Non-linear phenomena and dynamics of flame propagation

THEORETICAL ASPECTS AND IMPLEMENTATIONS

23 - 27 of September 2024

Burabay (Borovoe) National Nature Park Kazakhstan

Institute of Combustion Problems, Kazakhstan

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Conference Schedule

23 September, Registration (15:00) and Welcome Party (16:00)
26 September, Excursion and Banquet (14:00)
27 September, Farewell (16:00)

24.09.24	25.09.24	26.09.24	27.09.24
09:00 V. Bykov Z. Mansurov E. Fernández-Tarrazo *Chair: V. Gubernov*	09:00 S. Minaev V. Golub A. Kasimov *Chair: R. Schießl*	09:00 M. Atamanov A. Moroshkina G. Ashirova *Chair: D. Fernandez-Galisteo*	09:00 *Online presentations* *Presentation of the special issue of Journal*
10:30 *break*	*break*	*break*	*break*
11:00 U. Maas D. Goussis V. Gubernov *Chair: V. Bykov*	11:00 A. Dmitriev V. Volodin P. Shrotriya (online) *Chair: A. Kasimov*	11:00 E. Dats I. Aigerim L. Krikunova A. Kuznetsova *Chair: E. Fernández-Tarrazo*	11:00 *Round table discussion* *(all participants who interested in scientific collaboration)*
12:30 *lunch*	*lunch*	*lunch*	*lunch*
14:00 A. Gavrikov E. Sereshchenko A. Lopato *Chair: U. Maas*	14:00 D. Fernandez-Galisteo A. Ponomareva V. Pavlenko *Chair: S. Minaev*	*Excursion*	
15:30 *break*	*break*		
16:00 R. Schießl D. Rodríguez-Gutiérrez R. Fursenko *Chair: D. Goussis*	16:00 E. Fernández-Tarrazo S. Mokrin B. Lesbayev *Chair: V. Golub*	*Banquet*	*Farewell*

Tabulation chemistry: applications, implementation problems and perspectives

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Modelling of chemical kinetics for computation of combustion processes has become complicated in terms of a number of variables and physical parameters involved. This fact leads to demanding computations requiring extensive CPU time and memory storage. In order to perform computations of complex processes 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. Question - how to perform model reduction bringing “one-step” (several steps) and detailed models of chemical kinetics together for a specific application and a parameter range is answered in the proposed talk.

A tabulation chemistry approach to cope with this problem is revised and outlined. Principle key assumptions, technical and theoretical problems, i.e., what is tabulated, how initial and boundary conditions are taken into account, parameter dependence etc. are sorted out and generic solutions for those problems are outlined. Several applications - a detailed mechanism of methyl-methacrylate (MMA) in the ignition problem as well as flame propagation in blended complex combustion systems containing several fuels (i.e. hydrogen-methane) are considered for illustration.

Autoignition Delay Times of H_2-NH_3 mixtures

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Molecular hydrogen (H_2) is agreed upon as a key energy carrier to reach Net Zero greenhouse emission goals in 2050. The deployment of technology for hydrogen production tripled from 2020 to 2021, and the global demand reached about 2.5% of the total energy consumption in 2021. In particular, applications powered with hydrogen or fuels containing a non-negligible content of H_2 will further push the demand for hydrogen on a large scale.

Storage, transport, and use of hydrogen are plagued by technological problems that can be partially alleviated by the use of ammonia (NH_3) as a complement to hydrogen. For instance, because of hydrogen's low density, it has to be stored either at high pressures or at cryogenic temperatures to provide high energy density in the stored fuel. Interestingly, ammonia at ambient conditions has a higher content of H atoms per volume than molecular hydrogen. NH_3 can be stored more easily and safely than hydrogen gas at high pressure or low temperature.

Nevertheless, pure ammonia has low flammability and ignitability and NOx emissions might be an issue when used as a fuel. These difficulties can be mitigated by cracking the ammonia molecule prior to combustion to form a hydrogen-ammonia blend. H_2/NH_3 blends offer even more advantageous features over pure hydrogen as a fuel:

Hydrogen burns much faster than the commonly used hydrocarbon fuels. This can make the use of existing combustion hardware (which is designed for the smaller combustion speed of conventional fuels) with the fast-burning hydrogen difficult. However, if slow-burning ammonia is added to hydrogen, the resulting mixture might display similar flame speeds like the conventional fuels. Similarly, H_2/NH_3 mixtures could be tailored to match ignition delay times of conventional fuels.

While typical hydrocarbons and pure hydrogen are well characterized in terms of flame propagation velocity, extinction strain rate, and ignition delay time, there is a paucity of data on hydrogen-ammonia blends in the literature. To cover that gap, in this work, we aim to experimentally characterize autoignition times in H_2-NH_3 mixtures and check the performance of recently developed combustion mechanisms in predicting these ignition delay times.

Shock Tubes (ST) and Rapid Compression Machines (RCM) are commonly used instruments for ignition delay time measurements. STs are well suited to measure very short autoignition times (typically, not far above the millisecond second scale), while RCMs are a better option when ignition delay times are longer, on the order of a few to a few hundred milliseconds. The low reactivity of NH_3 suggests that RCMs are better suited to produce self-consistent sets of data.

