages. Without the mediation of radicals, the final product is not ormed. The most mobile and active radical is atomic hydrogen H which plays an important role in nearly all combustion mechanisms involving hydrogen or its compounds. If its activity is reduced with a help of some chemical additive, the reaction will slow down. A slowdown in the reaction does not diminish its energy: the additive could be flammable itself. A decrease in the hydrogen atom activity can be achieved in many ways, one of which is using an unsaturated hydrocarbon; its reaction with H eliminates the double bond between the carbon atoms. The resulting alkane radical is much less active than atomic hydrogen. The amount of inhibitor could be several percent by volume.

The lecture presents the results of theoretical and experimental research of transient modes between deflagration and detonation. The problems of detonation onset caused by accelerating flame or reflected shock waves are discussed. The lecture considers the influence of a hydrocarbon inhibitor on the developed detonation in a hydrogen-air or syngas-air mixture, on the destruction of the detonation front and subsequent decay of detonation cells. This work was supported by the subsidy of the Ministry of Science and Education of Russian Federation on the topic: “Investigation and development of detonation combustion chambers being used in perspective aerospace propulsion systems” (No. 075-15-2021-1385).

Numerical analysis of vortex formation and particle dispersion in a supersonic compressible particle-laden mixing layer

Assel Beketaeyeva, Gulzana Ashirova
Al-Farabi Kazakh National University, Almaty, Kazakhstan
azimaras@mail.ru

The numerical simulations of a supersonic mixing layer of hydrogen-nitrogen flow (upper high-speed) and air (bottom low-speed) with solid particles are performed. The system of Navier-Stokes equations for the multispecies gas phase and the system of ordinary differential equations for solid particles (Eulerian-Lagrangian representation) are taken. By quasi 2D-DNS approach, solution of the Navier-Stokes equations with the third-order ENO scheme is carry out. The system of the ordinary differential equations for the particles is solved with the explicit second order Euler method.

Both dynamics of the unsteady vortex system formation and its effect on the solid parti-cles distribution in the mixing layer for two values of the convective Mach number (low 0.4 and high 0.8). Also influence of the various hydrogen and nitrogen mass fraction.

On the structure and dynamics of flame front in premixed lean hydrogen-air mixture in a channel with counterflow

Ivan Yakovenko
Joint Institute for High Temperatures, Russia
yakovenko.ivan@bk.ru

The research is devoted to the development of the flame front instability in lean hydrogen-air mixtures of various compositions. The combustion is considered inside an opened channel with inflow and outflow conditions. A numerical analysis of various stages of flame front evolution is carried out. In particular, the characteristics of the linear stage of instability growth are determined, dispersion curves are obtained, and the dependence of the critical wavelength on the mixture composition is found. General trends of the nonlinear development, following the linear stage, are demonstrated. Based on the obtained results, a diagram of the dependence of the flame propagation velocity on the combustion front area is obtained. It is shown that for lean hydrogen-air mixtures, the dependence of the propagation velocity on the front area has a nonlinear behavior for small values of the combustion front area.

Acknowledgments: The reported study was funded by the Grant of the President of the Russian Federation for State support of young Russian scientists [MK-1784.2022.1.1].

Nonlinear analysis of flame hydrodynamic instability at large gas expansion ratio

Sergey Minaev, Vladimir Gubernov
P.N. Lebedev Physical Institute, Russia
minaevss@yahoo.com

In the context of the large thermal-expansion approximation, we derive an equation describing flame front dynamics under conditions of Darrieus-Landau instability. We show that the second-order theory leads to system of two evolution equations for the flame front perturbations and for the potential of the unburned mixture flow. In the limiting case of long evolution, the system of equations can be reduced to one equation with respect to the additive variable that is the sum of the front perturbations and the flow potential. The equation with respect to the additive variable at large gas expansion coefficients has the form of the Sivashinsky equation obtained for the case of small gas expansion coefficients.

Authors acknowledge the financial support provided within the Project RSF 21-13-00434.

