SAMARA,
RUSSIAN FEDERATION,
JUNE 30 - JULY 4, 2026

4th International Conference on Physics and Chemistry of Combustion and Processes in Extreme Environments

TECHNICAL PROGRAM and BOOK OF ABSTRACTS

LPI SAMARA

SAMARA UNIVERSITY

Russian Section of the Combustion Institute

P.N. Lebedev Physical Institute of the Russian Academy of Sciences

International Conference on Physics and Chemistry
of Combustion and Processes in Extreme Environments

(Samara, Russian Federation, June 30 – July 4, 2026)

TECHNICAL PROGRAMM
AND
BOOK OF ABSTRACTS

“Insoma-Press”

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This collection presents the program and abstracts of presentations at the 3d International Conference on Physics and Chemistry of Combustion and Processes in Extreme Environments (ComPhysChem’26) held at Samara on June 30 - July 4, 2026. The presentations covered a wide range of fundamental and applied topics in physics and chemistry related to combustion and processes occurring in extreme environments. These included fundamental physical-chemical processes, reaction kinetics and dynamics, quantum chemical studies of the potential energy surfaces of chemical reactions in flames and interstellar media, as well as waves and oscillations in solar, stellar, and interstellar plasma. Other topics covered included the kinetics and dynamics of elementary processes, the mathematical modeling of combustion processes, laser and optical diagnostics, the chemical, plasma, and laser initiation of combustion, the structure, formation, and destruction of polycyclic aromatic hydrocarbons (PAHs), soot, graphene, carbonaceous nanoparticles, and chromatography and measurement techniques related to combustion.

Intended for graduate students in the fields of physical chemistry, chemical physics, combustion science and technology, astrochemistry, and astrophysics, as well as for researchers and university professors.

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Conference Venue: ComPhysChem'26 is held in the "Univer Studia" of the Samara University. Address: 151, Molodogvardeyskaya str., Samara, 443001, Russia.

TECHNICAL PROGRAM

UTC +4	30 June, Tuesday
9:00-9:25	**Registration**
9:30-9:50	**Opening remark**
9:50-10:30	**Vyacheslav Bykov** (KIT, Germany) – «Mechanisms of chemical kinetics in combustion – modelling and model reduction» ***PLENARY***
10:35-11:15	**Alexander Eremin** (JIHT RAS) – «Kinetic methods for controlling the ignition of combustible mixtures behind shock waves» ***PLENARY***
11:20-11:35	Coffee break
11:40-12:00	**Egor Khodyko** (JIHT RAS) – «Study of the soot growth process in a flame using the LIF method»
12:05-12:25	**Anastasia Moroshkina** (LPI) – «Investigation of the methane-air flame oscillations by 2D LIF method»
12:30-12:50	**Vladimir Kislov** (FRC PCPMC RAS) – «Sulfur absorption during thermal disposal of acid tar and bitumen»
12:55-13:15	**Igor Zinchenko** (IAP RAS) – «New methanol maser lines related to episodic accretion on a massive protostar» ***Invited***
13:20-14:25	Lunch 13:20-14:25
14:30-14:50	**Vladislav Matyushkov** (ICKC SB RAS) – «The effect of hydrocarbons and oxygenates addition on kinetics of ammonia oxidation»
14:50-15:10	**Sergey Matveev** (Samara University) – «Hydrogen-Enriched Fuels for Gas Turbine Combustors: Stability, Emissions, and Burner Design»
15:10 - 15:30	**Vladislav Rogoveshko** (ICKC SB RAS) – Supramolecular Double Spin-Flip Transition in van der Waals Complexes of Isoprene with Oxygen as a Source of Singlet Oxygen $O_2(1\Delta g)$
15:30-15:50	**Maria Gagonova** (MSU) – «Radiation-induced transformations of benzonitrile in cryogenic matrices»
15:55-16:10	Coffee break
16:15-16:35	**Nikita Bystrov** (JIHT RAS) – «Study of kinetics of high temperature oxiditation of basic furan compounds under high-dilute conditions - furan and tetrahydrofuran»
16:35-16:55	**Evgeny Serechenko** (LPI) – «Numerical and experimental investigation of performance of thermoelectric generator based on porous counter-flow burner with passive air cooling»
16:55-17:35	**Alexander Mebel** (FIU, USA) – «From PAH to fullerenes: Closing a nano bowl with a nano lid» ***online***
17:40-19:10	**Poster**

UTC +4	1 July, Wednesday
9:30-10:10	**Nickolay Smirnov** (MSU) «System Effect of Obstacles and Inhibitors on the Deflagration-to-Detonation Transition in Hydrogen-Air Mixtures» ***PLENARY***
10:15-10:55	**Sergey Matveev** (Samara University) – «Polycyclic aromatic hydrocarbons: issues of formation and emission in the exhaust gases of engines and power plants» ***PLENARY***
11:00-11:20	**Leonid Chikishev** (IT SB RAS) – «On the effect of a weak DC electric field on a Bunsen flame» ***Invited***
11:25-11:40	Coffee break
11:45-12:05	**Alina Ponomareva** (LPI) – «Thermal radiation characteristics of a cylindrical hybrid porous-microchannel counterflow burner»
12:10-12:30	**Maxim Tsvetkov** (FRC PCPMC RAS) – «Thermodynamic evaluation of conditions for the Fe(III) oxide reduction during downdraft gasification of coal mixed with lean ores»
12:35-13:15	**Sergey Yakush** (IPMech RAS) – «Dynamics and statistical features of premixed flame propagation in narrow gaps» ***PLENARY***
13:20-14:25	Lunch 13:20-14:25
14:30-14:50	**Konstantin Khvostochenko** (LPI) – «Development of a reduced combustion model for rich hydrogen-air mixtures»
14:55-15:15	**Iakov Medvedkov** (SB LPI, Samara University) – «Unexplored HACA pathway: acetylene trimerization on phenyl radical» ***Invited***
15:20-15:40	**Departure to River Station 15:20**
15:50-16:30	**15:40 Boarding**
16:35-16:55	**16:00 - 21:00** **Ferry trip along the Volga River**
17:00-19:10	

UTC +4	2 July, Thursday
9:30-10:10	**Gleb Fedoseev** (XAO, CAS, China) – «Surface Chemistry of Interstellar Carbon Chains» ***online***
10:15-10:55	**Vyacheslav Tugaenko** (S.P. Korolev Rocket and Space Corporation "Energia") – «Formation of Complex Structures During the Passage of Cosmic Bodies Through the Atmosphere» ***PLENARY***
11:00-11:20	**Dmitri Wiebe** (INASAN) – «Complex organics in cold molecular clouds: more atoms, less understanding» ***Invited***
11:25-11:40	Coffee break
11:45-12:05	**Maria Murga** (INASAN) – «The history of carbonaceous grains in the Universe from cosmic dawn to the present day» ***Invited***
12:10-12:30	**Ekaterina Shiryaeva** (MSU) – «Spectroscopy of products of radiation-induced transformations of isolated dimethyl ether molecules in low-temperature matrices» ***Invited***
12:35-12:55	**Alexander Shevchenko** (SB LPI, SamGTU, UrFU) – «Screening of polycyclic aromatic hydrocarbons with sp- and sp^2-hybrid carbon atoms and analysis of their properties» ***Invited***
13:00-13:20	**Anton Vasyunin** (UrFU) – «Interstellar Ices Around Protostars: Chemical Composition and Spatial Distribution» ***Invited***
13:25-14:30	Lunch 13:25-14:30
14:35-14:55	**Vladimir Gubernov** (LPI) – «Diffusion-thermal instabilities: from non-linear models to a methodology for verifying combustion reaction mechanisms» ***Invited***
15:00-15:20	**Yulia Titova** (SamGTU) – «Self-propagating high-temperature synthesis of highly dispersed ceramic nitride-carbide composition based on SiC using sodium azide and polytetrafluoroethylene»
15:25-15:45	**Vasily Rogozhnikov** (LPI) – «Investigation of flat burner flame 2D structure by studying absolute OH concentrations utilizing saturated laser-induced fluorescence»
15:50-16:05	Coffee break
16:10-16:50	**Denis Knyazkov** (ICKC SB RAS) – «Mass spectrometric and numerical study of formation of positive and negative ions in flames» ***PLENARY***
16:55-17:35	**Alexey Kuznetsov** (UTFSM, Chile) «Computational design of novel building blocks for nanotechnology based on complexes of core-modified (metallo)porphyrins with different species» ***online***
17:40-19:10	

UTC +4	3 July, Friday
9:30-10:10	**Leonid Fershtat** (N.D. Zelinsky IOC RAS) – «Nitrogen Heterocycles as a Versatile Platform for the Construction of Energetic Materials» ***PLENARY***
10:15-10:55	**Vitaly Kiselev** (NSU) – «Quantum chemical kinetics of combustion and atmospheric reactions» ***PLENARY***
11:00-11:20	**Pavel Yatsenko** (JIHT RAS, ICKC SB RAS) – «A shock tube study of NH_3 pyrolysis under strong Ar dilution»
11:25-11:40	**Ivan Antonov** (SB LPI, Samara University) – «Hypergolic ignition in acoustic levitator» ***Invited***
11:45-12:05	
12:10-12:30	**Valery Azyazov** (SB LPI) closing remark
12:30-13:00	Coffee break
13:10-13:30	**Departure to Samara University, Moskovskoe shosse**
14:30-14:40	**Excursion to the Aircraft Engine History Center (Samara University) + Scientific Research Laboratory "Combustion physics and chemistry"**
14:45-15:05	
15:10-15:30	
15:35-16:10	
16:15-16:50	
16:55-17:35	
17:40-19:10	

UTC +4	4 July, Saturday
9:30-10:10	**Excursion to Shiryaevo village (9:45-15:45) is not include in the conference fee** **Departure to River Station to 9:45** **Arrival to Samara 15:45**
10:15-10:55	
11:00-11:20	
11:25-11:40	
11:45-12:05	
12:10-12:30	
12:30-13:10	
13:15-13:35	
14:25-14:40	
14:45-15:05	
15:10-15:30	
15:35-16:10	
16:15-16:50	
16:55-17:35	
17:40-19:10	

Day 1 — 30 June 2026 (Tuesday)

9:00–9:25	**Registration**
9:30–9:50	**Opening remarks**
Session 1.1 **Chairs:** N.N. Smirnov (Moscow State University, FSI FSC SRISA RAS, Moscow) S.G. Matveev (Samara National Research University, Samara)	
9:50–10:30	Vyacheslav Bykov (Karlsruhe Institute of Technology, Institute of Technical Thermodynamics, Germany) *(Plenary)* *Mechanisms of chemical kinetics in combustion – modelling and model reduction*
10:35–11:15	Alexander Drakon, Alexander Eremin (Join Institute of High Temperature Russian Academy of Science, Moscow) *(Plenary)* *Kinetic methods for controlling the ignition of combustible mixtures behind shock waves*
11:20–11:35	**Coffee break**
Session 1.2 **Chairs:** V. Bykov (Karlsruhe Institute of Technology, Institute of Technical Thermodynamics, Germany) V.V. Gubernov (P.N. Lebedev Physical Institute of RAS, Moscow)	
11:40–12:00	A.V. Eremin[1], E.S. Khodyko[1,2], R.N. Kolotushkin[1] ([1]Joint Institute for High Temperatures of RAS, Moscow, [2]Kutateladze Institute of Thermophysics, Siberian Branch of RAS, Novosibirsk) *Study of the soot growth process in a flame using the LIF method*
12:05–12:25	Anastasia Moroshkina, Vasilii Rogozhnikov, Evgeniy Sereshchenko, Vladimir Mislavskii, Vladimir Gubernov (P.N. Lebedev Physical Institute of RAS, Moscow) *Investigation of the methane-air flame oscillations by 2D LIF method*
12:30–12:50	Vladimir Kislov, Ekaterina Pilipenko, Yulia Tsvetkova, Andrey Zaichenko, Marina Salganskaya, Dmitry Podlesniy, Maxim Tsvetkov, Eugeny Salgansky (Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Moscow) *Sulfur absorption during thermal disposal of acid tar and bitumen*
12:55–13:15	Igor Zinchenko [1], Svetlana Salii[2], Andrey Sobolev[3] ([1] Federal Research Center A.V. Gaponov-Grekhov Institute of Applied Physics of RAS, Nizhny Novgorod, [2] Astronomical Observatory, Ural Federal University, Ekaterinburg, [3] Xinjiang Astronomical Observatory of the Chinese Academy of Sciences, Urumqi, China) (*Invited)* *New methanol maser lines related to episodic accretion on a massive protostar*
13:20–14:25	**LUNCH**
Session 1.3 **Chairs:** A.V. Eremin (Joint Institute for High Temperatures of RAS, Moscow) I.A. Medvedkov (Samara National Research University, Samara)	
14:30–14:50	Vladislav Matyushkov, Ksenia Osipova, Vyacheslav Olennikov, Andrey Shmakov (Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk) *The effect of hydrocarbons and oxygenates addition on kinetics of ammonia oxidation*
14:50–15:10	Sergey S. Matveev (Samara University, Samara) *Hydrogen-Enriched Fuels for Gas Turbine Combustors: Stability, Emissions, and Burner Design*
15:10–15:30	Vladislav Rogoveshko, Alexey Baklanov (Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk) *Supramolecular Double Spin-Flip Transition in van der Waals Complexes of Isoprene with Oxygen as a Source of Singlet Oxygen $O_2(^1\Delta_g)$*
15:30–15:50	Mariia Gagonova, Daniil Tyurin, Irina Baranova, Vladimir Feldman (Department of Chemistry, Lomonosov Moscow State University, Moscow) *Radiation-induced transformations of benzonitrile in cryogenic matrices*

15:50–16:10	**Coffee break**
Session 1.4 **Chairs:** D. Knyazkov, (Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk) A. S. Savchenkova (Samara National Research University, Samara)	
16:15–16:35	Nikita Bystrov, Alexander Emelianov, Alexander Eremin, Pavel Yatsenko (Joint Institute for High Temperatures of RAS, Moscow) «Study of kinetics of high temperature oxiditation of basic furan compounds under high-dilute conditions - furan and tetrahydrofuran»
16:35–16:55	Evgeniy Sereshchenko[1], Anastasia Moroshkina[1], Vasiliy Rogozhnikov[1], Alina Ponomareva[1,2], Vladimir Mislavskii[1], Vladimir Gubernov[1] ([1] P.N. Lebedev Physical Institute of RAS, 53 Leninskii prosp., Moscow [2] ITMO University, St. Petersburg) *Numerical and experimental investigation of performance of thermoelectric generator based on porous counter-flow burner with passive air cooling*
16:55–17:35	Lotefa Binta Tuli[1] Ralf. I. Kaiser[2] and Alexander M. Mebel[1] ([1]Department of Chemistry and Biochemistry, Florida International University, USA, [2]Department of Chemistry, University of Hawaii at Manoa, Honolulu, USA) *online* *From PAH to fullerenes: Closing a nano bowl with a nano lid*
Session 1.5 Poster session 17:40–19:30 **Chairs:** P. Yatsenko, (Joint Institute for High Temperatures of RAS, Moscow) A.A. Ponomareva (St. Petersburg State University, St. Petersburg)	

List of poster presentations 30 June, 17:40–19:30

P1	Daria Agapova[1,2], Dmitrii Zavershinskii [1,2], Elizaveta Yarunova[1] ([1] Lebedev Physical Institute, Samara Branch, [2] Samara National Research University, Samara) *The effect of thermal misbalance and thermal conductivity on the dispersion properties of MHD waves: thin flux tube versus magnetic slab models*
P2	Semyon Agarkin[1,2], Andrey Cherepanov[1,2], A.A. Chernov[1], Denis Knyazkov[1,2] ([1]Voevodsky Institude of Chemical Kinetics and Combustion, [2]Novosibirsk State University, Novosibirsk) *Ion Chemistry of Premixed Acetone and Butanone Flames: Experimental and Theoretical Investigation*
P3	Anton Albokrinov[1], Dmitrii Riashchikov[1,2] ([1]Samara National Research University, [2]Lebedev Physical Institute, Samara Branch, Samara) *The effects of magnetic field on gravitational stratification of the solar atmosphere*
P4	Nikita Azyazov[1,2], Luybov Krikunova[1], Ivan Antonov[1] ([1] Samara Branch of the Lebedev Physical Institute of RAS, [2]Samara National Research University, Samara) *Nitrile reaction pathways in Titan's atmosphere*
P5	Evgenia Batrakova[1,2], Sergey Tuchin[1,2], Ivan Antonov[1,2] ([1] Samara Branch of the Lebedev Physical Institute of RAS, [2]Samara National Research University, Samara) *Mechanism of Glycolamide Formation in the Reaction of Formamide with Methanol*
P6	Andrey V. Cherepanov[1,2], Denis A. Knyazkov[1,2], Semyon A. Agarkin[1,2], Vitaly G. Kiselev[1,2], Anatoliy A. Chernov[1,2], Andrey G. Shmakov[1,2] ([1]Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk; [2]Novosibirsk State University, Novosibirsk) *An experimental and theoretical study of formation of cations in premixed n-butanol flames*
P7	Elizaveta S. Kurbatova[1,2], Nikita S. Bystrov[1], A.A. Emelianov[1], Pavel I. Yatsenko[1,3] ([1]Joint Institute for High Temperatures, [2]Moscow Institute of Physics and Technology, Dolgoprudny, [3]Bauman Moscow State Technical University, Moscow) *A comprehensive study of diethyl ether high temperature oxidation*