The RCM facility at KIT has been used to measure ignition delay times in H_2/NH_3 mixtures under different initial conditions. The whole range of mixtures, from pure ammonia to pure hydrogen, has been considered under lean, stoichiometric and rich conditions. Different conditions for pressure p_0 and temperature T_0 after compression are considered, in the range $950K < T_0 < 1100K$ and $10 \text{ bar} < p_0 < 15$ bar.

Advances in Nanoscience and Nanotechnology

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Renowned scholar R. Smalley[1] outlined ten paramount challenges confronting humanity, including the preservation of clean air, water, sustainable energy, and public health. The Institute of Combustion Problems has been actively engaged in addressing these challenges through rigorous fundamental and applied research.

- *Producing carbon fibers from coal tar pitches using electrospinning technique. Coal tar pitches, derived from coal tar distillation, are complex mixtures rich in polycyclic aromatic hydrocarbons (PAHs).* With high carbon content, they serve as ideal precursors for carbon fiber production. Through controlled heating, these pitches undergo carbonization, resulting in highly ordered carbon structures akin to graphite. Their properties profoundly influence resulting carbon fibers' characteristics, including strength and conductivity. Advanced modification techniques tailor pitches for optimized performance in electrospinning processes, facilitating high-quality carbon fiber production [2].
- *Synthesis of nanocarbon sorbents for water purification from heavy metal ions*. The synthesis of nanocarbon sorbents for water purification from heavy metal ions involves innovative approaches in material science and environmental engineering. Nanocarbon materials, such as carbon nanotubes, graphene, and activated carbon, exhibit exceptional adsorption properties due to their high surface area (~3000 m^2/g), porosity, and surface chemistry. These sorbents effectively capture heavy metal ions from water sources, mitigating environmental pollution and providing a sustainable solution for water treatment challenges [3-4].
- *Synthesis of composites based on semiconductor metal oxides and carbon nanostructures for the detection of toxic gases and development of activated carbon for gas masks.* These composites leverage the unique properties of metal oxide nanoparticles and carbon nanostructures such as carbon nanotubes or graphene to detect toxic gases through interactions with gas molecules on their surfaces. This opens up promising avenues for gas detection technologies [5]. Additionally, research is underway for synthesizing activated carbon from plant waste for use in gas masks aimed at protecting against toxic gases [6]. These developments offer significant advantages in military applications, enabling effective detection and protection from hazardous chemical substances.
- *Gas generator compositions based on activated carbon from a gas mask for destruction of rocks.* Gas generator compositions utilizing activated carbon from gas

masks offer a novel approach to rock destruction. Activated carbon, known for its high porosity and adsorption properties, serves as a key component in these compositions. Through controlled combustion or chemical reactions, gases generated from the activated carbon interact with rocks, facilitating their disintegration. This innovative method presents a promising alternative for rock demolition in various applications, including mining and construction [7].

This thesis is intended to present the latest developments of the Institute of Combustion Problems in the fields of combustion and producing nanomaterials for various applications.

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Sensitivity of manifold-based reduced kinetic models with respect to model parameters and rate constants

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Reduced kinetic models are an important tool for reducing the computational effort in simulations of reacting flows. Manifold-based reduction methods have proven to allow a very accurate representation of the chemical kinetics and, in some cases, their coupling with molecular transport. However, such manifold methods are sensitive both to the underlying detailed chemistry and transport models, as well as to the assumptions used in the model reduction. In this study we investigate these sensitivities to better understand the impact on simulation accuracy and efficiency.

For manifold methods based on “intrinsic low-dimensional manifolds (ILDM)”, “global quasi-linearization (GQL)”, and “reaction-diffusion manifolds (REDIM)”, the sensitivities of the manifold-based simplified chemistry with respect to elementary reaction rate coefficients are investigated. In this case it is shown that the reduced model reproduces sensitivities very similar to those of the detailed mechanisms, which confirms that the reduced model captures the essential chemical kinetics effectively. This validation/investigation is crucial as it shows that despite of the simplification of chemical kinetics, the reduced chemical model keeps the accuracy required for reliable predictions of reacting flow behaviors.

For the REDIM-method we discuss in addition the sensitivity equations and their solution with respect to the model parameters. These model parameters are the estimate for the gradient field and the prescribed boundary conditions. It is shown that the sensitivity with respect to the model parameters decreases significantly as the dimension of the reduced model increases. This implied that higher-dimensional REDIM reduced systems are less sensitive to inaccuracies in model parameter estimation, improving the robustness of the REDIM method in practical application.

A hydrogen/air combustion system as well as the syngas/air system are used as illustrative examples. Moreover, it will be briefly discussed how the proposed sensitivity analysis can also be used in other manifold based methods.

Algorithmic determination of the propagation mechanism of premixed laminar flames

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The eloquent asymptotics introduced in the late 80s by Peters and Williams and their groups, advanced significantly our knowledge on the inner-structure of the flame and of the propagation mechanism of the flame front. Considering hydrocarbon fuels, these works highlighted the significance of the upstream diffusion of H and heat in generating chemical activity far from the flame front and in enacting convective motion. This type of paper-and-pencil type of analysis was relying heavily on the intuition and experience of investigator, since he had to produce a small reduced model for chemical kinetics, estimate accurately the length scales involved and provide the appropriate closures. The emergence of very large chemical kinetics mechanisms, made this type of analysis very cumbersome, to the point that no such asyptotics studies were performed.