Growth Rate of Laminar Flame Disturbances: Experiment and Theory

Vladislav Volodin
Joint Institute for High Temperatures, Russia
vlad@ihed.ras.ru

The experimentally measured dependences of the perturbation amplitude of a laminar spherically expanding flame front are compared with those calculated using 6 theoretical models. Experiments and calculations were carried out in an initially quiescent hydrogen-air mixture with a hydrogen content from 10 to 60 vol.%. Shadow video recording was carried out with a frame rate of up to 9000 fps. The initial amplitude of the perturbation was taken as the value of the amplitude on the first frame of the video recording, where this perturbation was recorded. The calculated dependences of the amplitude differ significantly both quantitatively and qualitatively. Based on a comparison of experimental and theoretical data, conclusions were drawn about the best analytical model describing the observed flame front instability.

Lifted jet edge flames: symmetric and non-symmetric configurations

Vadim Kurdyumov, Carmen Jimenez
CIEMAT, Spain
vadim.k@ciemat.es

The purpose of this work is to demonstrate that there are different stable configurations of lifted edge flames for the same set of parameters. It is shown that when a fuel jet is injected surrounded by oxidizer streams of equal velocity, there are configurations with symmetric and non-symmetric flame structures with respect to the symmetry line of the problem. These two kinds of solutions are both stable and the actual realization of one or another solution depends on the initial conditions, in particular on the flame ignition parameters. It is shown that this multiple solution phenomenon takes place when the fuel Lewis number is less than unity. The influence of the Zel'dovich number and the injection flow rate is also investigated.

Synthesis of a graphene film on the current collectors of supercapacitors in a flame

B.T. Lesbayev, N.G. Prikhodko, M.K. Atamanov, A.N. Batkal, N.B. Rakhymzhan, Z.A. Mansurov

Institute of Combustion Problems, Kazakhstan

lesbayev@mail.ru

The paper presents the results of studies on the synthesis of graphenes in a coaxial flame of ethanol with benzene, acetylene, and propane on the surface of a nickel substrate. It has been established that by organizing coaxial combustion and changing the types of fuels, it is possible to achieve the conditions for obtaining graphenes with a given number of layers. In a coaxial flame of propane with ethanol, graphenes are synthesized containing from 10 layers or more; graphenes containing from 5 to 10 layers are synthesized in acetylene with ethanol; one- and two-layer graphenes were synthesized in a coaxial flame of benzene with ethanol. The resulting graphene-coated nickel substrates were used as current collectors in supercapacitor electrodes.

Numerical modeling of filtration gas combustion in a cylindrical radiation burner for contactless heating of materials

Evgeniy Dats, Sergey Minaev
Institute of Applied Mathematics FEB RAS, Russia
datsep@gmail.com

The filtration gas combustion in a porous cylindrical tube with axial injection of combustible mixture is numerically investigated. This configuration can be potentially used as new type of heater for the contactless heating of materials in industrial processes. The material under treatment is placed inside the cylindrical porous tube and is heating by radiative flux from the cylindrical tube wall. The simulation of the filtration gas combustion in porous burner was carried out within the framework of the two-temperature thermal-diffusion model. Conducted numerical modeling yields qualitative description of the effects of heat removal from the burner on the limits of a stable combustion regime. The data about range of the gas flow rates and the intensity of the heat losses on the burner's inner surface corresponding to the stable combustion were obtained.

Computer simulation of combustion initiation processes in a hybrid solid-fuel engine

Lyuben Stamov, Veronika Tyurenkova, Elena Mikhalchenko
Scientific Research Institute for System Analysis RAS, Russia
lyubens@mail.ru

The purpose of this work is numerical investigation of unsteady processes in the combustion chamber of the hybrid solid fuel rocket engine. Three-dimensional modeling of the interaction of a supersonic inlet oxidizer flow with gaseous 1,3-butadiene and methyl methacrylate fuels obtained during the thermally decomposition of the Hydroxyl-Terminated Polybutadiene and Polymethyl methacrylate solid fuels respectively was carried out. Good consistency between solutions, analytics and experiments was demonstrated. The combustion chambers with various geometry parameters of the solid fuel were considered. The distributions of physical parameters inside the combustion chamber were received. The asymmetry of the flame propagation and diffusion mode in the combustion chamber were received. Significant influence of the kinetics on the ignition of the evaporated fuel was found.