P8	A.V. Drakon[1], A.V. Eremin[1], E.S. Khodyko[1], R.N. Kolotushkin[1] ([1]Joint Institute for High Temperatures, Moscow) *Mass spectrometric study of the effect of dimethyl ether additives on the formation of carbon nanoparticles in ethylene/air flame*
P9	Vasiliy Zolotarenko[1,2], Alexander Eremin[1], Maya Korshunova[1], Ekaterina Mikheyeva[1] ([1]Joint Institute for High Temperatures, Moscow, [2]Moscow Institute of Physics and Technology, Dolgoprudny) *Temporal and spectral measurements of LIF during pyrolysis of hydrocarbons of various chemical structures behind shock waves*
P10	Dmitry Idrisov, Matveev Sergey, Daria Yukina, Mayorov Vladimir (Samara National Research University, Samara) *Investigation of the laminar flame speed of traditional and alternative fuels*
P11	Egor A. Karakich, Emil R. Umerov, Aleksandr P. Amosov, Vladislav A. Novikov (Samara State Technical University, Samara) *Structure and properties of TiC-Cu cermet synthesized in combustion in coupled processes of thermal metal reduction and self-propagating high-temperature synthesis*
P12	Egor A. Karakich, Emil R. Umerov, Aleksandr P. Amosov (Samara State Technical University, Samara) *Combustion in coupled processes of thermal metal reduction and self-propagating high-temperature synthesis for producing TiC-Cu cermet*
P13	Anastasia P. Khrushchova[1], Mikhail M. Evseev[2], Oleg V. Kuznetsov[2], Iakov A. Medvedkov[1,2], Ivan O. Antonov[1,2], Valeriy N. Azyazov[1,2] ([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *The effect of mass discrimination in molecular beam time-of-flight mass spectrometry*
P14	Vladimir Kislov, Ekaterina Pilipenko, Yulia Tsvetkova, Andrey Zaichenko, Marina Salganskaya, Dmitry Podlesniy, Maxim Tsvetkov, Eugeny Salgansky ([1]Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry, Chernogolovka) *The effect of the oxidizer composition on sulfur absorption by calcium-containing additives during filtration combustion of sulfur fuels*
P15	Daria Konstantinova[1,2], Vladimir Mislavskii[1], Evgeniy Sereshchenko[1], Vladimir Gubernov[1]([1]Lebedev Physical Institute, Moscow; [2]Moscow Institute of Physics and Technology, Dolgoprudny) *Porous-microchannel burner with an optically open hot zone as an IR emitter*
P16	Vladislav Krasnoukhov (Ural Federal University, Ekaterinburg) *Investigation of Isomerization and Cyclization Pathways in the Reaction of Naphthyl ($C_{10}H_7$) and Propargyl (C_3H_3) Radicals*
P17	N.A. Kryukov, A.P. Amosov (Samara State Technical University, Samara) *Gel combustion synthesis of a highly dispersed ZnO powder with a high photocatalytic activity for phenol decomposition*
P18	N.A. Kryukov, A.P. Amosov (Samara State Technical University, Samara) *Solution combustion synthesis as a simple effective ZnO doping method for increasing photocatalytic activity*
P19	Andrey Kudashev, Alexander Semenikhin (Samara National Research University, Samara) *Calculation of thermodynamic functions for xylene and its radicals*
P20	Ruslan Kuramshin, Aleksei Torbin, Pavel Mikheyev (Lebedev Physical Institute, Samara Branch, Samara) *Influence of a dielectric barrier discharge on the combustion of lean methane-air mixtures*

P21	Alina Kuznetsova, Ivan Antonov (Lebedev Physical Institute, Samara Branch, Samara) *Theoretical study of reactions of boron trihydride with molecular oxygen*
P22	Ivan Loginov[1,2], Dmitri Wiebe[2], Maria Murga[2] ([1]Moscow State University, Chemistry Department; [2]Institute of Astronomy of the RAS, Moscow) *Chemical evolution of aromatic compounds in circumstellar envelopes of AGB stars*
P23	Anna Loyko[1], Dmitri Wiebe[2], Maria Murga[2] ([1]Moscow State University, Department of Physics; [2]Institute of Astronomy of the RAS, Moscow) *Cosmic ray irradiation of interstellar grain icy mantles*
P24	Sergey S. Matveev, Dmitry V. Idrisov, Gan E.O. (Samara National Research University, Samara) *Numerical and Experimental Investigation of the Combustion Processes of Methane–Hydrogen Mixtures and Hydrogen in a Cluster Microflame Burner*
P25	Sergey S. Matveev, Dmitry V. Idrisov, Gan E.O. (Samara National Research University, Samara) *Effect of Hydrogen Addition on the Lean Blowout Limit in a Premixed Swirl Burner*
P26	Vladislav Matyushkov[1,2], Tatyana Bolshova[1], Andrey Shmakov[1,3] ([1]Voevodsky Institute of Chemical Kinetics and Combustion; [2]Novosibirsk State University; [3]Kutateladze Institute of Thermophysics, Novosibirsk) *From detailed mechanism to skeletal model: MBMS study of TS-1 kerosene and its SU4 surrogate in lean and stoichiometric flames*
P27	Ouarmim Alaa Eddine, Dmitry Idrisov, Matveev Sergey, Kulakov Semyon (Samara National Research University, Samara) *Kinetic Mechanisms of Ammonia/Hydrogen Combustion: A Comparative Study*
P28	Maksim Ozhiganov, Kirill Skripov, Uliana Sapunova, Varvara Karteeva, Mikhail Medvedev, Gleb Fedoseev, Anton Vasyunin (Ural Federal University, Ekaterinburg) *Acid-base reactions of aniline at low temperatures*
P29	Andrey A. Pershin[1,2] ([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *Airy propagator method for calculation of cross sections for inelastic atomic scattering*
P30	Pivovarov P.S.[1], Mebel A.M.[1,3], Azyazov V.N.[1,2] ([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara; [3]Florida International University, Miami) *Investigation of the mechanism of formation of fluoranthene and pyrene in* the reaction *of benzyl and indenyl recombination*
P31	Andrei Pleshko, Nikita Trashkov, Dmitrii Glushkov (National Research Tomsk Polytechnic University, Tomsk) *Combustion characteristics of gel fuel in a hypergolic system*
P32	Ivan Pomelnikov[1,2], Dmitrii Ryashchikov[1,2], Dmitrii Zavershinskii[2,1], Nonna Molevich[1,2] (1 Lebedev Physical Institute, Samara Branch, Samara; 2 Samara National Research University, Samara) *On the evolution of an isochorically unstable medium*

P33	Alexander Ryabov[1], Dmitrii Riashchikov[1,2] ([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *A method for constructing the solar coronal heating function in a gravitationally stratified atmosphere*
P34	Alexandra Sabanina[1], Dmitrii Riashchikov[1,2], Dmitrii Zavershinskii[1,2], Roman Shevelev[1], Andrei Pershin[1,2] ([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *Methods for approximating longitudinal compressional waves in the magnetic structures of the solar corona*
P35	Uliana Sapunova, Maksim Ozhiganov, Igor Petrashkevich, Mikhail Medvedev, Anton Vasyunin (Ural Federal University, Ekaterinburg) *Detection of solid CN^- in the protostellar envelopes using the JWST data*
P36	Anna S. Savchenkova, Alexander S. Semenikhin, Sergey G. Matveev (Samara National Research University, Samara) *Methods for determining of PAHs concentration in hydrocarbon fuel emissions*
P37	Elizaveta Scoptsova[1], Alina Kuznetsova[1,2], Ivan Antonov[1,2] ([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *Theoretical study of the mechanism and kinetics of the reaction of the benzyl radical with hydroxyl*
P38	Alexander Semenikhin, Andrey Golenko, Anna Savchenkova, Sergey Matveev (Samara National Research University, Samara) *Theoretical study of gas-phase polymerization processes of p-xylylene*
P39	Roman Shevelev[1], Dmitrii Zavershinskii[1,2] (1 Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *The Effect of Thermal Conductivity and Thermal Misbalance on the Properties and Dynamics of Magnetoacoustic and Entropy Waves in Coronal Loops*
P40	I.V. Shishkov[1], V.S. Krasnoukhov[1,2], V.N. Azyazov[1,3] ([1]Samara National Research University, Samara; [2]Ural Federal University, Ekaterinburg; [3]Lebedev Physical Institute, Samara Branch, Samara) *Theoretical study of the i-C_4H_5 + O_2 reaction*
P41	Anastasia Shishova, Krikunova Lubov, Nikolayev Anatoly, Ivan Antonov (Samara National Research University, Samara) *Experimental and Theoretical Raman Spectroscopy Study of Novel Energetic Ionic Liquids*
P42	Anastasia Stolboushkina[1], Dmitrii Riashchikov[1,2], Anastasia Shishova[1], Ivan Antonov[1,2]([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *A method for acoustic potential manipulation in a bichromatic levitator for controlled droplet coalescence*
P43	Y.V. Titova, A.F. Yakubova, A.V. Ivanova (Samara State Technical University, Samara) *Preparation of Highly Dispersed TiN–TiC Nitride–Carbide Composites by the Azide SHS Method during Combustion of the Ti–NaN_3–C–C_2F_4–N_2 System*

P44	M.V. Tsvetkov[1,2], D.N. Podlesniy[1,2], A.Yu. Zaichenko[1,2], A.V. Danilov[1], A.V. Sergeev[1], Yu.Yu. Tsvetkova[2], E.V. Polianczyk[1,2] ([1]Fossil Fuels Institute – Scientific and Technical Center for Complex Processing of Solid Fossil Fuels, Moscow; [2]Federal Research *Center for Chemical Physics and Medicinal Chemistry, Chernogolovka)* *Thermodynamic evaluation of possibility of extracting industrial metals combined with downdraft gasification of metal-containing waste*
P45	Sergey Tuchin[1,2], Evgeniya Batrakova[1,2], Ivan Antonov[1,2] ([1]Lebedev Physical Institute, Samara Branch; [2]Samara National Research University, Samara) *Formamide ($HCONH_2$) formation in CO:NH_3 interstellar ice analogs*
P46	Elizaveta Yarunova, Daria Agapova, Ivan Pomelnikov, Dmitrii Riashchikov (Lebedev Physical Institute, Samara Branch, Samara) *Unified Description of Propagating and Non-Propagating Modes in Thermally Active Plasma and Broad-Area VCSELs*
P47	Alyona Yudina[1], Dmitrii Riashchikov[1,2] ([1]Samara National Research University; [2]Lebedev Physical Institute, Samara Branch, Samara) *Detection of quasi-periodic pulsations in stellar flare light curves using a convolutional neural network from Kepler telescope data*
P48	Daria Yukina, Dmitry Idrisov, Sergey G. Matveev, Olga Kolobova (Samara National Research University, Samara) *A Modified Kinetic Mechanism for the Combustion of Methane-Hydrogen Mixtures*
P49	Daria Yukina, Ivan V. Chechet, Sergey G. Matveev (Samara National Research University, Samara) *Enhancing the efficiency of gas turbine engine combustor component design through machine learning models*
P50	Alexandra Samadova[1], Dmitrii Riashchikov [1,2], Dmitrii Zavershinskii [1,2] [1] Samara National Research University, [2] SB LPI, Samara) *Thermal Misbalance Signatures in Wavelet Spectrograms of Coronal Slow Magnetoacoustic Wave Trains*

Day 2 — 1 July 2026 (Wednesday)

Shortened day — departure for the Volga river cruise at 15:30.

Session 2.1 **Chair:** Sergey Yakush (Ishlinsky Institute for Problems in Mechanics of the Russian Academy of Sciences (IPMech RAS))	
9:30–10:10	Nickolay Smirnov (Faculty of Mechanics and Mathematics, Lomonosov Moscow State University, Moscow,) (*Plenary)* *System Effect of Obstacles and Inhibitors on the Deflagration-to-Detonation Transition in Hydrogen-Air Mixtures*
10:15–10:55	Sergey G. Matveev (Samara National Research University, Samara,) (*Plenary)* *Polycyclic aromatic hydrocarbons: issues of formation and emission in the exhaust gases of engines and power plants*
11:00–11:20	Leonid Chikishev, A. Ponomarev, K. Lavronov, Vladimir Dulin (Kutateladze Institute of Thermophysics, 1 Lavrentyev Ave str., Novosibirsk) (*invited*) *On the effect of a weak DC electric field on a Bunsen flame*
11:25–11:40	**Coffee break**
Session 2.2 **Chairs:** Ivan Antonov (Samara National Research University; Lebedev Physical Institute, Samara Branch, Samara) Ekaterina Shiryaeva (Department of Chemistry, Lomonosov Moscow State University, Moscow, Russia)	
11:45–12:05	Alina Ponomareva[1,2], Anastasia Moroshkina[1], Vasilii Rogozhnikov[1], Evgeniy Sereshchenko[1], Vladimir Mislavskii[1], Vladimir Gubernov[1] ([1]Lebedev Physical Institute, Moscow; [2] St. Petersburg State University, St Petersburg) *Thermal radiation characteristics of a cylindrical hybrid porous-microchannel counterflow burner*
12:10–12:30	Maxim Tsvetkov[1,2], D.N. Podlesniy[1,2], A.Yu. Zaichenko[1,2], A.V. Danilov[1], A.V. Sergeev[1], Yu.Yu. Tsvetkova[2], E.V. Polianczyk[1,2] ([1] Federal State Budgetary Institution «Fossil Fuels Institute – Scientific and Technical Center for Complex Processing of Solid Fossil Fuels», Moscow; [2] Federal Research Center for Chemical Physics and Medicinal Chemistry of RAS, Chernogolovka) *Thermodynamic evaluation of conditions for the Fe (III) oxide reduction during downdraft gasification of coal mixted with lean ores*
12:35–13:15	Sergey Yakush[1], S.A. Rashkovskiy[1], M.M. Alexeev[2], O.Yu. Semenov[2] ([1]Ishlinsky Institute for Problems in Mechanics, Moscow; [2]Surgut State University, Surgut) *(Plenary*) *Dynamics and statistical features of premixed flame propagation in narrow gaps*
13:20–14:25	**Lunch**
Session 2.3 **Chairs:** V.Y. Tugaenko, S.P. Korolev Rocket and Space Corporation "Energia", Korolev, Russia V.M. Kislov, Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia	
14:30–14:50	Konstantin Khvostochenko[1], Evgeniy Sereshchenko[1], Vladimir Gubernov[1] ([1]Lebedev Physical Institute, Moscow) *Development of a reduced combustion model for rich hydrogen-air mixtures*

14:55–15:15	Iakov A. Medvedkov,[1,2] Vladislav S. Krasnoukhov,[1,2] Oleg V. Kuznetsov,[1,2] Mikhail M. Evseev,[1,2] Torbin A.P.,[1] Ivan O. Antonov,[1,2] Valery N. Azyazov[1,2] ([1]Lebedev Physical Institute, Samara Branch; [2] Samara National Research University, , Samara) (*Invited)* *Unexplored HACA pathway: acetylene trimerization on phenyl radical*
15:20	**Departure to the River Station**
15:40	**Boarding**
16:00–21:00 — Ferry trip along the Volga River	

Day 3 — 2 July 2026 (Thursday)