With the algorithmic methodologies that are available today, which can deliver asymptotic analysis results, flame dynamics studies can be performed without the obstacles hindering the conventional paper-and-pencil studies. Recently, such studies were performed by using the Computational Singular Perturbation (CSP), which is most suited for the study of complex multi-scale reacting systems and can generate, order by order, the results of asymptotic analysis. CSP can algorithmically identify (i) the low dimensional surface in phase space (a.k.a., slow invariant manifold) on which the reacting process is confined to evolve and (ii) the slow model that governs the evolution along the manifold. In the presence of both transport and chemistry, CSP can algorithmically (a) determine whether transport or chemistry drives the evolution along the SIM and (b) identify the dominant reactions involved.

In this presentation results on the premixed flame front propagation mechanisms will be presented, accounting for various fuels.

On the role of low temperature reactions in burner stabilized and propagating flames

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In this work we overview our recent findings on the investigation of the structure and dynamics of low- and high-temperature reactions based on two configurations: burner-stabilized methane-air flames at atmospheric pressure and hydrogen-air freely propagating flames at elevated pressure.

This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation (project No. FZNS-2024-0003).

CABARET-COMBUSTION code validation on combustion experiments of different scale and different combustion modes

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The aim of the presented work is to verify the CABARET-COMBUSTION code, which is based on the numerical vortex-resolving method CABARET and proposed for calculating turbulent combustion of mixed homogeneous and inhomogeneous hydrogen-air mixtures. Experimental data obtained in a series of experiments on the combustion of homogeneous and inhomogeneous hydrogen-air mixtures with different hydrogen contents in fast and slow combustion regimes at experimental facilities of different scale and are used as database for verification. A description of the mathematical models implemented in the CABARET-COMBUSTION code is presented, and the results of the code validation are given, characterizing its capabilities in terms of the propagation of a turbulent flame. It is shown that in order to refine the results of calculations in lean hydrogen-air mixtures, it is necessary to include models of radiant heat transfer and heat loss on the walls of the facility.

Study of chemiluminescence of methane-air flame stabilized on a flat porous burner

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In this work, the spatial distribution and spectral characteristics of the chemiluminescence of chemically excited species, OH^* and CH^*, are experimentally and numerically studied by using a stationary premixed methane-air flame stabilized on the surface of a flat porous burner for various equivalence ratio and normal pressure. Numerical simulations are carried out using detailed reaction mechanisms, and the experimental study includes high-resolution spatial and spectral optical measurements. Despite the data reported in the literature, it is found that (i) the rotational degrees of freedom of OH^* and CH^* are not in thermal equilibrium with the surrounding gas and therefore cannot be used to measure flame temperature; (ii) there is no correlation between the heat release rate and the distribution of OH^* and CH^*; (iii) the detailed reaction mechanisms not only quantitatively, and also qualitatively differ in description of the OH^* and CH^* concentrations. Since the chemically excited species are well localized in a direction normal to the flame surface, they are demonstrated to be a very accurate markers of flame location. The shape of the combustion front can be reconstructed and resolved up to the accuracy of tens of microns, which is very important for estimation of blow-off critical parameters and measurement of the laminar burning velocity.

Nonlinear effects of one-dimensional pulsating detonation propagating in a mixture with initial density non-uniformity

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The propagation of detonation waves in non-uniform gas mixtures has become an area of interest in recent years due to the development of rotating detonation engines. Theoretical studies of one-dimensional detonation have shown that perturbations to the parameters ahead of the detonation wave can cause a resonant amplification of internal pulsations over a specific range of wavelengths. This talk aims to clarify the mechanism behind this phenomenon.

One period of pulsations in the wave velocity curve is analyzed. Due to the supersonic speed of detonation, at each point in time, the state of the leading wave is determined by a characteristic that moves towards the front. Families of C0, C+ and C– characteristics were constructed during the calculation process for the time interval under consideration. From the C+ family, those that reach the extreme points of the leading wave are selected. The pulsation period of the parameters can be estimated as the time taken by the C+ characteristic to travel along the reaction zone to the point of maximum wave speed. Bounding C+ characteristics that enter and leave the reaction zone are found and run almost parallel to the front of the leading wave.

Signals in the opposite direction from the leading wave propagate along the C0 and C– characteristics. The C0 and C– characteristics are constructed from the points of the extreme velocity of the leading shock wave. Two possible mechanisms for pulsation development have been identified. One involves perturbations propagating along the C0 characteristic, as described by McVey and Toong (Comb. Sci. Tech., 1971), and the other, with perturbations propagating along the C– characteristic, as discussed by Leung et al. (Phys. Fluids, 2010). The dynamics of gas density changes in front of the detonation wave front have also been taken into account. When the wave front reaches its leftmost position during the time interval under consideration (simulations in the shock-attached frame has been used), a C0 characteristic emanates. The resonant amplification of oscillations behind the wavefront occurs due to the superposition of disturbances that propagate along the C0 and C– characteristics from the leading shock wave.