Russian Foundation for basic research is acknowledged for financial support (RFBR 20-07-00587).

Mass spectrometric and modeling study of low-stretched non-premixed methane/air flames stabilized in a planar channel

Denis A. Knyazkov, Roman V. Fursenko, Egor S. Odintsov, Andrey G. Shmakov, Vladimir V. Gubernov, Sergey S. Minaev

P.N. Lebedev Physical Institute, Russia

daknyazkov@gmail.com

The counterflow configuration is an ideal geometry for studies of non-premixed flame structure since provides a quasi-one-dimensional flame. However, most previous works were focused on the counterflow flames with relatively high stretch rates, as low-stretched flames in normal gravity conditions are difficult to stabilize due to natural convection. In this work, non-premixed counterflow methane/air flames confined in a planar micro channel (in a gap between quartz plates) were stabilized in a range of stretch rates 15-30 1/s due to the heat return from combustion products to unburned gases through the heat conducting plates. The flames were sampled by a quartz microprobe through the slit 7 mm long and 0.7 mm wide cut in the top plate. Spatial distributions of mole fractions of major flame species were measured in the flames and compared with the simulation using 1D-model and a detailed kinetic mechanism.

Authors acknowledge the financial support provided within the Project RSF 21-13-00434.

Chemical energy conversion in piston compressors

Robert Schießl
Karlsruhe Institute of Technology, Germany
robert.schiessl@kit.edu

Chemical energy conversion processes induced by compression of gases are prospective candidates for flexible energy technologies that help to close the gap between energy demand and supply. In this work, two prototypical such processes, namely the conversion of methane into hydrogen and unsaturated hydrocarbons, as well as dry reforming of CH_4/CO_2 mixtures into syngas (CO/H_2) are demonstrated by experiments in a Rapid Compression Expansion Machine (RCEM) and by numerical simulations involving detailed chemical kinetics. The dynamics of the conversion in a compression-expansion process is dominated by the strong endothermicity and the high activation energies of the desired reactions. The latter demand high temperatures to allow the reactions to commence; once reaction sets in, the former tends to inhibit further reaction progress by a negative feedback loop. It is shown how careful shaping of the compression process can help to gain good conversion and yield.

On the calculation of Minimum Ignition Energy for different fuel-air blends

Eduardo Fernández-Tarrazo, Mario Sánchez-Sanz and Raquel Gómez-Miguel
University Charles III of Madrid, Spain
eafernan@ing.uc3m.es

The Minimum Ignition Energy (MIE) of any fuel in air is a fundamental parameter to ensure safe operation that is relevant from a fundamental and practical point of view. This parameter is specially important in applications in which a small deposition of heat, such a spark or hot spot, might ignite a flammable mixture formed as a consequence of an uncontrolled fuel leak, producing a self-propagating flame front. The determination of the basic necessary parameters for successful ignition (in particular MIE) is therefore an important task to develop reliable safety protocols.

We present numerical analysis of the minimum ignition energy of two fuels in air: hydrogen-ammonia blends and methanol. After the pioneering works of Frendi and Sibulkin (1990) and Maas and Warnatz (1988) and the generic theoretical work developed, among others, by Vázquez-Espí (2001), Kurdyumov (2001, 2003, 2004), a useful methodology was developed. This methodology has been used to determine the MIE of fuels

On the weakly nonlinear analysis of detonations and deflagrations

Aslan Kasimov, Andrei Goldin, and Tatiana Medvedeva
Skolkovo Institute of Science and Technology, Russia
aslankasimov@gmail.com

In this work we investigate the dynamics of gaseous detonation propagating under periodic external conditions. It is well known that gaseous detonations are typically unsteady exhibiting periodic or aperiodic oscillations of propagation velocity in one dimension and cellular structures in multiple dimensions. A question arises as to how such dynamics is affected by the presence of periodic external influences. By analogy with periodically forced nonlinear oscillators, one expects that the answer to the question may involve a number of interesting and nontrivial phenomena. In particular, in the case of self-sustained nonlinear oscillations under periodic forcing, there may occur the phenomenon of synchronization [M. Rosenblum, 2003]. Since a detonation wave is self-sustained and behaves in many ways similar to a nonlinear oscillator, then its propagation in a periodic medium may be expected to result in synchronization. And this is indeed what we have found as reported in our recent publications [A.R. Kasimov, 2020; A.R. Kasimov, 2021; A.Y. Goldin, 2022]. In this talk, we present the main results in these papers as well as discuss some new ones concerning propagation of two-dimensional detonations in channels with either periodic mixture non-uniformities or channel wall properties, such as frictional losses. The novel phenomena and features observed are those of resonance, mode locking, synchronization, Arnold tongues and devil’s staircases.