Session 3.1 **Chairs:** Anton Vasyunin (Ural Federal University (UrFU), Ekaterinburg) Maria Murga (Institute of astronomy of Russian academy of sciences, Moscow)	
9:30–10:10	Fedoseev Gleb Sergeevich (Xinjiang Astronomical Observatory, Chinese Academy of Sciences, China) *(Plenary)* *Surface Chemistry of Interstellar Carbon Chains*
10:15–10:55	Vyacheslav Tugaenko[1], R.M. Khatsaeva[2], R.A. Voropaev[1] ([1]S.P. Korolev Rocket and Space Corporation "Energia", Korolev; [2]A.N. Severtsov Institute of Ecology and Evolution, Russian Academy of Sciences, Moscow, Russia) *(Plenary)* *Formation of Complex Structures During the Passage of Cosmic Bodies Through the Atmosphere*
11:00–11:20	Dmitri Wiebe[1], Anna Loyko[2], Maria Murga[1] ([1]Institute of Astronomy of the RAS; [2] Moscow State University, Department of Physics, Moscow) *Complex organics in cold molecular clouds: more atoms, less understanding*
11:25–11:40	**Coffee break**
Session 3.2 **Chairs:** Gleb Fedoseev (Xinjiang Astronomical Observatory, Chinese Academy of Sciences, China) Dmitrii Wiebe (Institute of Astronomy of the RAS, Moscow, Russia)	
11:45–12:05	Maria Murga (Institute of astronomy of Russian academy of sciences, Moscow) (*Invited)* *The history of carbonaceous grains in the Universe from cosmic dawn to the present day*
12:10–12:30	Ekaterina Shiryaeva, Vladimir Sulaev, D. Tyurin, Vladimir Feldman (Department of Chemistry, Lomonosov Moscow State University, Moscow) *(Invited)* *Spectroscopy of the products of the radiation-induced transformations of isolated dimethyl ether molecules in low-temperature matrices*
12:35–12:55	Alexander P. Shevchenko[1,2], Varvara V. Nikitina[2], Vladislav S. Krasnouhov[1,3] ([1]Lebedev Physical Institute, Samara Branch;[2] Samara State Technical University, Samara; [3]Ural Federal University, Ekaterinburg) *Screening of polycyclic aromatic hydrocarbons with sp- and sp^2-hybridized carbon atoms and analysis of their properties*
13:00–13:20	Anton Vasyunin (Ural Federal University (UrFU), Ekaterinburg) (*Invited)* *Interstellar Ices Around Protostars: Chemical Composition and Spatial Distribution*
13:25–14:30	**Lunch**

Session 3.3 **Chair:** Vitaly Kiselev (Institute of Chemical Kinetics and Combustion SB RAS, [2] Novosibirsk State University, Novosibirsk, Russia)	
14:35–14:55	Vladimir Gubernov (P.N. Lebedev Physical Institute of Russian Academy of Sciences, 53 Leninskii prosp., Moscow) (*Invited)* *Diffusion-thermal instabilities: from non-linear models to a methodology for verifying combustion reaction mechanisms*
15:00–15:20	Yulia V. Titova (Samara State Technical University, Samara) *Self-Propagating High-Temperature Synthesis of Highly Dispersed SiC-Based Ceramic Nitride–Carbide Composites Using Sodium Azide and Polytetrafluoroethylene*
15:25–15:45	Rogozhnikov Vasiliy[1], Anastasia Moroshkina[1], Alina Ponomareva[1,2], Evgeniy Sereshchenko[1], Vladimir Mislavskii[1], Vladimir Gubernov[1] ([1]Lebedev Physical Institute, Moscow, [2] ITMO University, St. Petersburg) *Investigation of flat burner flame 2D structure by studying absolute OH concentrations utilizing saturated laser-induced fluorescence*
15:50–16:05	**Coffee Break**
Session 3.4 **Chair:** Leonid Fershtat (N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow, Russia)	
16:10–16:50	Denis Knyazkov, Andrey Cherepanov, Vitaly Kiselev, Anatoly Chernov, Semyon Agarkin, Vladislav Nikolaev (Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk) (*Plenary)* *Mass spectrometric and numerical study of formation of positive and negative ions in flames*
16:55–17:35	Aleksey Kuznetsov (Departamento de Quımica, Campus Santiago Vitacura, Universidad Tecnica Federico Santa Marıa, Chile) *online* *Computational design of novel building blocks for nanotechnology based on complexes of core-modified (metallo)porphyrins and their derivatives with different species: fullerenes, alkali metal cations, semiconductor nanoparticles, etc.*

Day 4 — 3 July 2026 (Friday)

Closing day, followed by an excursion in the afternoon.

Session 4.1 **Chair:** V.N. Azyazov (Samara University, SB LPI)	
9:30–10:10	Leonid Fershtat (N.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow) (*Plenary)* *Nitrogen Heterocycles as a Versatile Platform for the Construction of Energetic Materials*
10:15–10:55	Vitaly G. Kiselev,[1,2] N.V. Muravyev,[3] I.N. Melnikov,[3] A.N. Pivkina[3] ([1] Institute of Chemical Kinetics and Combustion SB RAS, [2] Novosibirsk State University, Novosibirsk;[3] Semenov Federal Research Center for Chemical Physics RAS, Moscow) (*Plenary)* *New Accuracy Level of Computational Thermochemistry and Kinetics of Important Energetic Materials: from DFT to Modern Explicitly Correlated and Local CCSD(T) Modifications*

11:00–11:20	Nikita Bystrov[1,2], Alexander Emelianov[1], Elizaveta Kurbatova[1,3], Pavel Yatsenko[1,2] ([1]Joint Institute for High Temperatures of RAS, Moscow; [2]Voevodsky Institute of Chemical Kinetics and Combustion Siberian Branch of RAS, Novosibirsk; [3] Moscow Institute of Physics and Technology, Dolgoprudny) *A shock tube study of NH_3 pyrolysis under strong Ar dilution*
11:25–12:05	Ivan O. Antonov (Samara National Research University, SB LPI, Samara) *(Invited)* *Hypergolic ignition in acoustic levitator*
12:10–12:30	Valery N. Azyazov (Samara National Research University, SB LPI, Samara) *Closing remarks*
12:30–13:30	**Coffe break**
13:40–14:00	**Departure to Samara University (Moskovskoe shosse)**
Excursion to the Aircraft Engine History Center (Samara University) and the Scientific Research Laboratory "Combustion physics and chemistry"	

PLENARY AND INVITED TALKS

Kinetic methods for controlling the ignition of combustible mixtures behind shock waves

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Combustion processes have been the basis of industrial human civilization for many centuries, and despite the rapid development of other energy production methods, they will likely remain so for the foreseeable future. Humanity is constantly striving to invent new effective methods to control combustion, especially the initiation of this process, i.e., ignition. Research efforts are focused on two areas: firstly, accelerating and intensifying ignition where combustion serves as an energy source, and secondly, suppressing ignition where there is a risk of fire and explosion.

Among the methods of ignition initiation, the most obvious and widespread one is the additional energy input of some kind, like a spark discharge or local heating of the combustible mixture. Gas-dynamic and chemical methods, in which the mixture is either compressed or mixed with high-flammable components, are also well-known. A wide variety of methods are being developed to suppress ignition as well, primarily thermodynamic and gas-dynamic ones, which involve actively cooling the mixture or adding non-flammable substances with high heat capacity, and mechanical methods, such as limiting oxygen access to the mixture.

This review, though, focuses on purely kinetic effects affecting ignition initiation and suppression, i.e. ones alternating the pathways of the generation and consumption of active radicals involving in chain reactions of combustion. Numerous experimental studies of ignition kinetics details are performed using shock tubes which provide the possibility of almost instant and quite uniform heating of gas volume. The shock wave itself, while being an essential experimental tool, is a remarkable phenomenon that can have affect ignition in a unique way, making it quite distinct from, for example, spark-induced one. Thus, we further narrow the scope of this review, considering the kinetics of the ignition of flammable mixtures behind shock waves.

First, we describe two rather exotic ideas concerning nonequilibrium ignition initiation, namely super-equilibrium high-energy collisions in the shock wave front and quantum effects at elevated pressures — and demonstrate why they proved unrealistic. The following part of the review is devoted to more common methods of influencing the development of chain ignition mechanisms using minor chemically active additives. A large number of experimental results on the promotion and suppression of ignition of a wide variety of gaseous fuels when doped with various (in particular, hydrocarbon and halogen-carbon) impurities are presented. Finally, specific features of the kinetic impact of different admixtures on combustion in shock-heated gas flows are discussed and analyzed.

Surface Chemistry of Interstellar Carbon Chains

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The ubiquity of polycyclic aromatic hydrocarbons (PAHs) or graphite-like carbonaceous particles in space were postulated since 1960-ies. The presence of refractory hydrocarbons (carbonaceous material) on the surface of submicrometer sized dust particles and in the gas phase played a key role in various theories required to explain extinction and polarization of the visible light, as well as observations of unidentified infrared emission bands (UIE bands) and diffuse interstellar bands (DIBs). However, direct observations of individual PAHs were lacking. This was until several years ago, when a true "boom" in the detection of various carbon chain species and substituted PAHs had occurred [1, 2]. The detection of several dozens of such species coincided with the delivery of the first samples from asteroids Ryugu and, later, Bennu. The organic macromolecules in the Ryugu samples revealed the plausible presence of polyaromatic structures that are composed of small numbers of aromatic rings with short, cross-linked aliphatic chains and various oxygen- and nitrogen-bearing functional groups, like the insoluble organic material (IOM) from Orgueil and Murchison meteorites [3]. The possibility to obtain simple prebiotic molecules by erosion of this macromolecular organic material upon delivery to the early Earth raised interest to its possible role in the emergence of life. Although many independent studies point at the Interstellar Medium as the place of origin for the IOM in the asteroids, the universal and consistent theory of IOMs formation staring from synthesis of elemental carbon in carbon-rich stars to its incorporation into the refractory organic material detected in the asteroids and meteorites is still lacking. In this talk I will present the most recent laboratory results obtained at Xinjiang Astronomical Observatory (XAO) of the Chinese Academy of Sciences (CAS) and the Laboratory for Astrophysics at Leiden Observatory, Leiden University that provide some chemical links between these various independent observations [4, 5].

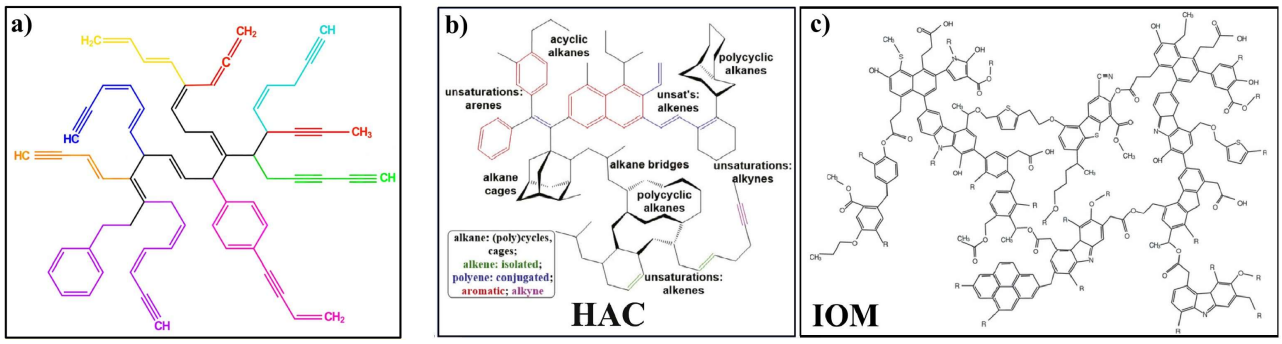

Fig. 1: The structures proposed for: (a) Refractory residues obtained by UV-photolysis of C2H2 under UHV conditions at 10 K, (b) "Hydrogenated amorphous carbon"(HAC) - one of the possible UIE carriers, (c) IOM in carbonaceous meteorites. Adapted from Samarth et al. (2026), Yang et al. (2017) and Derenne & Robert (2010).

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Nitrogen Heterocycles as a Versatile Platform for the Construction of Energetic Materials

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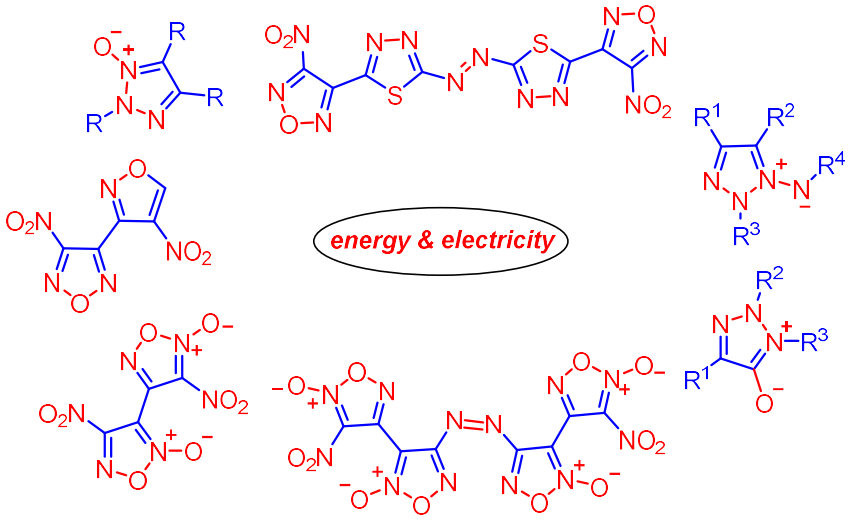
Nitrogen heterocycles are a key class of organic compounds and find application in pharmacology, medicinal chemistry, materials science, and the chemical industry. Developing new approaches to assembling such molecular systems using modern organic synthesis methods is a pressing and sought-after task. This report presents the latest achievements of our research group in developing new methods for the synthesis of polynitrogen heterocyclic structures. In recent years, we have developed promising synthetic strategies for assembling a wide variety of heterocyclic systems, including 1,2,5-oxadiazoles and their *N*-oxides (furazans and furoxans), isoxazoles, 1,2,3-triazole 1-oxides, and mesoionic 1,2,3-triazole 1-imines. Importantly, we have developed a series of approaches to the electroorganic synthesis of certain polynitrogen heterocycles, which is of interest for the environmentally friendly production of new functional materials.



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New Accuracy Level of Computational Thermochemistry and Kinetics of Important Energetic Materials: from DFT to Modern Explicitly Correlated and Local CCSD(T) Modifications

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Highly accurate theoretical values of formation enthalpies, bond energies, and activation barriers of elementary reactions are crucial for reliable quantitative modeling of reaction mechanisms and many related issues (e.g., estimations of the detonation parameters of energetic materials, EM). However, due to prohibitive computational cost, high-level ab initio calculations had been impractical for a large number of "medium-size" molecules, containing dozens of CNOF atoms. The widely used DFT calculations very often could not provide the uniform "chemical accuracy" (~1 kcal mol−1) and, ultimately, the convincing mechanistic evidence on the decomposition pathways of important EMs.

Here we report on the recent methodological advantages in the theoretical thermochemistry and kinetics achieved with the use of novel explicitly correlated (CCSD(T)-F12) and local modifications of the coupled cluster technique (DLPNO-CCSD(T)). The benchmarking on a representative set of EM revealed that both approaches do not deteriorate the quality of the conventional coupled cluster procedure. More specifically, we obtained the accurate bond energies and gas-phase formation enthalpies for a number of promising energetic materials, including high-nitrogen compounds and cyclic nitramines. These values are profoundly more accurate than the best available theoretical estimations so far. To this end, we proposed and benchmarked a "bottom-up" approach. First, highly accurate multi-level procedures W2-F12 and/or W1-F12 in conjunction with the atomization energy approach were utilized for smaller species. In turn, for medium-sized species (up to 30-40 non-H atoms), these values were complemented with the enthalpies of isodesmic reactions calculated using DLPNO-CCSD(T)/aVQZ. In addition, due to the very favorable scaling with the size of the molecule, this level of theory is still affordable, e.g., for the dimers of the latter species.

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

This work is supported by the Russian Science Foundation (project 22-13-00077-P). The support by the Supercomputer Center of Novosibirsk State University is also acknowledged.

Mass spectrometric and numerical study of formation of positive and negative ions in flames

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Ion-sensing technology is considered a promising tool for real-time monitoring and control of combustion processes in next-generation high-performance internal combustion engines [1]. Furthermore, electrically assisted combustion has recently emerged as an attractive approach to improve efficiency, stability, and controllability — particularly for fuel-lean mixtures, where ignition and stability remain challenging. Advancing these technologies requires a detailed understanding of ion–molecule interactions during combustion.