Automatic progress variable construction for reduced combustion models

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Reduced combustion models often use the concept of a so-called progress variable (PV), which are supposed to capture the progress of combustion in a suitable way. To be suitable, the PV is supposed to meet certain conditions regarding its monotonicity with increasing combustion progress, and also regarding the behaviour of the state variables when they are considered as functions of the PV. Also, for the sake of a simple use of the PV in combustion models, it is preferred that the PV can be expressed as a linear combination of the state variables.

Finding a suitable progress variable for a given combustion system has become a widespread problem. In the past, some methods have been described that attempt at automatically constructing such a progress variable so that it fulfills certain criteria.

In this paper, some aspects involved in the construction of progress variables (PV) from a given combustion data set (like from a flame or a trajectory) are addressed. A new method is outlined which can create a progress variable for given combustion data. Compared to the methods which have previously been introduced, this new method incorporates certain additional aspects regarding the “robustness” of the progress variable with respect to perturbations in the underlying combustion data. Moreover, it is potentially more efficient and robust.

The method is applied to a number of examples, including some where finding a progress variable is commonly been considered to be a difficult task.

It is shown that the method is successful, and can also successfully handle the case where one common PV is searched for a family of multiple related combustion data, e.g., for premixed flames at different equivalence ratios.

Quantification of combustion-generated acoustic energy and influence on the flame propagation dynamics

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This work resolves the flame propagation in a slender semi-open chamber filled in a premix of reactants. After local heating in the vicinity of the open end, an auto-sustained combustion process is induced, resulting in a laminar premixed deflagration flame freely propagating under the confinement of the walls of the channel. The interaction of the energy release with the acoustic waves cause a perturbation of the process which may trigger the appearance of the thermos- acoustic instabilities.

The aim of the work is the quantification of the acoustic energy, which is firstly introduced into the chamber during the ignition process, and then can be amplified or attenuated during its interactions with the flame front.

Results will be compared for two different sets of boundary conditions at the channel exit. First, an outlet calculated using Riemann Invariants will be used, this is an extensively used boundary condition in which pressure at the chamber exit is kept constant and uniform. On the other hand, the second case will solve the surrounding atmosphere, allowing to evaluate the acoustic energy losses and the phenomena associated with the exhaust jet, understanding the differences in the flame propagation processes between both models.

Macro-scale and pore-scale dynamics of upstream propagating filtration combustion wave in a one-layer porous burner

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Combustion in inert porous media has a number of applications including power engineering, energy conversion devices and heaters. Porous media combustion has been systematically studied over the last decades and many fundamental regularities of this process have been revealed. At the same time, there is a lack of fundamental knowledge on flame behavior at the pore-scale and its influence on the filtration combustion wave at the macro- or burner-scale. This is mainly due to the limitations of the existing experimental techniques and opacity of the porous media hampered visual observation of the flame front.

In this work the upstream propagation of filtration combustion wave in a one-layer porous burner is studied experimentally and theoretically. The burner design makes it possible to observe macroscopic propagation of the combustion wave as well as non-stationary flame behavior at the pore scale. It is shown that the macro-scale propagation of a flame is accompanied by local distortions of its front and the emergence and movement of hot spots and low-temperature regions at the scale of several pores. Macroscopic flame propagation can be accompanied by oscillations of some flame fragments at the pore-scale. These oscillations have the same nature as the flame repetitive extinction and ignition which can be observed in the non-uniformly heated channel. Experimental results show that large scale evolution of the filtration combustion wave affects the flame dynamics at the pore scale and vice versa. The interplay between macro-scale and pore-scale processes manifests itself in the multiple repetitions of some patterns of the flame propagation. Most typical and common patterns are (1) step-wise jump of the flame fragment into the upstream pore and (2) transition to the upstream pore after the series of flame oscillations. It is shown that reduced one-dimensional thermal-diffusion model of flame propagation in externally heated variable cross-section channel with thermally conducting walls captures main features inherent of these two patterns. Results of parametric study allow us to assess the effect of problem parameters on the regions of existence of one or another pattern of flame propagation. Presented results may be of interest for further physical understanding of the porous media combustion and for validation of pore-resolved modelling which is actively developed in the last decade.

Peculiarities of hydrodynamic flame instability developments in nonuniform gas flows

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The development of hydrodynamic instability of the premixed gas flame propagating in an inhomogeneous flow has peculiarities that are discussed in this report. The cases of flame propagating in the narrow flat channels, the flame propagating in rotating flows and the outward propagating flame at large gas expansion coefficients are considered.

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Axial propagation of a hydrogen-air flame front in narrow gaps

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Hydrogen-air flame propagation in narrow gaps plays a key role in various fields of engineering, including microelectromechanical systems and fuel cell development.

When hydrogen-air mixtures are burnt in a narrow gap, constant heat loss occurs into the walls of the combustion chamber. The combination of ultra-lean hydrogen-air mixtures and constant heat loss leads to a mode of flame propagation in the form of individual flame cells.