Numerical modeling of unstable hydrocarbon displacement from a porous reservoir in the presence of in-situ combustion

Evgeniya Skryleva
Scientific Research Institute for System Analysis RAS, Russia
jennyne@yandex.ru

The work is focused on unstable displacement of a viscous liquid from a porous medium in presence of chemical interactions between phases. The process of hydrocarbon displacement from a porous medium in the presence of in-situ combustion is considered. With the development of Suffman-Taylor instability, the initially flat interface is perturbed, and the area of contact between the phases increases. This phenomenon must be taken into account when modeling the displacement process with chemical reactions between phases, since the extension of the contact line between the reacting phases leads to an increase in the rate of the chemical reaction. The paper describes mathematical models for a multiscale description of the combustion process in a porous medium. The results of numerical simulation based on the mathematical models developed by the authors are presented.

3D simulation of turbulent reacting flows in rotating detonation engine

Elena Mikhalchenko, Valeriy Nikitin, Lyuben Stamov
Scientific Research Institute for System Analysis RAS, Russia
MikhalchenkoLena@yandex.ru

A rotation detonation engine combustible chamber is modeled numerically. When modeling the hydrogen-oxygen mixture chemical kinetics, six mechanisms were used: Maas–Pope–Warnatz (19 react.), Hong (20 react.), Williams (22 react.), Gri-Mech 3.0 (20 react.), Lie–Zhong–Kazakov–Dryer (18 react.), and the author's kinetic mechanism (20 reactions). The influence of the additional oxygen supply from the side injection system on the traction characteristics was studied. Different geometry of the chamber was tested so that the length of the internal body was varied extending beyond the exit nozzle of the chamber. Influence of internal rings inside the annular combustion channel was tested to examine stability of the detonation wave.

This work was supported by the subsidy of the Ministry of Science and Education of Russian Federation on the topic: “Investigation and development of detonation combustion chambers being used in perspective aerospace propulsion systems” (No. 075-15-2021-1385).

Influence of momentum loss on hydrodynamically unstable premixed flames

D. Fernández-Galisteo, A. Dejoan, J. Melguizo-Gavilanes, and V.N. Kyrdyumov
CIEMAT, Spain
d.galisteo@ciemat.es

The propagation of an isobaric premixed flame into a quiescent gas mixture contained between two adiabatic parallel plates separated by a small distance h is investigated numerically in three dimensions. The mixture is assumed to be lean in fuel and the model employs a single-step reaction, constant heat capacity, and unity fuel Lewis number. Transport properties are considered to be temperature-dependent or constant, which allows us to decouple two different instability mechanisms of hydrodynamic nature: (i) Darrieus-Landau and (ii) Saffman-Taylor. The overall propagation rate is analyzed as a function of the dimensionless parameter $a=h/\delta f$, where δf is the thickness of the planar flame. Results show that, as the distance between the plates decreases, loss of momentum enhances the hydrodynamic instability in comparison with that of a freely propagating flame, and that viscosity contrast brings about an additional destabilizing mechanism.

Flame-Ball-to-Deflagration Transition in Ultra-Lean Hydrogen-Air Mixtures: Mechanism and ”Magic” Numbers

Igor A. Kirillov
Russian Research Centre Kurchatov Institute, Russia
kirillov.igor@gmail.com

Two specific features of the ultra-lean hydrogen-air combustion are well known – 1) its incompleteness (von Humboldt & Gay-Lussac, 1805) and associated under-adiabaticity (Ural&Zalosh, 1985) and 2) the difference in the concentration limits for the ascending and descending flames in vertical tubes (Coward, 1914).