This work reports recent findings from the Laboratory of Combustion Kinetics (ICKC) on developing of predictive kinetic models of ion chemistry in flames of various hydrocarbons. Positive and negative ions naturally occurring in laminar premixed near-stoichiometric flames were detected using flame-sampling molecular beam mass spectrometry. H_3O^+, $C_2H_3O^+$, $C_3H_3^+$ are found to be the major cations the flames of C_1-C_3 hydrocarbons, while flames of heavier hydrocarbons produced numerous $C_xH_y^+$ cations. When nitrogen was used as a diluent, NO^+ was also detected in the post-flame zone. The dominant anions were O_2^-, OH^-, O^-, CHO_2^-, CHO_3^-, CO_3^-. Spatial profiles of all identified ionic species were obtained under various flame conditions.

The experimental data served first as the basis for constructing a detailed ion chemistry model and then as a target for its quantitative validation. Thermochemical data for all charged species were calculated using the highly accurate W2-F12 quantum chemical methodology. The updated ion chemistry model includes an improved submechanism for negative ions and is extended with reactions for NO^+ formation. The spatial distributions of charged and neutral species in the flames were simulated using the open-source chemical kinetics solver Cantera (v.2.6.0). The model is shown to reproduce the experimental data adequately. Major reaction pathways for cation formation in flames and directions for further model refinement are discussed.

This work was supported by Russian Science Foundation (project 25-13-00383), https://rscf.ru/en/project/25-13-00383/.

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Computational design of novel building blocks for nanotechnology based on complexes of core-modified (metallo)porphyrins and their derivatives with different species: fullerenes, alkali metal cations, semiconductor nanoparticles, etc.

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Tetrapyrrole macrocycles—porphyrins and their derivatives—are among the most studied macrocyclic systems because of their various prominent characteristics and versatile applications. The porphyrin molecule contains an 18 π-electrons conjugated system within a square-planar or quasi planar framework giving rise to the aromatic character responsible for the porphyrin species stabilization. Metal complexes of tetrapyrrole macrocycles are of particular interest because the metal centers can govern various chemical and physical properties of metalloporphyrins and thus their potential applications. Furthermore, different ways of modifying the tetrapyrrole macrocycle in order to tune its structural, electronic, reactivity, and photophysical features, have been elaborated, including partial or complete replacement of pyrrole nitrogens with other elements. Since 2012, we have been doing computational studies of metalloporphyrins and their derivatives with all four pyrrole nitrogens replaced with P-atoms, $MP(P)_4$, or by other elements, e.g., As, S, Se, etc. We have demonstrated that the prominent structural feature of the completely core-modified tetrapyrrole derivatives is their significant bowl-like distortion from planarity which would result in their various properties noticeably different from regular (metallo)porphyrinoids. Motivated by the fact that studies, either experimental or computational, on different complexes of completely core-modified porphyrinoids are either scarce or absent at all, we have been focusing on computational design of complexes of completely core-modified porphyrins and their derivatives with different partner species, such as fullerenes, graphene nanoparticles, other porphyrin units, alkali metal cations, etc. The results of our computational studies clearly demonstrate formation of different types of novel building nanoblocks based on the complexes of core-modified (metallo)porphyrins and their derivatives with other species. Such complexes show noticeable stability, often comparable to that of similar complexes of regular (metallo)porphyrins, and interesting electronic and other properties, thus paving new ways in nanotechnology and related areas.

Polycyclic aromatic hydrocarbons: issues of formation and emission in the exhaust gases of engines and power plants

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Aviation gas turbine engines (GTE) and hydrocarbon-fueled power plants contribute significantly to environmental pollution. Aviation, however, is unique in that pollutant emissions occur in the highly sensitive upper layers of the atmosphere. On the other hand, intensive air traffic leads to environmental pollution in the vicinity of airports. Similar problems exist at the operational sites of ground-based gas turbine power plants. In light of the above, international and governmental organizations are introducing increasingly stringent requirements for harmful emissions and air quality in the working environment. During the combustion of hydrocarbon fuels in the combustion chambers of GTEs, power plants, internal combustion engines, and thermal power units, various hydrocarbon compounds and soot particles are formed. These can be emitted into the atmosphere with exhaust gases in the form of unburned hydrocarbons, smoke, or non-volatile Particulate Matter (nvPM). The term "unburned hydrocarbons" encompasses a wide spectrum of organic compounds, ranging from simple aliphatic ones to complex polycyclic aromatic hydrocarbons (PAH), many of which are potent carcinogens capable of causing cancer and cellular mutations in living organisms. Furthermore, PAH are the primary reactants in the soot particle formation process. Therefore, studying the mechanisms of PAH formation during the combustion of hydrocarbon fuels as applied to the combustion processes in combustion chambers, along with the development of predictive models to determine the emission of these chemical compounds in the exhaust gases of GTEs and power plants, is a crucial and highly relevant task. This research is essential for addressing the challenge of developing environmentally friendly and highly efficient aviation engines and power plants.

The processes of PAH formation in a flame depend on temperature, pressure, fuel chemical composition, and the characteristics of turbulent two-phase flows (including droplet heating and evaporation), as well as the mechanisms governing the gas-phase reactions of hundreds of chemical species. For this reason, predicting PAH emissions from GTE combustion chambers is feasible only through the simultaneous application of Computational Fluid Dynamics (CFD) and detailed chemical kinetics, or by employing combined modeling techniques.

From PAH to fullerenes: Closing a nano bowl with a nano lid

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Development of new technologies to produce hydrogen and carbon materials, e.g., thermal or plasma-assisted pyrolysis of natural gas and the gas-phase production of carbon black and nanotubes, requires detailed understanding of the formation of carbonaceous particles from hydrocarbons. While PAHs are firmly established as molecular precursors of carbonaceous particles and their growth mechanisms at the pyrolysis/combustion conditions have been revealed in recent years, the physico-chemical processes leading from small PAHs to fullerenes and nanotubes remain poorly understood. Here, we demonstrate that the formation of C_{60} can be accounted for in terms of PAH growth mechanisms proceeding in a particular order. In particular, quantum chemical DLPNO-CCSD(T)/cc-pVDZ//B3LYP/6-31G(d) calculations have been performed to unravel the formation mechanism of buckminsterfullerene (C_{60}) via the reaction of the C40 nano bowl ($C_{40}H_{10}$) and corannulene ($C_{20}H_{10}$). The generated potential energy surfaces and molecular properties were further utilized to evaluate equilibrium constants and rate constants of elementary chemical reactions involved in the C_{60} synthesis. The overall $C_{40}H_{10} + C_{20}H_{10} \rightarrow C_{60} + 10H_2$ reaction is shown to be highly exoergic and hence thermodynamically favorable at temperatures above 700 K and a kinetically feasible pathway under high-temperature conditions was revealed. This route involves hydrogen atom abstraction steps to activate closed-shell reactants/intermediates alternating with cyclodehydrogenation reactions eventually zipping the edges between the reacting C40 and C20 units by consecutive closures of six- and five-membered rings between them. The reaction is driven/catalyzed by hydrogen atoms which carry out the hydrogen abstractions from $C_{60}H_x$ and are later recovered on the cyclodehydrogenation stages. The initial association reaction, $C_{40}H_9 + C_{20}H_{10} \rightarrow C_{60}H_{18} + H$, linking the two units by a covalent C-C bond appears to represent the kinetic bottleneck of the whole multistep process. This reaction is fast at low temperatures but slows down and has its equilibrium shifted toward the reactants at high temperatures. The feasibility of the proposed mechanism corroborates the hypothesis that C_{60} can be produced through a series of elementary reactions typical for the PAH growth.

System Effect of Obstacles and Inhibitors on the Deflagration-to-Detonation Transition in Hydrogen-Air Mixtures

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Research on combustion and detonation processes in combustible mixtures has a long history and great significance for the development of human society. Of particular interest is the regime of fast supersonic combustion – detonation, since it is both the most efficient combustion regime and the most destructive one due to the rapidity of the processes involved and the resulting damage. Therefore, studying various methods of its initiation has great practical importance both from the standpoint of triggering detonation, for example, in advanced propulsion systems based on detonative combustion of fuel, and from the standpoint of its prevention and minimization of the destructive consequences of explosions, e.g., during the transport and storage of various fuels. Transition processes, when slow combustion under certain conditions can transition into detonation, occupy a special place.

One of the interesting and relevant problems related to flame propagation and detonation onset is combustion in channels filled with premixed combustible mixtures containing various objects and obstacles. The presence of obstacles leads to distortion of the flame front and an increase in its speed. Therefore, from a safety perspective, it is important to comprehensively study the mechanism of flame interaction with obstacles.

The lecture examines the effect of obstacles on the formation and propagation of detonation in a stoichiometric hydrogen-air mixture. The research is carried out numerically using three-dimensional modeling in a region shaped as a rectangular parallelepiped filled with the combustible mixture.

It was found that for the chosen ratio of obstacle height to transverse channel dimensions, placing obstacles accelerates the flame front, but the number of obstacles does not affect the propagation speed of the front after passing these obstacles. When considering a tube completely filled with obstacles along its entire length, the flame propagates in a periodic regime with a constant average speed without detonation onset. It was shown that obstacles stabilize the flame front. After passing the obstacle zone, detonation may occur in the mixture (deflagration-to-detonation transition). The presence of up to a certain number of obstacles accelerates the deflagration-to-detonation transition. A further increase in the number of obstacles leads to an increase in the predetonation time.

When the ignition energy is reduced, detonation in the considered region occurs later and farther from the ignition point.

Formation of Complex Structures During the Passage of Cosmic Bodies Through the Atmosphere

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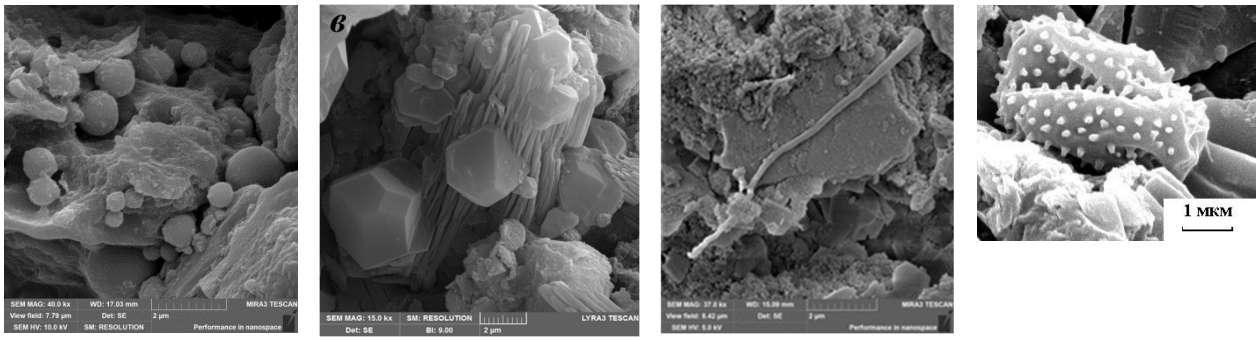
Natural and artificial cosmic bodies, when passing through the Earth's atmosphere, are subjected to significant loads due to the impact of a high-velocity gas flow on their surface. Tons of cosmic material, consisting of cosmic dust and meteoroids, enter the Earth's atmosphere daily. Transformed cosmic dust particles and meteoroid disintegration products, ranging in size from 10 μm to 2 mm, reach the Earth's surface, forming cosmogenic balls (spherules) with characteristic, sometimes very beautiful structures during their passage through the atmosphere. Meteoroids with sizes (conditionally) in the meter range and larger, under the action of aerodynamic forces that increase as the bodies penetrate denser atmospheric layers, and strong heat fluxes from the heated gas between the body's surface and the shock wave front, break apart, forming relatively large fragments that reach the Earth's surface. For the Chelyabinsk asteroid, which was 17–20 m in diameter, the largest found fragment had a mass of 650 kg. In-situ measurements of the dust particle characteristics that made up the aerosol trail of the Chelyabinsk asteroid showed the presence of large micron-sized particles. Among the dust that settled on the snow cover, faceted carbon particles several tens of micrometers in size were unexpectedly discovered, most likely formed during the passage of fragments through the atmosphere.

Artificial cosmic bodies move through the atmosphere, mostly maintaining their orientation in space, and reach the surface intact due to their high strength and the use of "soft" landing. For such bodies, only their outer surface undergoes destruction, mainly due to strong heat fluxes. During the ablation of the surface of reentry spacecraft during atmospheric passage, the material comprising the thermal protection coating enters the plasma layer formed as a result of interaction with the high-velocity incoming airflow. In the descent vehicle (DV) of the Soyuz transport spacecraft, which returns crews from the International Space Station, the temperature on the surface of the forward heat shield reaches 2000 K, and the temperature in the compressed layer, which is 10–15 cm thick, can reach 8000–10000 K. In [1], it was shown that on the leeward surface of the Soyuz descent vehicle, after atmospheric passage, various microparticles formed by the interaction of the plasma flow with the spacecraft were discovered.

As a first approximation, the physicochemical processes of material deposition from the plasma flow onto the descent vehicle surface are equivalent to chemical vapor deposition (CVD),

widely used in various technological and scientific applications. However, under the considered conditions of cosmic body passage through the atmosphere, significant differences from CVD methods include the presence of a dust component in the gas-plasma flow, a wide variety of elements in the plasma composition, the presence of local turbulence zones in the boundary layer as the flow moves along the body's forward surface, and the melting of thermal protection components with the formation of droplets that enter the plasma flow. Obviously, the extreme conditions of material transformation realized in the described cases for materials comprising the surfaces of cosmic bodies and the upper atmosphere cannot be adequately reproduced in laboratory settings (CVD technologies, plasma torch setups). In [1], a classification based on morphological features was proposed for microparticles found in the deposit on the descent vehicle surface. The formation of "large" particles (solid particles, agglomerates, droplets) with dimensions (at least in one dimension) exceeding several tens of micrometers undoubtedly involves erosion or melting processes of thermal protection coating components. However, on the surface of these particles, as well as independently within the deposit, smaller particles and submicron-scale formations were also discovered (see Fig. 1), and the study of their characteristics will be presented in the report.



a b c d

Figure 1. Microscopic and sub-microscopic particles formed during the passage of the descent vehicle through the atmosphere: (a) – droplets, (b) – faceted particles, (c) – filamentary particles, (d) – particles with nanoscale spikes.

The elemental composition of the thermal protection coating consists of several dozen elements, the main ones being carbon, oxygen, nitrogen, and silicon. Given the prevailing role of carbon in the composition of the spacecraft surface, the report will present data on the formation of organic molecules during atmospheric passage. The possible connection of the obtained results with the presence of organic matter in carbonaceous chondrites is discussed, as well as the results of studying samples from the surface of asteroids.

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Dynamics and statistical features of premixed flame propagation in narrow gaps

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Flame propagation in narrow space between two closely spaced plates (Hele-Shaw cell) is of high fundamental interest because it provides insight into the intrinsic flame instabilities of hydrodynamic and thermal-diffusive nature, cellular flame structure, and global flame dynamics [1]. In this work, recent experimental and theoretical results on premixed methane and propane flames (including the fuels with hydrogen addition) are presented. The channels were formed by two glass walls, with side walls and internal barriers; the flame front dynamics is captured by video recording with subsequent processing that allowed the statistical features of the cells on the flame front to be derived [2].

Flame propagation in Hele-Shaw cells is considered in two geometry configurations: the diverging channel (diffuser) with straight side walls with the spreading angle from 5 to 25 degrees, and a rectangular channel with a transverse barrier having a hole connecting the closed and open channel sections; ignition was performed at the closed channel end.

For the diffuser channels, it is shown that flame propagation in a channel with small gap width (up to 5 mm) is featured by the initial rapid stage due to gas expansion from the ignition point, followed by the stage where the flame propagates at a constant visible speed. However, in wider-gap channels, self-oscillations of the flame are developing, leading to alternating fast and slow flame propagation intervals. The frequency of these oscillations is much lower than the acoustic frequency of the channel, they are of relaxation nature due to thermal interaction with the cold channel walls (Figure 1).