This work presents experimental studies on the combustion of hydrogen-air mixtures with a volumetric hydrogen concentration of 7 and 10% in gaps with a thickness of 3 to 5 mm. Visualization of the process using an infrared camera recording wavelengths from 1.5 to 5 μm made it possible to obtain images of the flame front at the initial stage and its subsequent decay into individual cells.

The propagation speed of the flame front and flame cells was obtained. The obtained speed was compared with the rate of hydrogen diffusion. The shape of the flame cell front is considered to be cup-like. The decay of the deflagration front is a critical case of thermal diffusion instability, in which local attenuation of the curved flame front in concavities occurs.

The dynamics of combustion waves in periodic media

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The talk discusses recent advances on the dynamics of detonations and flames in periodic media. One of the main new results is the existence of a mode locking phenomenon whereby the periodic conditions in the combustible medium lead to the regularization of the combustion wave dynamics. The phenomenon will be illustrated with the examples of gaseous detonations and flames propagating in periodically nonuniform mixtures or in channels with variable properties.

Experimental and numerical study of hydrogen flame doped with tetraethoxysilane

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Flame synthesis is a scalable technology for the continuous production of inorganic oxide-based functional materials used for energy storage, catalysis, sensing, medical applications, and many other applications. However, development of these technologies proceeds mainly through empirical trial and error, since the complexity of the physicochemical processes of transformation and growth of particles in a flame does not allow establishing a clear connec-tion between the synthesis parameters and the final properties of the resulting particles. One of the problems here is the lack of reliable knowledge about the detailed mechanisms of py-rolysis and oxidation of precursors [1].

For the very beginning we chose SiO_2 precursor, tetraethoxysilane (TEOS). In this work we studied kinetics of TEOS oxidation in a hydrogen flame. Laminar premixed flames of $H_2/O_2/Ar$ mixtures of different stoichiometry with a small TEOS additive were investigated. The flames were stabilized over a flat flame burner at atmospheric pressure and examined with the molecular-beam mass-spectrometric setup. The reactants, stable and intermediate products of TEOS decomposition including radicals were detected. To get insights to the TEOS oxidation kinetics the mechanism of TEOS oxidation from the work of Fang et al. [2] was adopted. The rate of production and sensitivity analyses were performed to elucidate the key reaction pathways.

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Flame propagation in a channel with peripheral ignition

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An experimental and analytical investigation of the combustion of hydrogen-air mixtures with hydrogen concentrations of 12, 13 and 15 vol.% in channels with central and peripheral ignition is presented. The flame propagation was recorded using shadow and infrared high-speed photography in the transverse direction and along the axis of the channel. When ignited at the center of the channel end wall, the well-known “finger flame” is formed. The flame front stretches along the channel axis. The flame speed when approaching the side wall of the channel tends to the laminar flame speed. In this case, the flame speed at the axis is determined by the rate of production of combustion products, which is proportional to the front area. The main mechanism of flame acceleration is due to the front area growing. When ignited along the line connecting the side wall of the channel with the end wall, the flame also rapidly stretches along the axis of the channel in other words the use of peripheral ignition. As with a “finger flame,” the speed of the part of the front propagating toward the channel axis decelerates to the laminar flame speed. But, unlike the “finger flame”, the radius of the cylindrical part of the front decreases. This leads to more intense acceleration in the early stages and a noticeable slowdown in the later stages. Analytical models were used to describe the dynamics of the flame front in both cases. A model of a “reverse finger flame” generated by peripheral ignition is presented. It was experimentally discovered that with peripheral ignition the flame front speed is up to 1.7 times higher compared to central ignition. In a closed channel, the maximum pressure with peripheral ignition is achieved in a time 1.1 times less than with central ignition. The results obtained can be used in the design of hydrogen internal combustion engines with a reduced knock effect.

Model reduction “*on the fly*” using reaction-diffusion manifold (REDIM) approach

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Model reduction based on reaction-diffusion manifolds (REDIM) provides the detailed chemical kinetics effects at a reduced computation cost in the simulation of reacting flows. Chemistry and transport properties are provided in a tabulated form and all the components of the detailed thermoskinetic state vector are retrieved from the REDIM table when solving the reduced transport equations. The generated manifold using REDIM accounts for both reaction and diffusion processes. The REDIM approach offers the main advantage over other manifold based chemistry approaches that a minimum of prior knowledge is required about the type of the combustion system during generation of manifold. One of the reason behind this is that the information on transport processes, varying from one combustion system to another, can be provided “on the fly” as an external input parameter during the generation of REDIM so that the manifold can be evolved accordingly, and one does not need to assume a type of combustion system a priori. This external input parameter in REDIM is known as the gradient estimates, and in the “on the fly” approach, the generation process of REDIM is coupled with the reduced calculations itself such that the gradient estimates generated from reduced calculations are updated in the iterative process until the convergence of both the manifold and gradient estimates is achieved.

This “on the fly” approach using REDIM is assessed for both laminar and turbulent partially-premixed combustion. Laminar triple flames and Sydney turbulent partially-premixed flames with inhomogeneous inlets are selected as the target cases. The good agreement between calculated and measured values for temperature, major and minor species mass fractions are observed. Also in the work in progress, the same approach would be validated for the challenging thermos-diffusive unstable hydrogen premixed flames too.