Report is focused on a third (currently under-explored) specific feature, which was named “Flame Ball-to-Deflagration-Transition” (FBDT) (Kirillov, 2018).

Goals of this report are to describe – 1) separate phenomenological features of the FBDT, observed in the prior art research works under the Earth gravity and microgravity conditions, 2) mechanism of the FBDT during gradual changes of the initial hydrogen concentration in initial mixture, revealed in recent experiments in horizontal Hele-Shaw cell (Denisenko et al., 2018-2022) for 2dim and in vertical tubes (Anikin et al. 2022) for 3dim cases, 3) open fundamental questions for the further studies of the FBDT phenomena in the ultra-lean hydrogen-air gas mixtures.

Selection of global reaction mechanisms rate constants by optimization approach

Aleksander Zakharov, Roman Fursenko
Khristianovich Institute of Theoretical and Applied Mechanics SB RAS, Russia
roman.fursenko@gmail.com

In the paper, an optimization approach to determining global chemical reaction rate constants is proposed. This method allows to select reaction rate parameters (i.e. activation energy, preexponential factor, etc.) on the basis of experimental data or simulations with detailed reaction mechanisms. Computer program implementing proposed method was developed and the features of the application and operation of the optimization approach were investigated. Examples of one, two and four step mechanisms optimization with respect to laminar burning velocity and concentration profiles in counterflow diffusion flame are discussed. Studies of optimization problem solutions uniqueness demonstrate that for considered global mechanisms the minimum value of objective function is reached in some subdomain of the parametric space. Hence, any values of rate parameters from this subdomain results in almost the same deviations of chosen flame characteristic from its reference value.

Preparation and kinetic analysis of thermal decomposition of a copper based coordination complex

A. Akhinzhanova, S. Sultahan, Z. Beksultan, E. Maral, M. Atamanov
Institute of Combustion Problems (Kazakhstan)
mk.atamanov@gmail.com

Coordination complexes based on metal cations and oxidizing anion ligands have been considered as candidates for energetic composites. These composites are important in the area of energy storage, they are environmentally friendly, have high-energy and power density for thermal management. As a most widely investigated complex, $Cu(NH_3)_4(NO_3)_2$ (tetraamminecopper(II) nitrate (TACN)), has high energy density, low decomposition temperature and considered as relatively cheap.

The carbon nanomaterials (CNM) effect strongly on the thermal decomposition TACN, but the influence is still not investigated. In this study the graphene oxide (GO) sheets were found to have strong catalytic effects on thermal decomposition. The TACN complexes with or without GO as a doping agent were successfully synthesized and investigated. It was shown that these nanocomposite materials are uniformly deposited on the surface of CuC. The decomposition kinetics and mechanisms of GO on TACN have been investigated.

Numerical investigation of the premixed and diffusion flames dynamic under low Lewis number conditions

Evgeniy Sereshchenko, Roman Fursenko, Sergey Minaev, Vladimir Gubernov
P.N. Lebedev Physical Institute, Russia
s_evgeniy@yahoo.com

Recently, there are a trend towards a transition to the ecofriendly technologies, more sparing to the environment. Examples of such promising technologies are the methods of lean hydrocarbon fuels burning and the transition to hydrogen power. In this regard, the study of the combustion of lean gas mixtures with low Lewis numbers is a relevant task. This work is devoted to a numerical study of the propagation dynamics of the combustion front of a premixed gas mixture in straight channels, as well as a spherical diffusion flame. In both cases, mixtures with low Lewis numbers are considered. Numerical results shown that the combustion wave can propagate both as a continuous flat front and in the form of a cellular flame, as well as in the form of a sporadic flame consisting of sets of individual flame spots. The regions of existence of each of the flame propagation modes are determined depending on the fuel flow rate and its composition.

The work was supported by the Russian Science Foundation (project no. 21-13-00434). The numerical simulations were carried out using the supercomputer facilities of the Equipment Sharing Center "Mechanics" of ITAM SB RAS.