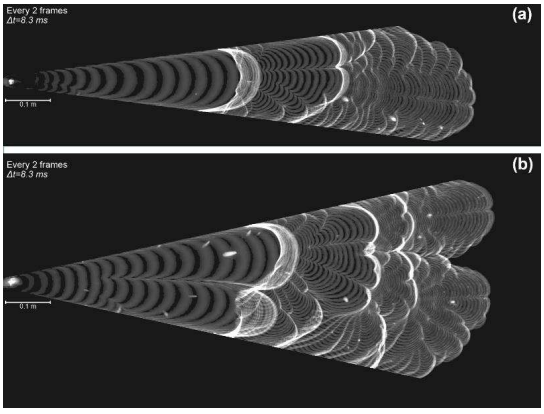

Fig. 1. Composition of frames a video recording of the propagation flame front of a methane-air mixture in a diffuser with an opening angle of 15° (a) and an angle of 25° (b).

By processing the cell properties (size, amplitude, shape) from a large experimental set, statistical properties were derived. In particular, it was shown that the cell size are described quite well by the gamma distribution function, and the cell shape can be approximated by a skewed parabola. Also, the probability of cell splitting is obtained as a function of cell size. With these observations in hand, a model is developed that predicts the motion of the cusps (corner points) between the cells, cell merging and splitting; also, the post-ignition gas expansion at taken into account. The model is shown to reproduce quite well the global cell statistics, flame shape, as well as the trajectories of the corner points.

Another set of experiments was devoted to the study on passage of a premixed flame through an opening (hole) in the internal barrier [3, 4]. Such studies are highly relevant to fire safety problems. Experiments were performed for rectilinear Hele-Shaw channels divided into two equal-volume parts by a rectilinear divider with a centrally located hole of varying width. Stoichiometric methane-air and methane-hydrogen-air mixtures were ignited at the closed end of the channel, propagating towards the barrier.

It was found that flame passage through the hole, or, alternatively, flame extinguishment, exhibited probabilistic behavior: for the same hole geometry and initial conditions, the fraction of cases where the flame passed through the hole (the passage probability) was shown to depend on the hole width. Unexpectedly, non-monotonic behavior was found where the passage probability decreased with the increase in the hole size. This indicates that different extinguishment mechanisms are present: the thermal losses play the predominant role for small hole sizes, whereas for larger holes the alternating direction flow across the hole becomes the principal reason for flame extinguishment. In the latter case, extinguishment occurs due to the impact of a short-duration cold gas jet directed towards the flame approaching the hole (Figure 2).

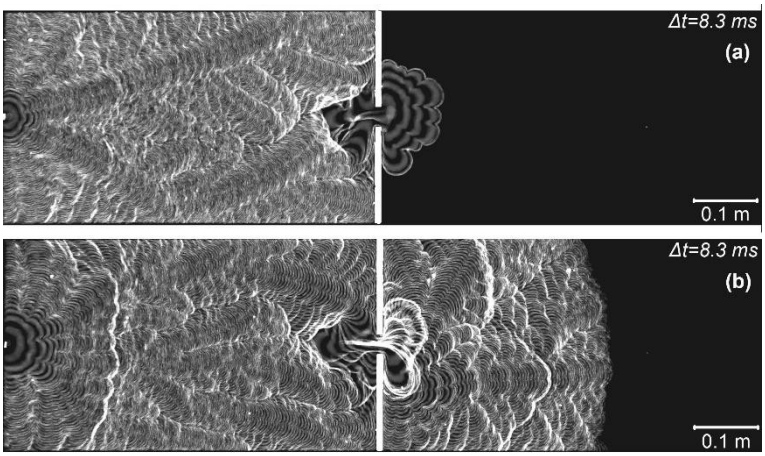

Fig. 2. Photographs of the flame front of a methane-air mixture in a straight channel 3 mm high without hydrogen (a) and with the addition of hydrogen (b).

Experiments with various fuels have shown that addition of hydrogen to methane increases the reactivity of the mixture and promotes flame passage through the hole in the barrier.

Thus, the studies have confirmed that Hele-Shaw cell is a useful configuration for studying the dynamics and statistical features of premixed flames. The quasi-two-dimensional arrangement makes flame recording more convenient than for three-dimensional flames; yet, the fluid dynamic structure of the flow remains complex enough in comparison with flames propagating in tubes (quasi-one-dimensional).

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Hypergolic ignition in acoustic levitator

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The development of next-generation “green” rocket propellants based on hypergolic ionic liquids (HILs) is critically dependent on understanding the fundamental mechanisms governing their ignition. A major obstacle is the inability to directly correlate molecular structure, particularly the functional groups of the cation and anion, with the energy barriers and kinetic bottlenecks that dictate ignition behavior. Traditional research often prioritizes the synthesis and characterization of new HILs, with comparatively less effort devoted to detailed mechanistic ignition studies. This challenge is compounded by the condensed-phase nature of the initial reaction steps and the inevitable wall effects (heat loss, quenching, and perturbed fluid dynamics) inherent in conventional drop-test methods.

To overcome these limitations, we have developed a novel experimental platform based on a bichromatic acoustic levitator. This approach enables containerless, contactless manipulation of droplets, eliminating wall effects and allowing for precise control over the initiation of hypergolic reactions. The device, operating at 25 and 40 kHz, uses a two-stage process: droplets are held in adjacent nodes of a 40 kHz acoustic field, and coalescence is triggered by activating the 25 kHz field. This causes a selective destabilization of the upper droplet while enhancing the trapping force for the lower one, resulting in a deterministic merging process. This method achieves a coalescence success rate of over 95% with a precise, predictable timing delay (20-30 ms), ideal for synchronized diagnostics.

The platform integrates high-speed video diagnostics with time-resolved emission spectroscopy, enabling synchronized observation of both the physical dynamics of merging and the chemical evolution of the flame. We have used this system to conduct the first comprehensive model study of hypergolic ignition in a series of novel HILs based on the 1,2,5-oxadiazole (furazan/furoxan) heterocycle. Key findings include the measurement of reproducible ignition delay times and in-situ flame temperatures. Notably, our results reveal significant discrepancies in ignition delays compared to traditional drop tests, highlighting the importance of containerless conditions. Concurrently, complementary theoretical calculations have been performed to model the molecular structure and vibrational spectra of the ionic liquids, particularly the effect of ion-pair formation on spectral features, which is crucial for interpreting future in-situ spectroscopic data.

On the effect of a weak DC electric field on a Bunsen flame

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The paper presents the results of an experimental study on the effect of a weak transverse electric field on temperature and velocity distribution in a laminar Bunsen methane/air flame. The temperature and velocity fields in the flame are measured by planar laser-induced fluorescence and particle image velocimetry methods, respectively, with and without the electric field. The results show that the electric field alters the shape of the flame front, but its effect on the local flame propagation speed or the temperature distribution behind the flame front is small.

The effects are compared based on the three-dimensional direct numerical simulations of the flame response to the external electric field for complete and reduced models of the charged particle distributions. The complete model involves the diffusion of the electrons and ten most abundant ions in an internal electric field, while the reduced model simulates only the electric force effect for the dominant cation H_3O+. Both models successfully reproduced the flame skewness toward the cathode.

However, the reduced model without other important ions significantly overestimates the electric force on the flame and leads to flame detachment from the burner rim, which is not observed in the experiment. The flow in this case is directed towards the cathode. The complete model reasonably predicts both the flame skewness and the flow field compared to the experimental data. The flow velocity and temperature distributions are measured during the experiment by particle image velocimetry and two-line planar laser-induced fluorescence of hydroxyl radicals, respectively. The velocity field demonstrates the ion wind in the combustion products in the direction of both the anode and the cathode, caused by anions and cations, respectively. The ion wind is concluded to be the reason for the flame deflection and the blurring of the flame cone tip, also observed in the experiment. The blurring effect arises because the charge distribution in the flame front is such that it results in forces acting on the flame cone tip in both the cathode and anode directions, with a dominant component toward the cathode. In addition, the simulation results show that the charged species in the flame front and combustion products completely screen the electric field in the zone between the flame cone and an electrically neutral burner rim, regardless of the external electric field intensity.

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Diffusion-thermal instabilities: from non-linear models to a methodology for verifying combustion reaction mechanisms

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Diffusive-thermal instabilities arising during flame propagation in fuel-air mixtures with a Lewis number different from unity are well known and studied. At Lewis numbers greater than unity and a sufficiently large Zel'dovich number, they lead to flame pulsations. This regime is observed, for example, during the combustion of hydrogen- and methane-air mixtures stabilized on a flat porous burner and can be described within a whole hierarchy of models: evolutionary equations for the front position and temperature, single-step reaction thermal diffusion models, and models with detailed kinetics and gas dynamics in one- and two-dimensional geometries. As we have previously shown, experimentally measured characteristics of thermal diffusion pulsations can be used to verify combustion mechanisms and models. For testing and developing detailed reaction mechanisms, the most productive approach is to use mathematical formulations with one-dimensional spatial geometry, as this eliminates computationally expensive modeling of the gas dynamics of the reacting flows. Obviously, the assumption of one-dimensional flow may not hold for both steady and pulsating flames for a variety of reasons. This work will review our theoretical, computational, and experimental work aimed at studying the factors influencing the deviation of flame pulsation regimes stabilized on a flat porous burner from spatially one-dimensional ones and elucidating the conditions for using these regimes to verify combustion reaction mechanisms.

Unexplored HACA pathway: acetylene trimerization on phenyl radical

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The formation and growth of polycyclic aromatic hydrocarbons (PAHs) are central to understanding soot formation in combustion and the chemical evolution of the interstellar medium. While the hydrogen-abstraction–acetylene-addition (HACA) mechanism is a cornerstone of aromatic growth, it is known to has a "naphthalene ceiling" – further ring expansion beyond naphthalene kinetically inefficient. This work presents a comprehensive investigation into a novel acetylene trimerization (AcT) pathway on the phenyl radical to yield biphenyl, which may provide a "hidden door" to bypass this limitation.

We utilized a synergistic approach combining high-level *ab initio* calculations (G3(MP2,CC)//ωB97XD/cc-pVTZ), RRKM calculations, kinetic modeling augmented with molecular beam experiments. Experiments were conducted at temperatures of 800–1200 K using a high-temperature pulsed flow microreactor coupled with single-photon ionization reflectron time-of-flight mass spectrometry (SPI-MB-ReTOF). A critical component of the study involved comparing the phenyl (C_6H_5) + acetylene (C_2H_2) reaction system with a phenyl radical self-reaction (C_6H_5+ C_6H_5) reference to isolate the AcT pathway from background radical–radical recombination signals.

The identified AcT channel offers a way for bypassing structural limitations at low temperatures (500–800 K), where it maintains a branching ratio of approximately 40%. However, its significance in high-temperature combustion or astrochemical environments is limited by competition with traditional HACA channels leading to naphthalene and phenylacetylene. These findings refine our understanding of PAH assembly.

The study was funded by the state assignment of the Ministry of Science and Higher Education of the Russian Federation, project code FSSS-2026-0010.

The history of carbonaceous grains in the Universe from cosmic dawn to the present day

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Polycyclic aromatic hydrocarbons (PAHs) and carbonaceous dust play a key role in the chemical, thermodynamic, and ionization processes of the interstellar medium, serving as the primary absorbers of ultraviolet (UV) radiation and as important indicators of the chemical evolution of galaxies. This talk will present an overview of the evolution of carbon dust from the epoch of the first stars to the present day. It will examine the formation and growth of carbonaceous particles in various astrophysical environments: in the envelopes of asymptotic giant branch (AGB) stars, in the powerful outflows of Wolf-Rayet stars, as well as the processes of fragmentation in the interstellar medium and dust grain growth in cold molecular clouds.

Special attention will be paid to the spectral signatures of carbonaceous particles, particularly the interstellar UV extinction curve. The nature of the broad absorption feature at 2175 Å, attributed to small carbonaceous particles, will be explained, and its variations from object to object will be analyzed. Recent observational breakthroughs will be highlighted, in which the James Webb Space Telescope (JWST) plays a key role. Operating in the infrared range, JWST has opened an era of direct observation of dust properties in the most distant galaxies, allowing us to indirectly reconstruct the characteristics of UV absorbers at the dawn of cosmic history. Comparing the extinction curves in local galaxies and systems at high redshift ($z > 4–6$) allows us to trace how dust abundance and grain sizes have changed throughout the evolution of the Universe.

The review will outline the main challenges facing theory and experiment: 1) developing models of dust nucleation in stellar atmospheres under different physical parameters, 2) laboratory measurements and quantum-chemical calculations of the spectra of various carbonaceous compounds, and 3) accounting for dust destruction processes in environments with intense star formation for the correct interpretation of observations at high redshifts.

Spectroscopy of the products of the radiation-induced transformations of isolated dimethyl ether molecules in low-temperature matrices

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Dimethyl ether (DME) is one of the relatively complex organic molecules detected in the interstellar environment. It plays an important role in the astrochemical evolution of organic substances in space. In this respect, the chemical transformations of DME under the action of vacuum ultraviolet (VUV) and ionizing radiation under astronomical conditions are of considerable interest.

We report the systematic study on the radiation-induced transformations of isolated DME molecules in various rigid media under X-rays irradiation using FTIR and EPR spectroscopy.

The DME/Ng (1:1000-1:3000; Ng=Ne, Ar, Kr, Xe), DME/$CFCl_3$/Ng (1:1:1000-1:1:1500), DME/SF_6/Ng (1:1:1000-1:1:1500) and DME/M (1:300-1:1000; M=CO, CO_2, N_2) mixtures were deposited in the temperature range of 4.5-35 K. The deposited samples were irradiated with X-rays at 4.5-7 K. To refine the identification of the cationic products of DME radiolysis, we have applied the *ab initio* quantum-chemical calculations at the CCSD4T level with the L2a_3 basis set.

The main products of DME radiolysis were identified and their accumulation curves were obtained [1]. The formation of CH_3OCH_2 radical, and methane plus formaldehyde were detected as the principal products of C–H and C–O bond cleavage of DME, respectively. In addition, the products corresponding to the C–O bond rupture with subsequent hydrogen atoms loss namely HCO radical and carbon monoxide were detected. One of the most intriguing result is the observation the products containing C–C bond, which correspond to the molecular backbone rearrangement (i.e., ethanol, acetaldehyde, etc.). Furthermore, based on comparison with EPR results and *ab initio* calculations we assigned for the first time absorptions attributed to the $CH_3OCH_3^{+\bullet}$ radical cation, which are quite prominent in the presence of electron scavengers (SF_6, $CFCl_3$). The preliminary scheme of DME radiolysis involving the observed products and probable short-lived intermediates was suggested.

The experimental assistance of I.V. Tyulpina is gratefully acknowledged. This work was supported by the Russian Science Foundation (project no. 25-13-00103).

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Spectroscopy of the products of the radiation-induced transformations of isolated dimethyl ether molecules in low-temperature matrices

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Complex organics in cold molecular clouds: more atoms, less understanding

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Recent years have seen a dramatic increase in the number of known interstellar organic species. Their list now comprises long carbon chains, branched molecules, and numerous aromatic compounds [see 1–3 and references therein]. This raises the question of potential gas-phase reaction pathways (or lack thereof), which may lead to the formation of these compounds in extremely cold and rarified gas.

One of the major problems is the origin of kinetic information on the formation of branched and cyclic molecules, which mainly comes from combustion chemistry. Thus, most well-studied reactions leading to the formation of aromatic compounds possess quite high activation barriers, which makes them irrelevant to cold molecular clouds, which necessitates a search for new chemical pathways controlling their synthesis and destruction in a low-temperature environment [4–6].

In this contribution, I will present a review of our understanding of organic chemistry in molecular clouds with a special emphasis on aromatic molecules. I will review major mechanisms, leading to formation of complex organic molecules in cold molecular clouds, including both gas-phase processes and processes in icy mantles induced by high-energy particles.