Ultra-lean hydrogen-air mixtures in an excess-enthalpy burner

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Conditions under which a burner can sustain combustion of an extremely lean hydrogen-air mixture are investigated numerically in the framework of the one-dimensional flame theory. The burner is of the excess-enthalpy type and consists of multiple small-scale counter-flow channels. The transverse heat transfer between the opposing channels causes super adiabatic temperatures and thus enables burning of mixtures far below the standard lean limit of flammability. The range of steady burning is shown for detailed chemical kinetics as a function of the mass flow rate, the effective heat-exchange coefficient and the length of the burner, and it is compared satisfactorily with a one-step reduced kinetics previously derived. The computations show that, theoretically, there is no limit to the burning of very lean mixtures if the length of the burner is sufficiently large.

Thermal decomposition of coals and biofuels: similarities and differences

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In recent years, the most pressing issues have been the efficient and environmentally acceptable burning of coal ("clean coal") and the use of new fuels, including the use of low-calorie, brown coals, the use of new technologies when using coal as fuel and the active involvement of biofuels in the energy sector. To improve the combustion of various fuels, many researchers are inclined to consider the structure of single fuel particles and their physical and technical characteristics as well as taking into account the nature of their ignition and burnout in the development of combustion systems and burner devices. The study of efficient combustion of fossil fuels is relevant for the search for optimal modes of combustion of coal particles in various domestic and industrial boilers and power plants.

Thermal decomposition of coals and biofuels is accompanied by processes of destruction and polycondensation, which determine the amount and rate of release of gaseous and resinous substances, and the ratio of these processes largely depends on the rate and temperature of heating, as well as on the structural features of the analyzed substances. As the material heats up, endothermic and exothermic effects occur, the effect of which and the position on the temperature scale depend on the heating rate. The lack of information about the structure of complex molecules makes it difficult to develop ideas about the mechanism of thermal decomposition of coals, especially in a gas environment of variable composition.

In this work, a study of the physical and chemical parameters of thermal decomposition of various types of fuels, such as brown coal, black coal and biomaterial belonging to the category of waste from wood-processing enterprises, has been carried out. Additionally, the study of changes in the chemical structure of fine particles of brown and hard coal during heat treatment at temperatures up to 350 °C in the air atmosphere and with limited air access was carried out using ATR (attenuated total reflection) infrared spectroscopy. The thermal effects that occur during the processing of coals in each temperature range under similar atmospheric conditions have been studied.

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Modern methods for obtaining nanoporous carbon materials

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The report will present data on the nomenclature and methods for obtaining the most intensively studied classes of nanoporous carbon materials, which are increasingly finding practical application in science, medicine and various fields of the national economy. The objects of consideration are both activated carbons, the production of which is carried out by conventional methods of processing biomass and fossil hydrocarbon raw materials, and nanoporous carbon materials obtained using modern synthetic methods. Recommendations on the use of template synthesis methods for carbon materials with a controlled nanopore structure will be provided. As promising areas, the methods of "self" template synthesis for obtaining porous carbon materials with a special morphology of particles from metal-organic precursors are highlighted, as well as environmentally friendly methods of using various "self" templates based on available organic salts, which make it possible to significantly reduce the cost of template synthesis of nanoporous carbon materials. The methods for obtaining functional materials with an ordered architecture of micro- and mesopores, as well as the use of modern methods of functionalization and doping are considered. A separate chapter is devoted to methods of using nanoporous carbon materials to create water purification systems, energy and hydrogen storage, gas mixture separation, as well as catalysts, sensors and other science-intensive products. In conclusion, the presentation summarizes the experience of research into various methods for obtaining nanoporous carbon materials, identifies the most problematic areas of their development and practical application at the present time, and provides our own vision of the further development of this area of materials science.

Ultra-lean hydrogen premixed flames propagation in channels

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Flame propagation in channels is a topic of technological and fundamental interest, especially in the new golden age of hydrogen. The effects of confinement, heat transfer to the wall, differential diffusion (Lewis number effect) and thermal diffusion make the understanding of the problem a difficult task. Recently, exotic regimes of hydrogen ultra-lean premixed flames of hydrogen in air have been found which raises questions on the safety procedures that should probably be revised.

In this work, we will consider ultra-lean hydrogen flame propagation in narrow channels, aiming to understand the true limits of flame propagation in such channels. Hydrogen is a fuel that leaks easily and such ultra-lean mixtures could be formed in the small cavities that surround any system. In these circumstances, a small deposition of heat, such a spark or hot spot, might ignite a flammable mixture producing a self-propagating flame front. The determination of the basic necessary parameters for successful flame propagation is therefore an important task to develop reliable safety protocols.

We present numerical analysis of the flame propagation of H_2-air mixtures in ultra-lean mixtures. The methodology is based on the low Mach number approximation of the reactive Navier-Stokes equations to determine flame propagation velocity a function of equivalence ratio and channel width.

Full reactive Navier-Stokes equations coupled with detailed chemical kinetics (San Diego mechanism for hydrogen). Results, including the effects of equivalence ratio and channel width are presented.

A new thermodiffusive model, that can be used with full chemistry, is proposed. We show that this model captures the essence of the physics, at a fraction of the cost of the full equations, eliminating the uncertainty associated with the chemistry models, typical of simplified thermodiffusive models.