Flame stabilization in two-layer porous burner: pore-scale simulation

Igor Yakovlev
Tomsk Scientific Center SB RAS, Russia
yakovlev-i-a@yandex.ru

Local flame stabilization phenomenon has been studied in the synthetic two-dimensional model porous burned using the pore-scale approach. The media consisted of two regions: upstream fine-pored section and downstream coarse-pored section. It has been shown that the flame front anchors the interface between sections in wide range of the flow rates. In this case the effect of flame stretching in the region of velocity gradient plays an important role. The radiative heat losses from the external surface influences the stable flame limits – the larger downstream region thickness, the larger flow velocities are allowed without the flame flashback.

Author acknowledges the financial support provided within the Project RSF 21-79-10445.

Unusual flame behavior in a thin layer geometry transition from a fractal shape flame to a finger flame

Mike Kuznetsov

Institute for Nuclear and Energy Technologies of the Karlsruhe Institute of Technology, Russia

mike.kuznetsov@kit.edu

For the first time, unusual flame behavior in a thin layer geometry was found approaching the flame extinction. Due to heat losses and local extinction, the flame character at Pe < 20 changes from a fractal shape typical for Darrieus-Landau instability to finger flames typical for filtering and smoldering combustion. There is a branching of the fingers with the formation of a tree structure at 10 < Pe < 15. As long as the gap is thinner or hydrogen concentration is lower, the branches degrade to multiple or single fingers at 5< Pe < 10. They behave more stable being a double-head or they behave very chaotic being a one-head in nature. The characteristic velocity of two-heads finger flames is almost two times higher than the one-head finger flame of the same reactivity.

The analysis of flame dynamics in a narrow gap shows that turbulence does not play a role in the fragmentation of the flame. The heat transfer to the wall might be the governing mechanism of flame fragmentation.

Kinetics of oxygen allotropes

Valeriy Azyazov, Andrey Pershin, Aleksei Torbin, Ivan Medvedkov, Galiya Galimova, Anna Ghildina Alexander Mebel
Samara Branch of P.N. Lebedev Physical Institute, Russia
azyazov@rambler.ru

Radiation, energy exchange and chemical processes involving species composed of oxygen atoms O_n(n=1 - 4) including its own O, molecular oxygen O_2, ozone O_3 and collisional complex O4 occur in various natural objects and technical devices. Recently, there has been an increased interest in studies of processes involving excited oxygen O_n* due to their importance in understanding the physics and chemistry of the Earth's atmosphere, oxygen-containing plasma, oxygen–iodine laser, and combustion of fuel-air mixtures. The presence of even small fractions of O_n* in the fuel-air mixture makes it possible to accelerate the production rate of radicals and thereby significantly reduce the induction time, as well as the ignition temperature.

The presentation will overview results of measurements of kinetic constants for the radiation, energy exchange and chemical processes involving O_n. In addition, the report will present the results of ab initio calculations of potential energy surfaces in conjunction with the RRKM-Master Equation theoretical approach that was employed to evaluate temperature- and pressure-dependent total and product specific rate constants and product branching ratios for oxidation of polycyclic aromatic hydrocarbons (PAH) by oxygen species.

Features of the synthesis of Ni-Al alloys when burning a fluidized powder environment

Alexander Kirdyashkin
Tomsk Scientific Center SB RAS, Russia
kirdyashkin_a@mail.ru

Using the methods of video shooting, thermocouple and pyrometric measurements, as well as hardening reaction, studies of temperature and structural-phase dynamics of the synthesis of Ni-Al alloys while burning the powder mixture Ni+20wt.%Al with a different amount of $CaCO_3$ additive as a fluidizer of the system. An analysis of the mechanism of structural chemical transformations of the system was carried out at different stages of reaction development.

The research was funded by Russian Science Foundation (project № 21-79-10445).