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New methanol maser lines related to episodic accretion on a massive protostar

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Cosmic masers provide important information about the physical conditions and processes in the interstellar and circumstellar media. There are many masering molecular transitions, which belong to various molecules. Among them, a large fraction are methanol transitions. Methanol is an asymmetric top molecule with a very rich microwave spectrum. It is widespread in the interstellar medium and many lines are very bright. There are advanced theoretical models of methanol excitation (e.g. [1]), which predict maser effect in many transitions. Nevertheless, sometimes unpredicted maser lines are detected. Such a line was detected at 349.1 GHz in our observations of the S255IR high-mass star-forming region with ALMA in 2016 [2]. It was interpreted as a Class II methanol maser. Such masers are excited by IR radiation. This region attracted a great attention due to the luminosity outburst related to the disk-mediated accretion event detected in 2015 [3], one of the first such events observed in massive protostars. There are evidences of episodic accretion events on this protostar which resulted in several ejections observed as knotty narrow ionized jets and wide-angle molecular outflow [4,5]. Our observations in 2019 with the SMA and IRAM-30 telescopes showed a decay of the maser flux at 349.1 GHz and a likely maser effect in some other lines of the same series [6]. Our further ALMA observations in 2021 with a much higher angular resolution show an increase of the maser flux at 349.1 GHz in comparison with 2019. They reveal new Class II methanol maser lines [7] and show that their excitation is caused by the protostar radiation. In addition, highly likely a Class I methanol maser line was detected in the areas of the water maser emission (Salii et al., in preparation). These masers are excited by collisions and are usually associated with shocks.

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ORAL TALKS

Study of the high-temperature oxidation kinetics of furan and tetrahydrofuran under highly diluted conditions

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This work presents a comprehensive experimental and theoretical study of the high-temperature oxidation kinetics of furan and tetrahydrofuran. These two compounds are key representatives of the furan family and serve as parent compounds for the development of combustion kinetic models for more complex substituted furan oxygenates. The importance of this study lies in the need for a fundamental understanding of their elementary oxidation pathways. Such an understanding is required to predict efficient and environmentally benign combustion regimes for promising fuel blends based on these compounds.

The experiments were carried out in a high-vacuum shock tube at temperatures of 1700–3500 K and pressures of 2–3 bar using atomic resonance absorption spectroscopy. Numerical simulations were performed using the Cantera software package. Time-resolved measurements of $O(^3P)$ atom formation and consumption during the oxidation of furan and tetrahydrofuran in mixtures with O_2 and N_2O were obtained for the first time. This made it possible to directly characterize the radical kinetics of these systems over a wide temperature range. The main oxidation pathways leading from the reactants to the final products were identified. These included channels responsible for the formation of toxic aldehydes, cyanides, and polyynes. Rate parameters were also estimated for reactions that cannot be measured directly under the present experimental conditions. The results show that existing kinetic models have significant limitations in describing these systems. These limitations arise from uncertainties in the branching ratios of furan and tetrahydrofuran, the rate constants of multistep chain reactions involving C, H, and CH radicals in the presence of O_2, and the insufficient treatment of the oxidation submechanisms of propenylidene (C_3H_2) and methylene (CH_2). Characteristic features of high-temperature C_0–C_4 oxidation of saturated and unsaturated heterocyclic compounds were identified. On this basis, refinements to the high-temperature core of both baseline and modern kinetic models for the combustion of furan compounds were proposed and implemented.

The results obtained deepen our understanding of the mechanisms governing the high-temperature decomposition and oxidation of furan oxygenates. They also provide a foundation for the development of more accurate kinetic models required for predicting efficient and environmentally safe combustion regimes for new types of fuel blends.

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Radiation-induced transformations of benzonitrile in cryogenic matrices

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Benzonitrile (PhCN), recently detected in space environment [1], is an astrochemically significant molecule. Its polar CN group may be used as a tracer for PAHs (polycyclic aromatic hydrocarbons) and this molecule may be a precursor for biologically relevant molecules containing aromatic moiety.

In this work, we investigated the radiation-induced transformations of benzonitrile in cryogenic media in order to get a model insight into the mechanisms of its evolution in interstellar ices, following the approach outlined previously [2]. The experiments on X-ray radiolysis or VUV photolysis (185 nm) of benzonitrile molecules isolated in solid noble-gas matrices at 5-7 K were carried out using a combination of FTIR and EPR spectroscopy. The results indicate formation of benzonitrile radical ions ($PhCN^{+\cdot}$ and $PhCN^{-\cdot}$). The formation of benzonitrile radical cation ($PhCN^{+\cdot}$) was supported by additional EPR experiments in halocarbon matrices and comparison with the results of quantum-chemical calculations. Regarding molecular products, we observed formation of phenyl isocyanide (PhNC) as a result of isomerization of benzonitrile after X-ray radiolysis or VUV photolysis. The formation of CN-substituted phenyl radicals was also tentatively suggested, however, their structure was not identified directly. Moreover, we observed the IR absorptions, tentatively assigned to the CN-substituted 1,3-hexadien-5-yne (product of the aromatic ring cleavage) after prolonged X-ray irradiation in an argon matrix. It is worth noting that we did not observe formation of unsubstituted phenyl radicals or cyano radical in any experiment, which demonstrates minor importance of the Ph–CN bond cleavage.

In summary, the formation of primary ionic products is an important feature of the radiation-induced processes, whereas the VUV photolysis mainly leads to isomerization of PhCN. Further studies are necessary to establish the detailed mechanism.

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Study of the soot growth process in a flame using the LIF method

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Knowledge about the mechanisms of formation and properties of polycyclic aromatic hydrocarbons (PAHs) and ultrafine (≤ 5 nm) carbon nanoparticles or precursors of soot particles with sizes smaller than ordinary soot (10-50 nm) formed during hydrocarbon combustion and pyrolysis is extremely necessary for prediction and reducing such a harmful for climate [1] and human health [2] emissions. To predict the properties and environmental influence of "mature" soot particles, it is necessary to understand the process of their formation and, in particular, to investigate its early stages, the key participants of which are PAHs and ultrafine carbon nanoparticles which are practically transparent to visible radiation.

One of the informative methods in this field is the well-known and widely used laser-induced fluorescence (LIF) technique, which allows measuring the relative concentrations of PAHs formed in a flame. According to the quantum chemistry calculations, it is well-known that PAHs of various structures and sizes are characterized by specific fluorescence wavelength bands [3]. Thus three detection wavelengths (330, 400, 520 nm) were used to distinguish PAHs with a different number of aromatic rings in their structure. The laminar flat premixed flame was stabilized with a kinetic McKenna type burner. The combustion of ethylene-air flames of various stoichiometries (φ = 1.9, 2.1, 2.22, 2.34) was investigated. The UV fluorescence radiation of flame molecules initiated by Nd:Yag laser (266 nm) was registered with PMT, focus lenses and narrow band filters. The obtained time-resolved data was then processed using the deconvolution method [4].

As a result, the intensities and decay times of LIF signals from PAH, ultrafine carbon nanoparticles and mature condensed soot particles formed in a laminar premixed ethylene-air flame depending on the registration wavelength, the flame stoichiometry and height were obtained. A sequential transition of emission with flame height was identified among the various groups of PAHs and soot particle precursors. The zones of existence of PAHs, ultra-fine carbon nanoparticles, and condensed soot particles in the flame were determined.

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Development of a reduced combustion model for rich hydrogen-air mixtures

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A reduced-order model for describing the combustion of fuel-rich hydrogen–air mixtures is proposed in the present work. The detailed chemical kinetic scheme is reduced to a system of partial differential equations governing the evolution of the mass fractions of H and O_2, as well as the temperature field. For the OH, O and HO_2 radicals, the quasi-steady-state approximation is employed, allowing their profiles to be determined from algebraic relations without solving additional differential equations. The model has been validated using two standard combustion problems: the one-dimensional freely propagating planar adiabatic flame and a flame stabilized on a flat porous burner. For stationary combustion regimes, it is shown that the results obtained with the reduced-order model – including temperature and radical concentration profiles, as well as the dependence of the flame propagation velocity on the equivalence ratio – are in good agreement, for hydrogen equivalence ratios greater than two, with the corresponding results obtained using various detailed chemical kinetic mechanisms, as demonstrated in Fig. 1. In addition, the proposed model has been tested at elevated pressures (up to 10 atm), where it also demonstrates good agreement with detailed kinetic models. Unsteady solutions associated with thermo-diffusive pulsations have also been investigated. In particular, it is shown that the pulsation frequencies at the bifurcation point predicted by the reduced-order model fall within the range of values obtained from detailed kinetic models.

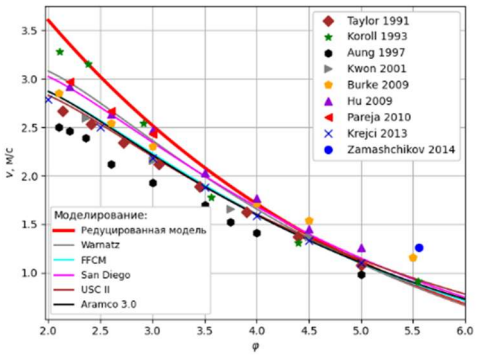

Fig.1. Dependence of the flame propagation velocity on the equivalence ratio. Solid lines correspond to numerical simulations, while markers denote experimental data [1].

The proposed approach provides a compromise between the accuracy of detailed kinetic models and computational efficiency, and may serve as a convenient framework for further investigations of combustion instabilities in fuel-rich hydrogen–air flames.

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Sulfur absorption during thermal disposal of acid tar and bitumen

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Due to the high (up to 7%) sulfur content, the utilization of heavy hydrocarbons is a complex and expensive process. The main direction of their processing is various thermal methods, which mainly produce thermal energy.

The aim of the work was to determine the degree of sulfur absorption by various finely dispersed calcium-containing materials and the optimal amount of absorbers used, as well as to verify the possibility of their reuse.

A study was conducted in a muffle furnace on the combustion of mixtures of oil waste (bitumen and acid tar) with various types of finely dispersed calcium-containing absorbers (limestone, chalk, seashells, quicklime). The influence of the type and composition of the calcium-containing additive on the degree of absorption of sulfur contained in bitumen and acid tar has been revealed, and the prospects for reuse of the absorber have been verified.

Experiments have shown that when burning compositions with tar, with an increase in the amount of the absorber additive, the concentration of sulfur in solid combustion products decreases, however, due to an increase in the mass of the absorber, the total amount of absorbed sulfur increases, reaching a maximum with a mass content of 75% of the absorber (chalk, limestone – ~80%, shells – 67% and quicklime – ~90% of the absorbed sulfur). Further, the degree of sulfur absorption practically does not change with an increase in the proportion of the absorber.

When burning compositions with bitumen, an increase in the addition of an absorber also leads to a decrease in the concentration of sulfur in solid combustion products, however, unlike compositions with acid tar, the type of this dependence differs significantly from the linear one. As the content of all types of additives (chalk, limestone, quicklime) increases, the proportion of sulfur absorbed by solid combustion products increases, reaching 100% with an additive content of 75% in the mixture.

When using the absorber repeatedly, the concentration of sulfur in it increases, but the efficiency of its absorption of sulfur is significantly reduced.

The measurements of the elemental composition of the materials used and the combustion products were carried out using the equipment of FRC PCP MC RAS.

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Hydrogen-Enriched Fuels for Gas Turbine Combustors: Stability, Emissions, and Burner Design

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The transition of gas turbine power systems toward low-carbon operation requires lower greenhouse gas emissions without sacrificing reliability or operational flexibility. In this context, hydrogen and methane-hydrogen mixtures are increasingly viewed as promising fuels for gas turbine applications. Methane-hydrogen mixtures are of particular practical interest because they allow a gradual increase in hydrogen content while preserving much of the existing gas infrastructure and combustion hardware.

At the same time, the use of hydrogen in gas turbine combustion chambers creates serious engineering challenges. Hydrogen has a high laminar flame speed, wide flammability limits, short ignition delay, and strong diffusivity. These properties improve lean-burn capability, but they also increase the risk of flame flashback, local overheating, and thermoacoustic instability.

A key issue is the choice of combustion concept. Diffusion-based combustion systems are generally more tolerant to high hydrogen fractions and offer good flame stability. However, they often produce higher NOx emissions. Lean premixed systems have a stronger potential for low-emission operation, but they require much tighter control of residence time, local flow velocity, flow structure, and fuel distribution between circuits.

For this reason, staged fuel supply, separate pilot and main circuits, and intensified mixing become especially important. As the hydrogen fraction increases, dedicated burner designs become essential. Their role is to prevent flashback, maintain stable flame anchoring, and keep wall temperatures within acceptable limits. Multichannel and other specialized burner concepts are therefore of great interest for hydrogen-containing fuels.

Experimental studies with model burners and combustion chambers make it possible to assess the effects of fuel composition, excess air ratio, inlet air temperature, and fuel split between circuits on flame stability and emissions. These results show that methane-hydrogen mixtures should be seen not only as a tool for reducing CO2 emissions, but also as a factor that requires a broader redesign of the combustion process in gas turbine chambers.

Effective use of methane-hydrogen mixtures therefore depends on a coordinated choice of fuel composition, mixing strategy, flame stabilization method, and fuel supply parameters. This makes further experimental and numerical research highly relevant for the development of low-emission and stable combustion chambers for hydrogen-containing fuels.

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Investigation of the methane-air flame oscillations by 2D LIF method

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In the current work the dynamics and morphology of the diffusive-thermal oscillations of burner stabilized methane-air flames are experimentally studied by laser-induced fluorescence method (LIF) in two cases: (i) small amplitude pulsations for φ = 1.15 and mixture flow rate M = 0.215 kg/m^{2}s near the boundary of stability and (ii) large scale relaxational pulsations at M = 0.1 kg/m^{2}s far away from the stability boundary. The influence of nitrogen co-flow on the formation of secondary diffusion flame is investigated. The local concentration of OH radical was measured with 50 um spatial resolution by exciting the R2(10) rotational line of the A-X (1, 0) transition band. It is shown, that near the stability limit and in the presence of sufficient co-flow the flame has one-dimensional structure. In contrast to this, the dynamics of flame oscillations at parameter values far from the stability boundary becomes complex two-dimensional, this is shown in Fig. 1, where the photo of the flame (a) and two-dimensional distribution of [OH] in two different phases (b-c) obtained by interpolating about 200 points are demonstrated for φ = 1.15, M = 0.1 kg/m^{2}s and the presence of sufficient N2 co-flow. The results are consistent with [1].

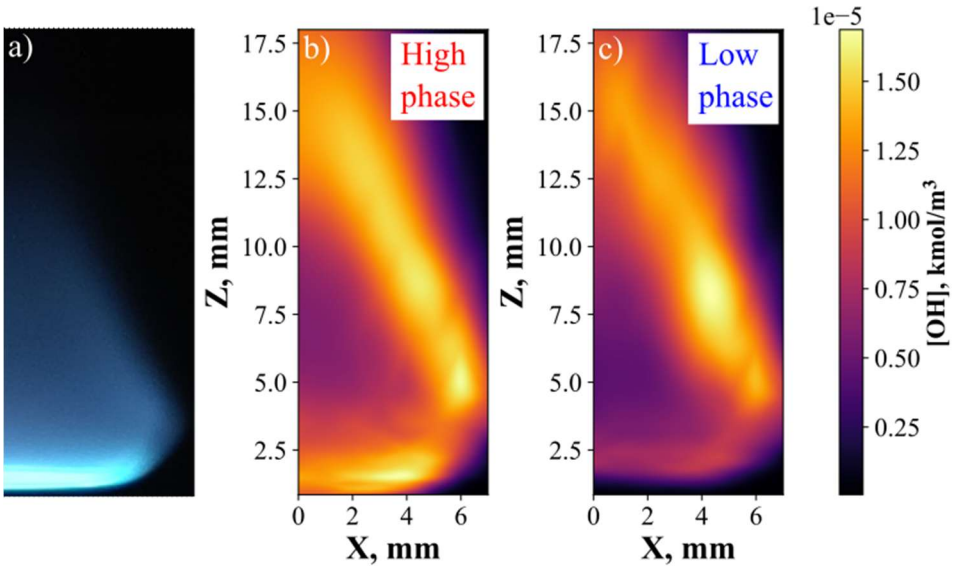

Fig.1. Picture of the methane-air flame (a) and distribution of the [OH] (b-c) for φ = 1.15, M = 0.1 kg/m^{2}s.

For the first time, the dynamics and structure of the pulsating methane-air flames were studied using the LIF method. The dependency on nitrogen co-flow was investigated. Obtained data about flame structure in pulsating regimes can be implemented for verification of detailed mechanisms.

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The effect of hydrocarbons and oxygenates addition on kinetics of ammonia oxidation

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Ammonia is a prospective chemical carrier of hydrogen as well as carbon-free fuel. However, due to its specific combustion characteristics, pure ammonia is unsuitable for use as a fuel in modern engines. One way to improve its combustion properties is the co-firing with highly reactive fuels (e.g., hydrocarbons and oxygenates). However, the potential application of such blends is impossible without reliable detailed chemical kinetic mechanisms of their oxidation and combustion. The development of such mechanisms is based, in particular, on testing them against experimental data obtained over a wide range of conditions.