Weak flame stabilized in planar channel with external heating

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The combustion modes of ultra-lean low-stretched methane-hydrogen-air flames stabilized in narrow planar channel with external heat source were experimentally studied. It was shown, that decrease of equivalence ratio and stretch rate value leads to transition of burner stabilized planar flame to unstable FREI regime and two stable ball-like weak flame occurrence. At further reducing of mixture of mixture content and flow parameters single ball-like weak flame stabilized at flow stagnation point. The effect of autoignition of ball like flame was also observed. The results show the possibility of detailed experimental investigation of weak flame with dominant diffusion transport processes under normal gravity condition.

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Obtaining porous carbon from plant raw materials by pyrolysis method for hydrogen storage

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Hydrogen is currently one of the promising fuels that can solve the world's growing energy needs without causing environmental damage to the planet. On the other hand, one of the key issues slowing the widespread use of hydrogen as an alternative fuel is the lack of safe, economical and efficient hydrogen storage systems. The proposed study examines the possibilities of using nanoporous carbon obtained from rice husks as a material for storing hydrogen. A new approach to controlling the process of pore formation in nanoporous carbon when it is obtained from plant raw materials using pyrolysis and chemical activation methods is proposed. The work presents and discusses the results of studies on optimizing the conditions for producing nanoporous carbon with a maximum content of micropores and studying their hydrogen sorption characteristics. It has been established that in nanoporous carbon obtained from rice husks and processed under identified optimal conditions of mechanical activation, compared with untreated rice husks, the specific surface area according to BET increases from 2386 to 2715 m^2/g, the specific surface area of micropores calculated using the Dubinin-Radushkevich method from 2754 to 3099 m^2/g and the total pore volume calculated by the BJH method from 0.251 to 1.625 cm^3/g, which makes it possible to increase its hydrogen adsorption capacity by 29.7% compared to nanoporous carbon obtained from rice husk and not subjected to mechanical activation.

Comparison of thermal activation methods of biomass for producing high-performance supercapacitor electrodes based on activated carbon

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This study provides a comprehensive investigation into the thermal activation methods used to convert biomass, specifically rice husk and walnut shell, into high-porosity activated carbon for application as electrode materials in supercapacitors. The research focuses on comparing two activation methods: chemical activation using potassium hydroxide (KOH) and physical activation using carbon dioxide (CO_2). The CO_2 activation method is highlighted for its environmental benefits and cost-effectiveness, demonstrating superior rate performance and lower charge transfer resistance compared to the traditional KOH method. These advantages make CO2 activation a promising alternative for the production of sustainable electrode materials.

Despite these benefits, KOH-activated samples showed higher specific capacitance and energy density, which can be attributed to their larger surface area and higher microporosity. This difference underscores the effectiveness of chemical activation in enhancing the electrochemical properties of activated carbon, particularly at lower charge-discharge rates. The study also delves into the critical role that the chemical composition of the biomass plays in determining the properties of the resulting activated carbon. The presence of inorganic components, such as silica in rice husk, influences the effectiveness of the CO_2 activation process, while the absence of such components in walnut shells leads to more favorable outcomes.

Furthermore, the research explores the structure-performance relationship, revealing that CO_2-activated carbons possess a well-developed mesoporous network, making them highly suitable for fast charge-discharge cycles in supercapacitors. In contrast, KOH-activated carbons excel at lower scan rates due to their extensive microporous structure, which enhances ion adsorption and storage. These findings suggest that the choice of activation method should be tailored to the specific performance requirements of the supercapacitor application.

In conclusion, this study offers valuable guidance for the selection of activation techniques and biomass sources in the development of high-performance, environmentally friendly electrode materials for energy storage devices. By providing a detailed comparison of CO_2 and KOH activation, the research contributes to the advancement of sustainable technologies in the field of energy storage, emphasizing the balance between performance and environmental impact.

Investigation of critical phenomena of the methane-air flames at normal and elevated pressure

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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.

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Numerical simulation of supersonic hydrogen combustion in the channel with transverse jet injection

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This study presents a numerical simulation of supersonic hydrogen combustion with transverse jet injection in a channel. The governing equations are the 3D Favre-averaged Navier-Stokes equations, closed by the k-ω turbulence model. These equations are solved using a third-order Essentially Non-Oscillatory (ENO) scheme. Two combustion mechanisms are investigated: the Spark mechanism, consisting of 7 species and 7 reactions, and the Keromnes mechanism, comprising 9 species and 19 reactions. Both mechanisms are used in validating against experimental data from Gamba et al. The objective is to compare the accuracy and performance of these mechanisms in modeling the combustion process.

Efficiency of cylindrical porous burners with heat return by radiative heat exchange

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The present study is devoted to theoretical estimates of the maximum achievable efficiency of radiative cylindrical burners with gas combustion in a porous medium. The theoretical estimates obtained for a burner with two coaxial porous shells, between which the flame is stabilized, and for a single-layer porous burner with filtration combustion of combustion gas. In the first case, heat regeneration is carried out due to radiation heat exchange between the layers, and in the second case, it occurs due to the thermal conductivity of the porous frame. It has been shown that the radiation efficiency of the burners is approximately the same and does not depend on the heat recovery way. At the same time, a two-layer system has an obvious advantage over a single-layer burner due to significantly lower material consumption and lower hydraulic losses when filtering gas through a porous medium.