Predicting Oxidation-Limited Lifetime of Ni-Al-Cr Porous Radiant Burners Made by Combustion Synthesis

Anatoly Maznoy
Tomsk Scientific Center SB RAS, Russia
maznoy_a@mail.ru

Ni-Al intermetallic alloys have superior high-temperature properties such as excellent oxidation resistance and high yield strength, making them particularly attractive as materials for the fabrication of porous components of energy conversion and combustion devices. In this study, the cyclic oxidation resistance of highly permeable Ni-Al-Cr alloys has been investigated. The porous alloys with a structure of irregular porous scaffold comprised of welded mm-sized spheroidal strut elements forming a net of mm-sized interconnected pore channels (porosity of 0.55–0.60, specific surface area below 10−3 m^2/g) were manufactured by the combustion synthesis method using μm-sized Ni, Al, and Cr powders of commercial purity as starting reagents. The surface area of alloys exposed to oxidation was calculated with an accuracy of 6% using quantitative 2D stereological method. The cyclic oxidation tests were conducted in dry artificial air at 1150 ℃ for 100 h. The Ni-Al-Cr alloys, compared to Ni-Al alloys, exhibited a twofold increased oxidation resistance because of decreased scale spallation. The porous alloys were also tested in a combustion environment. The lifetime prediction showed that Ni-Al-Cr radiant burners could be used for > 10000 h at a temperature of 1000 ℃, which makes them relevant for application in domestic combustion appliances such as water heating boilers.

The research was funded by Russian Science Foundation (project № 21-79-10445).

On the issues of the use of carbon-containing materials in filter ventilation installations of civil defense protective structures

S.D. Sharipkhanov, A.A. Zhaulybayev, Yu.V. Ilyin,
K.K. Kudaibergenov, Z.A. Mansurov
Academy named by M. Gabdullin MES Republic of Kazakhstan
shsyrym@rambler.ru

Copper oxide (NP) nanoparticles deposited on a carbonized sorbents were synthesized by a simple method to increase the adsorption capacity of carbon dioxide (CO_2). The structural and chemical properties of the carbonized sorbents (CS) were characterized by optical digital microscopy, SEM, IR and BET analyses. The results of the SEM and optical microscopy studies strongly indicate that carbonization is a suitable method for improving the porous structure of the sorbents particles compared to the virgin samples.

The CO_2 adsorption properties of the carbonized sorbents modified by CuO nanoparticles were investigated by gas chromatography analysis. Results showed that the CO_2 removal efficiency of carbonized apricot stone (CAS) and rice husk (CRH) were 98, and 91%, respectively. This research provides the basis for the development of a new environmental material with optimal characteristics, providing efficient sorption of CO_2 from gas mixture.

Flame spread reduction on wood surface with paint-and-varnish coatings

D.S. Sabitova
Academy named by M. Gabdullin MES Republic of Kazakhstan
danasabitova@mail.ru

According to the analysis studies result of thermo-oxidative process of wood decomposition with various flame retardants there has been effective reduce of the rate and oxidation heat of the coal layer. Thermal analysis has established, which determines the effectiveness of flame retardants for wooden construction.

Modern ways to protect the personnel of companies from intense thermal radiation

A.A. Zhaulybayev
Academy named by M. Gabdullin MES Republic of Kazakhstan
zhaulybaev.aa@emer.kz

Currently, many industrial enterprises use fire- and explosion-hazardous technological processes in production, including tanks with liquefied carbon gas (LPG). The presence of a large amount of LPG at the facility creates a danger for the personnel of enterprises in case of emergency depressurization of the tank, the formation of a gas–air mixture (DHW) with oxygen in the air, and in the presence of ignition sources - to an explosion or combustion of a DHW cloud, the formation of a fireball.

Determination of characteristic parameters and activation energy of a solid fuel thermal decomposition using thermogravimetry data

Alina Ponomareva, Vera Sitnikova, Sergey Minaev
ITMO university, Russia
alina.a.ponomareva@gmail.com

The thermal decomposition of coals and biomass is accompanied by degradation and polycondensation processes, which determine the amount and release rate of gaseous and resinous substances. Moreover, the ratio of these processes mostly depends on the heating rate and temperature as well as on the petrographic composition and rank of metamorphism. The study of pyrolysis at different heating rates and of oxygen content influence on decomposition such materials can help to find the common tendency of its combustion in dependence on chemical structures. As the fuel substance is heated, endo- and exothermic effects occur, whose duration and position on the temperature scale depend on conditions. The lack of information about kinetic and energy parameters of thermal decomposition and oxidation hinders developing new approaches of solid fuel processing, especially in a gaseous environment of variable composition.