In this work the new experimental data on the flame structure of ammonia blends with hydrocarbons and oxygenates were obtained. These data are combined with the results on ammonia/hydrocarbons (oxygenates) blends oxidation at low temperatures. Molecular beam mass-spectrometric setup with the soft electron-impact ionization was used for flame structure measurement. The measurements were performed both at atmospheric and elevated (3 and 5 atm) pressures, whereas equivalence ratio was 0.8-1.2. Botha-Spalding type burner was used for flame stabilization and its temperature was 368K in all experiments. In high-pressure experiments the burner was placed in a special chamber pressurized with nitrogen. Thin S-type thermocouples were used for temperature measurements. Experiments on low-temperature oxidation were performed using the jet-stirred reactor. The speciation was measured at atmospherics pressure, in the temperature range from 600 to 1300 K, and at constant residence time of 1s. Numerical simulation was performed with the CHEMKIN package. For flame structure simulation PREMIX module was used, whereas oxidation in jet-stirred reactor was simulated with the PSR code. Several published detailed chemical kinetic mechanisms of ammonia/hydrocarbons (oxygenates) oxidation were tested in order to assess their predictive capability. The effect of different additives on ammonia oxidation was analysed in terms of intermediates formation and the temperature range of the blend oxidation. Special focus was given to the cross-reactions of carbon-and nitrogen-containing species interactions. The effects of initial composition, pressure and temperature were analysed as well.

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Thermal radiation characteristics of a cylindrical hybrid porous-microchannel counterflow burner

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Filtration combustion of gas in an inert porous medium has a number of advantages that provide wide possibilities for practical application such as high specific power, low emissions, wide power range, combustion stability in a wide range of excess fuel coefficient and high thermal efficiency. Thermal inertia of the porous medium determines favorable conditions for combustion and flame stabilization. That provides ample opportunities for controlling the combustion process by changing the flow rate, the composition of the combustible mixture or the structure of the porous medium. The main focus in this work is paid to the study of the thermal radiation characteristics of a cylindrical porous burner of a new design.

In this work a novel configuration of the burner is proposed as a hybrid concept of counterflow mircro-channel and cylindrical porous combustors. The fresh mixture is supplied from the ends of two mirco-channels aligned along the axis of symmetry with a gap between them, through which the combustion products are exiting. This system of capillaries is encircled by a porous media made of zirconium grains placed in an quartz tube. The flow of hot combustion products is thus reverted and preheats both the porous cylindrical layer and feeding tubes. It is found that the heat recuperation allows to steady burn propane-air mixture with variation of the flow rate in an order in magnitude. The heat released from the chemical reaction is effectively converted in the thermal radiation flux, the power and spectral characteristics of which are studied. It is demonstrated that with the use of axillary optical system the power density can reach several units of W/cm^2.

It is shown that the burner can be successfully used as a source infra-red radiation with a fraction of chemical power of fuel converted into the power of electromagnetic field reaching the value as high as 80 %. Due to the divergent flow of hot combustion products discharged from the gap space between the capillaries through which the fresh mixture is fed into the burner, the volume of the heated zirconium filling can be significantly increased as compared to [1] and can attain several centimeters in axial length. The gain in the surface of the porous filling emitting thermal radiation results in the enhancement of its power so that the same power density can be attained at lower flow rates.

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Investigation of flat burner flame 2D structure by studying absolute OH concentrations utilizing saturated laser-induced fluorescence

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In current work, a two-dimensional flame diagnostic technique based on saturated laser-induced fluorescence (LIF) was developed by measuring the absolute concentration of hydroxyl radicals (OH). The method was tested on methane–air flames stabilized on a flat porous burner. It was shown that, for fuel-rich mixtures ($\varphi = 1.15$), the structure of the flame front is significantly two-dimensional due to the formation of a secondary conical diffusion flame at the interface with the surrounding air. Use of a coflowing nitrogen shielding flow with a linear velocity equal to that of the fuel–air mixture completely suppresses the secondary flame and ensures a one-dimensional front structure in the central region of the burner up to distances of 20 mm from its surface. Based on processing of the two-dimensional OH concentration distributions the flame front surface was reconstructed as a function of radius. It was demonstrated that in the central region the front is flat within the measurement uncertainty (50 μm), whereas edge distortions caused by heat exchange with the surroundings do not exceed 100 μm in height and 1 mm in radius. For the first time, it was experimentally shown that, for pores with diameter of 400 μm, flow nonuniformities on the scale of the porous structure do not lead to deformation of the combustion front.

Experimental setup consists of a solid-state laser system based on a Ti:sapphire laser, a LIF signal collection and detection system, and a flat porous burner. The laser system was tuned to excite the isolated R2(10) transition of the (1–0) vibrational band of the $A^2\Sigma - X^2\Pi$ electronic transition of OH radical at a wavelength of 281.9 nm. The LIF signal was detected in the wavelength range defined by an Edmund Optics 313 nm filter with an FWHM of 5 nm. The experimental setup is described in detail in [1]. A spatial resolution on the order of 50 μm was achieved, which is substantially smaller than the thermal flame thickness and the characteristic scales of the heat-release zones.

Developed technique enables high-precision determination of the laminar burning velocity under critical flame blow-off condition and may also be used for verification of detailed kinetic mechanisms and validate combustion models.

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Numerical and experimental investigation of performance of thermoelectric generator based on porous counter-flow burner with passive air cooling.

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Over the past two decades, small-scale combustion-based power generation systems have attracted significant attention due to the much higher specific energy of hydrocarbon fuels compared to batteries, leaving room for combustion-based devices despite rapid advances in battery technology. This work focuses on the thermoelectric method of converting heat into electricity, which offers the advantages of no moving parts and minimal maintenance requirements. While water-cooled thermoelectric generator (TEG) systems have achieved efficiencies of 3–4%, air-cooled systems have generally remained below the 1% threshold. A key challenge is the stabilization of the combustion process when heat is extracted for power generation. To address this problem, we developed a highly stable hybrid counterflow microchannel porous burner that converts approximately 2/3 of the fuel's chemical energy into thermal radiation without altering the combustion mode. This radiant energy flow is highly promising for integration with a TEG. The aim of this work was to couple our developed burner with a commercial Bi_2Te_3-based thermoelectric generator via radiative heat transfer that ensures the combustion regime remains unchanged, as well as to develop a mathematical model for predicting and optimizing system performance.

As a result, the radiative heat flux from the burner, the hot and cold side temperatures of the TEG, and the electrical power at optimal load were experimentally measured and numerically simulated as functions of the distance between the burner wall and the TEG, as well as of the burner thermal regimes. The simulation results demonstrated good agreement with the experimental data. The proposed model allowed us to predict the optimal operating conditions of the generator, in particular, to estimate the minimum propane-air mixture flow rate required to achieve the maximum hot side temperature of the TEG and the maximum generated power (1.2W per TEG module).

Ultimately, we demonstrated that an overall system efficiency of approximately 1% (consistent with literature data for air-cooled thermoelectric generators) can be achieved using a standard commercial TEG module, highlighting the potential of the proposed approach for portable power generation when using more advanced thermoelectric modules or their cascaded configurations, as well as pending future advances in TEG technology.

Screening of polycyclic aromatic hydrocarbons with sp- and sp²-hybridized carbon atoms and analysis of their properties

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Polycyclic aromatic hydrocarbons (PAHs) are present in the interstellar medium of galaxies, where they control the heating of neutral gas and the charge balance of molecular clouds. PAHs are formed in the outflows from late type stars through chemical processes similar to those occurring in soot-forming flames, as well as through ion–molecule reactions and neutral radical reactions in dense cloud cores. To assess the diversity of PAH composition and structure, it was of interest to collect up-to-date statistics on all currently known crystalline structures of PAHs and their properties. The results of such an analysis are presented in this study.

A dataset of more than 3000 crystalline PAH structures containing only sp- and sp²-hybridized carbon atoms was prepared. Based on the collected information, we analyzed their properties and molecular structural features, identified secondary structural units, and classified the mechanisms of topological crystal assembly. In addition, common cyclic fragments that make up PAHs were determined. The collected information can be useful for explaining the mechanisms of PAH formation and for searching for them in the interstellar medium.

PAH formation can occur via various chemical mechanisms (HACA, HAVA, MAC, RRR, etc.) or their combination, which can be described as sequences of chemical reactions leading to specific products. Among the main parameters for estimating reaction rates are the rate constant and the activation energy. These characteristics are stored in kinetic parameter databases and determine the predominance of PAHs of a particular composition and structure in the interstellar medium. To gather current information on the kinetic parameters of chemical reactions involving PAHs, a comparison was performed of the following databases: the NIST Chemical Kinetics Database (SRD 17, for gas-phase reactions), the Process Informatics Model (PrIMe, for combustion modeling), the Open Reaction Database (ORD, for organic chemistry), and the KInetic Database for Astrochemistry (KIDA, for astrochemistry).

The screening of PAH data and their analysis were carried out as part of a state assignment.

Self-Propagating High-Temperature Synthesis of Highly Dispersed SiC-Based Ceramic Nitride–Carbide Composites Using Sodium Azide and Polytetrafluoroethylene

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To realize the potential advantages of SiC-based ceramic composites, it is critically important to use starting powders with a high degree of dispersity. The transition from micron powders to submicron and nanoscale components makes it possible to reduce the sintering temperature, decrease the porosity of finished products, and significantly improve their mechanical properties [1]. However, obtaining highly dispersed powder compositions is associated with certain difficulties. The traditional ex-situ approach, which involves mechanical mixing of ready-made TiN (Si_3N_4, AlN) and SiC nanopowders, has serious drawbacks: the high cost of nanopowders and the tendency of nanoparticles to form strong agglomerates that are difficult to break during mixing, leading to inhomogeneity of the composite structure.

In this regard, in-situ methods that involve the chemical synthesis of composition components directly during the production of the powder mixture from cheaper starting reagents are more preferable. Among such methods, self-propagating high-temperature synthesis (SHS) occupies a special place [2]. The azide SHS process has already been applied to produce Si_3N_4-SiC, AlN-SiC, and TiN-SiC powder composites; however, the phase compositions of the synthesized composites differ significantly from the calculated theoretical compositions, showing a much lower SiC content or its complete absence, as well as the presence of a large amount of impurities [3]. At the same time, it is known that the use of a catalytic additive of powdered polytetrafluoroethylene (PTFE), a fluoroorganic polymer, in SHS processes can greatly promote SiC formation due to chemical activation and participation in carbidization, but this approach has not been used in azide SHS [3].

Therefore, it is relevant to investigate the azide SHS process using an activating and carbidizing PTFE additive instead of the traditionally employed gas-forming halogen salts, in order to bring the phase composition of synthesized highly dispersed Si_3N_4-SiC, AlN-SiC, TiN-SiC powders significantly closer to the desired theoretical composition.

For the investigations, charge compositions consisting of mixtures of elemental Si, Al, Ti, and C, as well as PTFE and NaN_3, were selected with five molar ratios of the nitride to carbide phases: 4:1, 2:1, 1:1, 1:2, and 1:4. Four PTFE contents in the charges were used: complete replacement (100%) of technical carbon with PTFE, as well as partial replacement (10, 20, and 30%).

Thermodynamic calculations showed that for all formulated reaction equations using PTFE, the adiabatic temperatures (2348–3348 K) are sufficient for the reactions to proceed in the combustion mode. It was experimentally established that when partial replacement of technical carbon with PTFE is used, the synthesized powders are highly dispersed with particle sizes below 1 μm, and the phase composition of the composites is substantially closer to the calculated theoretical composition due to an increased silicon carbide content compared to using halogen salts. At the same time, the consumption of expensive and toxic sodium azide is significantly reduced.

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Thermodynamic evaluation of conditions for the Fe (III) oxide reduction during downdraft gasification of coal mixted with lean ores

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This paper presents a thermodynamic assessment of the conditions for Fe (III) oxide reduction during downdraft gasification of a coal mixed with lean ore. Downdraft gasification provides favorable conditions for Fe_2O_3 reduction: high temperature (800-1200°C) and a reducing environment (producer gas, primarily comprising CO and H_2). The discharge of solid gasification products (along with the reduced iron) occurs with the filtration of the producer gas through them, preventing reoxidation of Fe. The calculation is based on the minimization of the Gibbs free energy, which allows for the prediction of the equilibrium composition of the reaction products and the determination of the most favorable temperature regimes for the extraction of pure metals. The study examined a system containing only iron oxide and gaseous coal gasification products (a typical producer gas composition). The conditions for Fe_2O_3 reduction were investigated depending on the temperature of the producer gas and its excess relative to Fe_2O_3. It was shown that carbon is present in the system at a producer gas temperature below 900K. A threefold excess (by stoichiometry) of the reducing components of the producer gas (CO and H_2) provides condition for Fe_2O_3 reduction to metal Fe.

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A shock tube study of NH_3 pyrolysis under strong Ar dilution

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Ammonia is increasingly recognized as a promising carbon-free energy carrier and synthetic fuel [1], making a deep understanding of its high-temperature pyrolysis kinetics essential for the development of predictive combustion models.

This work presents an experimental study of high-temperature (2000–3000 K) ammonia pyrolysis under conditions of high dilution (500/3300 ppm NH_3 in Ar) at pressures of 2–3 bar using vacuum ultraviolet (VUV) absorption spectrometry. An *in situ* diagnostic method in the band 129.9–131.1 nm was developed to obtain direct time-resolved NH_3 absorption profiles. The temperature dependence of the ammonia absorption cross-section $\sigma(T)$ for the considered spectral area was measured for the first time, which made it possible account for potential ammonia adsorption in shock tubes. The effect of shock tube pre-passivation on the accuracy and reproducibility of kinetic measurements was also analyzed. The results clearly demonstrate the urgent need for monitoring ammonia concentrations under highly dilution conditions.

Thus, the reliable NH_3 concentration profiles obtained *via* the described method have significant value for validation of kinetic mechanisms. Subsequent kinetic modeling, complemented by rate of production and sensitivity analyses, identified several mechanisms that satisfactorily reproduce the experimental data. In addition, the obtained results made it possible to estimate the uncertainty of the key dissociation rate constant $NH_3 + M \rightleftarrows NH_2 + H + M$, which is essential for the development of kinetic models for the combustion chemistry of nitrogen-containing compounds.

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POSTER TALKS

The effect of thermal misbalance and thermal conductivity on the dispersion properties of MHD waves: thin flux tube versus magnetic slab models

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Nonadiabatic processes — heating, radiative cooling, and parallel thermal conduction— determine the space-time structure of the solar corona plasma and significantly affect the excitation, propagation, and attenuation of acoustic, magneto-acoustic (MA), and Alfven waves. In an optically thin medium, the thermal balance is maintained by a generalized heat loss source, and parallel thermal conductivity redistributes energy along magnetic lines, forming the temperature profile and dynamics of the plasma. Slow magnetoacoustic waves are particularly sensitive to these effects, which makes them a powerful tool in coronal seismology for diagnosing the solar atmosphere.

Studies of the effect of thermal conduction and thermal misbalance on slow MA waves show qualitatively consistent results in two main models: a thin flux tube and a magnetic slab. In the long-wave (low-frequency) limit, the behavior of waves in both models is determined by thermal misbalance, which leads to a modified adiabatic velocity taking into account the heating and cooling power. In the short-wave (high-frequency) limit, the phase velocity is determined by parallel thermal conduction and tends to the isothermal sound speed.

The fundamental difference between the models lies in the spectrum of their solutions. The thin flux tube, modeled as a narrow-isolated waveguide, supports a single mode - the slow magnetoacoustic wave. In contrast, a magnetic slab of finite thickness generates a whole spectrum of transverse harmonics ($n = 1, 2, 3 ...$). Each of them forms an independent dispersion branch with its own transverse structure. In the region of short periods, these branches diverge, but as the wavelength increases, they asymptotically converge. Accordingly, the phase velocity dispersion in the thin flux tube model is weakly pronounced and is determined by the physical parameters of the medium. In the magnetic slab model, a strong geometric dispersion is added to these effects, related to the final slab thickness, which leads to a complex dependence of velocity on the wavenumber.