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Morphological features of Fe_3O_4 nanoparticles obtained by solution combustion synthesis

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Magnetite (Fe_3O_4) nanoparticles have the potential to provide innovative solutions to various problems and promote technological advancement in many fields due to their low toxicity, low cost and high magnetic properties. The versatility and biocompatibility of magnetite make it a candidate for a wide range of applications in biomedical, environmental and industrial fields.

In this work, magnetite was synthesized by solution combustion method using various fuels such as urea, citric acid, glycine and glucose. Morphological, structural and elemental analyses of the synthesized magnetite nanoparticles were carried out using SEM, EDS and XRD. The corresponding characterizations are presented in Table 1.

Table 1. Main characteristics of synthesized magnetite nanoparticles

Characteristics	Fe_3O_4 (urea)	Fe_3O_4 (citric acid)	Fe_3O_4 (glycine)	Fe_3O_4 (glucose)
Average crystallite size, nm	20.365	20.431	19.178	30.294
Average particle size, nm	102.15	69.68	-	70.40
Fe content, %	66.26 ± 0.12	68.47 ± 0.10	29.65 ± 0.04	34.59 ± 0.07

X-ray diffraction patterns confirmed the presence of Fe_3O_4 crystal structure, with average crystallite size in the range of 19 to 31 nm, calculated according to the Debye-Scherrer formula. The surface area of magnetite nanoparticles was determined using the Brunauer-Emmett-Teller (BET) method. Magnetite Fe_3O_4 samples obtained with urea and citric acid showed surface areas of 9.925 m^2/g and 58.451 m^2/g, respectively.

The synthesis of the AC/Fe_3O_4 composite involved the preparation of activated carbon (AC) from biomass through a heat treatment process. SEM analysis reveals that the AC exhibits a highly porous structure, while the BET analysis indicates a remarkable specific surface area exceeding 2000 m^2/g.

The combination of this high-quality AC with Fe_3O_4 magnetite presents significant potential for the development of an efficient filter capable of retaining Pb^{2+} ions, thereby effectively purifying water. This study highlights the importance of studying combustion processes in solution to obtain unique and high-quality nanomaterials that can further advance water treatment technologies.

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Theoretical study of the Reaction of Acetonitrile CH_3CN ($X^1\Sigma^+$) with Methylidine Radical (CH $X^2\Pi$) in cold rarefied molecular clouds

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The reaction of the methylidyne (CH; $X^2\Pi$) radical with Acetonitrile (CH_3CN; $X^1\sum+$) molecule was studied at a collision energy of 4.0 kJ/mol with ab initio calculations of the potential energy surface (PES). At low temperatures in deep space, a large amount of nitriles are present in the atmosphere of Saturn's moon Titan [1, 2], as well as in interstellar molecular clouds. Reactions of nitriles with the methine radical CH are of interest, as potencial initial step in the study of biological molecules. In particular, in the course of the reaction with cyanide molecules, a nitrogenous base, structural blocks in DNA chains, can be formed. In addition, the formation of linear and cyclic radicals is possible with the release of the corresponding products: atoms, molecular particles, ethylene, etc.

Geometries and potential energies of reactants, products, intermediates and transition states for the reaction were found by means of ab initio quantum chemical method ωB97xd/cc-pVTZ [3, 4] and the higher-level corrections were evaluated at the CCSD(T)-F12 level of theory[5, 6, 7] with the cc-pVQZ-f12 (E_1) basis set [8, 9].

Those results were utilized in Rice−Ramsperger−Kassel−Marcus calculations of the product branching ratios at the zero pressure limit – common approach in modelling of the cold molecular clouds chemistry. Mechanism identified emphasizes importance of the CH+CH_3CN reaction as an important supplier of the initial bricks for building heterocyclic hydrocarbons in extreme environments [10, 11].

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Theoretical study of the benzyl radical oxidation reaction

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Aromatic compounds are used as components of automotive and aviation fuels. They are a source of polycyclic aromatic hydrocarbons (PAHs) and soot particle formation, as reported in many studies. Toxicological studies show that PAHs have mutagenic and carcinogenic properties. In addition to their toxic properties, the high octane number of aromatic compounds motivates the interest in better understanding their combustion properties.

Developing an accurate kinetic model for toluene radicals combustion is also important for extension to larger aromatic components in diesel or jet fuel or even beyond to assess the reactivity of monoaromatic hydrocarbons and PAHs emitted from thermal processes of biomass.

In this paper, we present the results of a quantum chemical study of the oxidation reaction of benzyl radical with molecular oxygen. The results were obtained at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. In this paper we present the results of a quantum-chemical study of the oxidation reaction of benzyl radical with molecular oxygen. The results were obtained at the G3(MP2,CC)//B3LYP/6-311G(d,p) level of theory. This approach provides chemical accuracy of relative energies and molecular parameters. For the studied reaction pathways, the values of rate constants were calculated for various external conditions within the framework of the RRKM-ME theory with kinetic accuracy of the reaction products were obtained.