The work was supported by the Ministry of Science and Higher Education of the Russian Federation (Project No. 075-15-2020-806).

Influence of the combustion process on formation of the axial region in the vortex-type cyclone primary furnace

Tatiana Soloveva, Konstantin Shtym
Far Eastern Federal University, Russia
mtasta@mail.ru

A gas-oil vortex cyclone primary furnace (VCPF) is a preliminary combustion chamber (CC) with a combined supply of air and gas, which enables efficient mixing of fuel and air at great thermal stresses and high flow turbulence.

The results of pneumometric tests in the VCPF CC with the power capacity of 65 MW have shown that burning of gas in the VCPF slightly increases the axial velocity of the swirling flow in the quasipotential zone. When the temperature of the flow rises, the axial velocity also rises, as the flow moves to the exit from the combustion chamber toward the constriction. As compared to the values of the cold flow, combustion contributes to the increase in the axial velocity of the flow in the quasi-solid zone by 2 to 10 times.

As a result of the combustion process, the axial velocity is comparable to the tangential velocity and even exceeds it by values in paraxial and axial regions. When performing design calculations of the vortex cyclone primary furnace, the conditions of non-isothermicity should be kept in mind.

Quenching rate constants of the nitrogen molecule

Vladimir Mislavskii, Vladimir Gubernov
P.N. Lebedev Physical Institute, Russia
vmislavskii@gmail.com

The emission spectroscopy methods are used to measure the lifetime of the excited states of nitrogen molecules and ions corresponding to the second positive and first negative systems of its radiation. The measurements are carried out in mixtures of molecular nitrogen with hydrocarbons in the afterglow of a repetitive high-voltage nanosecond discharge. The method used was verified by measuring the lifetime of the excited states of nitrogen molecules and ions in pure nitrogen and in a mixture with oxygen. After processing the data and obtaining the values of the quenching rate constants, the results were compared with those obtained by other authors [Pancheshnyi S.V., 2000; Valk F., 2010]. In this work, the time of the exponential fall of the radiation intensity is measured at various pressures of the studied gas mixtures with a known proportion of the incoming components, which makes it possible to vary the values of $[N_2]$. We find the quenching constants and the radiative lifetime of the vibrational levels $N_2(C^3\Pi_u, v' = 0, 1, 2, 3 \rightarrow B^3\Pi_g, v)$ and $N_2^+(B^2\Sigma_u^+, v' = 0 \rightarrow X_2\Sigma_g^+, v)$. The quenching constants of excited states of nitrogen molecules in mixtures containing hydrocarbons, in particular ethane and propane, have been measured. The second positive $N_2(C^3\Pi_u, v' = 0,1,2,3 \rightarrow B^3\Pi_g, v)$ and the first negative $N_2^+(B^2\Sigma_u^+, v' = 0 \rightarrow X_2\Sigma_g^+, v)$ nitrogen emission systems were studied.

Authors acknowledge the financial support provided within the Project RSF 21-13-00434.

Measurement of activation energy of combustion of methane-air mixture using the thin-fiber pyrometry method

Anastasia D. Moroshkina, Vladimir V. Gubernov, Vladimir V. Mislavskii
P.N. Lebedev Physical Institute, Russia
moroshkina.ad@phystech.edu

The latest results of the experimental measurement of activation energy of methane-air mixture are presented. The thin-fiber pyrometry method is used. The experimental setup includes the flat porous burner which position can be regulated vertically, the gas mixture flowing from the burner, thin filament made of silicon carbide (SiC) to measure the gas temperature, and the thermal imager OPTRIS PI. The flow rate of the gas can be adjusted by Bronkhost Elflow controllers. By measuring the gas temperature dependence on the height above the burner the maximum flame temperature is determined. According to theoretical calculations changing the mass flow of the gas and measuring the maximum temperature it is possible to find the overall activation energy for certain methane concentration in the mixture. This experiment was carried out for various methane-air mixtures with different ϕ. The results are compared with the numerical calculation that uses the GRI 3.0 method.

Authors acknowledge the financial support provided within the Project RSF 21-13-00434.