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Ion Chemistry of Premixed Acetone and Butanone Flames: Experimental and Theoretical Investigation

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Interest in the combustion of acetone and butanone is motivated by several factors. First, acetone and butanone are the simplest ketones; therefore, their combustion mechanism can serve as a basis for the development of a generalized mechanism describing the homologous series. Second, acetone is an important intermediate in the oxidation of more complex organic compounds, implying the presence of similar intermediates in the flames of heavier fuels. Third, acetone and butanone themselves are considered as fuel additives and alternative fuels [1,2].

Ionization in carbon-based fuel flames is a natural process. Ions are primarily formed via the chemiionization reaction: $CH^+ + O^- \rightarrow HCO^+ + e^-$. Despite the low concentration of charged species in the flame, the ionic structure can influence combustion kinetics due to the high rates of ion–molecule reactions. To develop next-generation high-performance in-ternal combustion engines, ion-sensing technology is considered a promising tool for real-time monitoring and control of in-cylinder combustion processes.

Neutral combustion mechanisms for acetone and butanone are well established in the literature, whereas the mechanisms governing the formation and redistribution of charged species in these flames remain largely unexplored. The main cations were experimentally identified and reported by Fialkov [3]; however, detailed mechanisms incorporating reactions involving these species are currently lacking.

Positive ions naturally formed in laminar premixed burner-stabilized acetone/O2/Ar and butanone/O2/Ar flames were sampled and analyzed using modified Hiden HPR-60 – molecular beam system coupled with quadrupole mass spectrometer. The burner consisted of a perforated matrix with a diameter of 16 mm, its temperature maintained at 368 K. Liquid fuel was delivered by a syringe pump to vaporizer, where it was evaporated and mixed with oxygen and argon. Flame gases were sampled by a nickel conical nozzle at various distances from the burner. Mass spectra were recorded over the m/z range of 1-300. Temperature profile was determined via the «pneumatic probe» method.

The spatial distributions of charged and neutral species in the flames were performed using the Cantera 2.6 software package [4]. Using a detailed chemical-kinetic model for the transformation of natural components for the acetone and butanone flame, as well as spatial distributions of ions discovered in the experiment, a chemical-kinetic mechanism was developed.

Thermochemical data of ions were calculated using high-precision methods of quantum chemistry W2-F12 type.

Was found that proposed mechanism correctly describes the relative contents of H_3O^+, CH_5O^+, $C_2H_3O^+$, $C_3H_7O^+$, $C_4H_9O^+$, $C_5H_{11}O^+$. The proposed model was analyzed and the main reaction pathways involving ions were established.

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The effects of magnetic field on gravitational stratification of the solar atmosphere

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The solar coronal heating problem remains one of the key unsolved issues in solar physics. Heating models are traditionally divided into stressing (DC) and wave (AC) mechanisms. Their verification requires reliable constraints on the heating function, usually written as a power-law dependence on density and temperature.

One established approach uses MHD seismology: observed properties of magnetoacoustic waves (damping times, phase shifts) impose limits on the heating power indices through the thermal misbalance effect.

An independent method, developed in paper [1], relies on observed gravitational stratification of the solar atmosphere. Using forward-modelled EUV data from SDO/AIA, altitude profiles of density and temperature are obtained. Assuming local thermal balance between heating and radiative cooling together with hydrostatic equilibrium, the method directly yields a set of allowed values for the heating power indices.

The original formulation assumed a constant magnetic field that does not affect vertical force balance. The present study removes this limitation by including the full Lorentz force in the stationary MHD equations. We consider realistic magnetic configurations such as expanding flux tubes typical of coronal loops, horizontal or weakly inclined fields.

Quantitative comparison shows that magnetic effects are negligible only in weak-field quiet-Sun regions. In regions with strong magnetic fields and large gradients of magnetic pressure or curvature of field lines (such as loops, plumes, and coronal holes), the allowed domain of heating indices shifts noticeably.

Inclusion of realistic magnetic geometry makes the gravitational-stratification diagnostic both more accurate and more powerful. It opens the way for joint seismological and stratification constraints on the coronal heating function.

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NITRILE REACTION PATHWAYS IN TITAN's ATMOSPHERE

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The orange-brown color of the aerosol haze in the atmosphere of Saturn's moon Titan is due to the presence of hydrocarbon nitrogen-containing compounds $C_xH_yN_z$ [1]. These compounds absorb high-energy radiation in the upper layers of Titan's atmosphere, protecting other complex organic molecules from ultraviolet solar radiation in its lower layers, just as Earth's ozone layer protects all life on Earth. Despite extensive study of Titan's chemistry, the complex and diverse atmospheric kinetics of the low-temperature formation and destruction of $C_xH_yN_z$ remains insufficiently understood.

In this study, optimized geometries and energies of compounds on the potential energy surface (PES) of the C_4H_4N molecular system are found using electronic structure calculations at the ωB97X-D density functional theory level with the cc-pVTZ basis set. The goal is to identify reaction pathways leading to the formation of mononitriles (z=1) observed in the atmosphere of Titan, a moon of Saturn. Of the 14 bimolecular reactions occurring on the PES of the C_4H_4N molecular system, 11 contain entry barriers that are insurmountable under Titan's atmospheric conditions, while the remaining reaction pathways have barrier energies lower than the sum of the energies of the separated reactants. During the barrier-free addition of the methylidene radical (CH) to acrylonitrile (CH_2CHCN), the cyano radical (CN) to allene (CH_2CCH_2), and to propyne (CH_3CCH), primary adducts C_4H_4N are formed, releasing chemical energy sufficient to overcome all barriers to both heterocyclic pyrrole radicals c-C_4H_4N and the mononitriles detected in Titan's atmosphere: hydrogen cyanide (CHN), hydrogen isocyanide (HNC), cyanoacetylene (HCCCN), acrylonitrile (CH_2CHCN), acetonitrile (CH_3CN), and cyanopropyne (CH_3CCCN) (Fig. 1). In the lower layers of Titan's atmosphere, pyrrolyl radicals can be stabilized by collisions with N_2 and subsequently participate in processes of increasing the molecular mass of prebiotic N-containing polycyclic hydrocarbons.

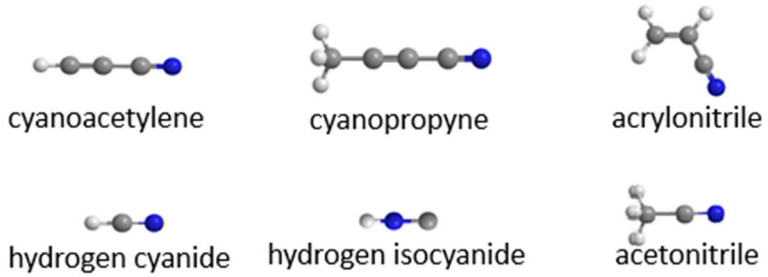

Fig. 1. Mononitriles detected in Titan's Atmosphere

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Mechanism of Glycolamide Formation in the Reaction of Formamide with Methanol

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Formamide ($HCONH_2$) is an important prebiotic molecule found in the interstellar medium. Its reactions with other common compounds, such as methanol (CH_3OH), are considered a possible route to the synthesis of complex organic molecules, including isomers of the amino acid glycine ($C_2H_5NO_2$). One such isomer, glycolamide, was detected in 2023 in the star-forming region Sgr B2 [1]. In this work, using high-level *ab initio* calculations (CBS-QB3 method) and automated conformational analysis, four products of radical–radical recombination of formamide and methanol were studied. For each product, the relative stability and adiabatic ionization energies (AIE) were determined, the latter being necessary for laboratory identification using photoionization mass spectrometry.

Table 1. Characteristics of $C_2H_5NO_2$ conformers

Reaction product	N_{conf}	ΔH_{conf}, kJ·mol^{-1}	AIE, eV
Methyl carbamate	2	0.0-32.3	10.11-10.27
Glycolamide	2	27.1-29.6	9.64-9.66
N-(hydroxymethyl)formamide	7	49.5-64.5	9.89-10.20
N-methoxyformamide	3	241.2-264.3	8.86-9.17

The most thermodynamically stable isomer is methyl carbamate. However, the less stable glycolamide is the one observed in the interstellar medium. This is explained by kinetic reasons: glycolamide is formed via recombination of the carbamoyl (•$CONH_2$) and hydroxymethyl (•CH_2OH) radicals, the most accessible and energetically favorable precursors. The more stable methyl carbamate would require the participation of the less likely methoxy radical (CH_3O•). Moreover, glycolamide has a significantly larger dipole moment, which facilitates its radio astronomical detection. Based on the calculated AIE values, schemes are proposed for the identification of all four isomers in laboratory experiments using photoionization mass spectrometry. Gradually increasing the photon energy would allow registering signals in the following order: N-methoxyformamide (~8.9 eV), glycolamide (~9.7 eV), N-(hydroxymethyl)formamide (~9.9 eV), methyl carbamate (>10.1 eV).

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An experimental and theoretical study of formation of cations in premixed n-butanol flames

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Oxygenated biofuels such as butanol reduce greenhouse gas and soot emissions while offering high energy density and compatibility with existing gasoline engines, making them promising renewable alternatives for energy diversification and climate mitigation [1]. Among its isomers, n-butanol exhibits the highest reactivity, highlighting its practical relevance and the potential of ion-sensitive diagnostics for combustion control. However, ionic chemistry in n-butanol flames remains poorly understood due to the limited availability of relevant experimental data.

The aim of this work was to develop an ion chemistry model for flames n-butanol based on the novel experimental data on spatial distribution of ions in laminar premixed flames of n-butanol. The data was obtained from the molecular beam mass spectrometry of $C_4H_9OH/O_2/Ar$ flames with different equivalence ratios (ϕ = 0.75, 1.00, 1.25), stabilized on a flat-flame burner at atmospheric pressure. Multiple new cations with the general formula $C_xH_yO^+$ (x=1-4) were identified and their thermochemical data was calculated using W2-F12 method. A chemical-kinetic mechanism with reactions involving charged species was developed to describe ion chemistry.

Using the obtained mechanism, numerical calculations of the cationic structure of flames were carried out using Cantera 3.2 software [2]. Based on a comparison of experimental and simulation data, it was found that the proposed mechanism correctly describes the relative contents of H_3O^+, $C_2H_3O^+$ and $C_3H_6OH^+$, but underestimates the $C_3H_8OH^+$, $C_4H_{10}OH^+$ content. The proposed model was analyzed and the main reaction pathways involving discovered ions were established. The results obtained in this work will serve as the basis for further improvement of the model of ionic chemistry in oxygenated-fuel flames.

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Theoretical study of gas-phase polymerization processes of *p*-xylylene

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Para-, *ortho*-, and *meta*-xylene are aromatic hydrocarbons consisting of a benzene ring substituted with two methyl groups. Xylenes are widely used as solvents and are common components of both biofuels and petroleum-derived fuels. However, the presence of aromatic compounds in fuel formulations promotes increased emissions of polycyclic aromatic hydrocarbons (PAHs), many of which are potent carcinogens and key precursors in the formation pathways of solid soot particles. Given these considerations, investigating the mechanisms of PAH growth during xylene combustion becomes particularly important.

Previous studies have indicated that during the combustion of fuel-rich xylene–oxygen mixtures, the dominant mechanism for PAH growth is presumed to follow the HACA pathway initiated by styrene. Additionally, the increased methylation of the benzene ring enhances the formation of benzyl intermediates, which raises the probability of radical recombination and, consequently, promotes PAH yields. At the same time, structural differences among the isomers account for alternative PAH growth pathways that are unique to each specific isomer. For instance, H-abstraction from a methyl group of *p*-xylene yields the *p*-xylyl radical — a resonance-stabilized species featuring a delocalized radical center (Fig. 1). Its subsequent dehydrogenation (H loss) results in a loss of aromaticity and the formation of *p*-xylylene, a compound known to readily undergo polymerization, as extensively demonstrated in the vapor deposition of Parylene protective coatings. However, the role of this pathway under combustion and pyrolysis conditions remains poorly understood. Therefore, the present study aims to perform quantum chemical calculations of the rate constants for the relevant reactions to enable subsequent detailed kinetic modeling.

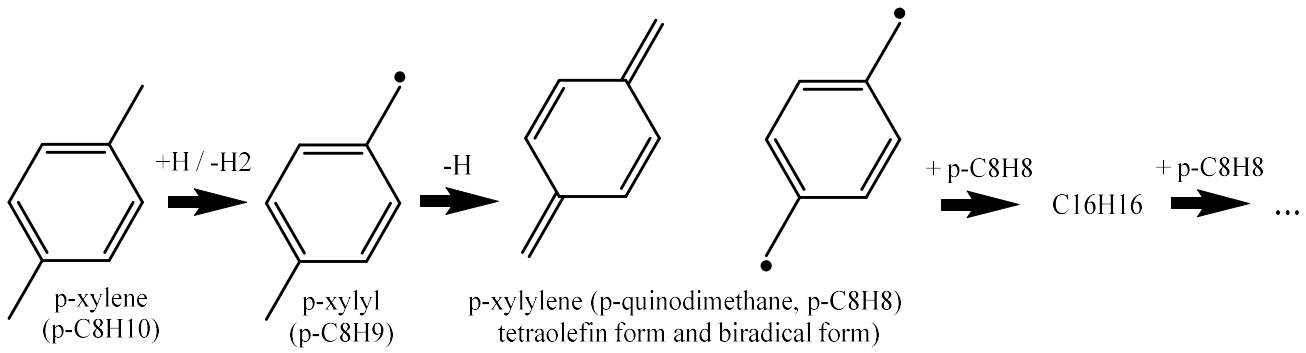

Fig. 1. Schematic representation of poly-*p*-xylylene formation

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Investigation of the laminar flame speed of traditional and alternative fuels

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Increasing the hydrogen content in traditional and alternative fuels is viewed as a means to enhance combustion stability and combustion chamber efficiency; in this context, the laminar flame speed serves as a key parameter governing flame stability and characteristics. Investigating the influence of composition, temperature, and pressure on the laminar flame speed for methane, kerosene, n-decane, and ammonia – specifically when blended with hydrogen – is essential for the safe and efficient design of combustion systems.

This study presents a combined computational and experimental investigation into the laminar flame speed of methane, kerosene, n-decane, and ammonia, as well as their mixtures containing hydrogen additives. The experiments were conducted at Samara University's test facility using the Heat Flux method. Numerical simulations were performed utilizing various kinetic mechanisms. The investigations covered a range of equivalence ratios – spanning from lean to rich mixtures – with hydrogen volume fractions reaching up to 50%. The obtained data reveal distinct, systematic differences among the various fuels and demonstrate a pronounced influence of hydrogen on the normal flame speed.

N-decane and kerosene exhibit significantly lower flame speeds compared to methane, a disparity attributed to their more complex combustion kinetics. Nevertheless, the addition of hydrogen accelerates the flame front and enhances flammability; the magnitude of this effect depends on the completeness of evaporation and the homogeneity of the vapor mixture – specifically, the influence of hydrogen is attenuated under conditions of incomplete evaporation. Among the fuels examined, ammonia demonstrates the lowest laminar flame speed, a characteristic linked to the presence of slow, nitrogen-containing reaction steps. However, the introduction of hydrogen dramatically improves the laminar flame speed, even at low hydrogen concentrations.

Thus, the addition of hydrogen to the fuels under consideration serves as an effective strategy for increasing the laminar flame speed and enhancing combustion stability; notably, the magnitude of this effect is strongly contingent upon the specific nature of the fuel, the degree of liquid-phase evaporation, and the initial temperature and pressure conditions.

Acknowledgment

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Structure and properties of TiC-Cu cermet synthesized in combustion in coupled processes of thermal metal reduction and self-propagating high-temperature synthesis

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The authors of this work have recently proposed a method for producing ceramic-metal composites (cermets) TiC–Cu, which retain to a large extent the electrical conductivity of the copper matrix when it is hardened with high-hardness refractory titanium carbide (TiC), by using combustion in the coupled processes of thermite formation of copper melt by reaction ($2Al+3CuO=Al_2O_3+3Cu$) and self-propagating high-temperature synthesis (SHS) of a porous refractory TiC skeleton by the reaction (Ti + C = TiC) with its infiltration by a thermite copper melt [1, 2]. The aim of the work was to study the effect of the addition of copper to the SHS charge (Ti+C) and its compacting pressure on the processes of infiltration of the copper melt, the formation of the structure and physico-mechanical properties of TiC-Cu cermets produced by a combination of metallothermy and SHS without the use of crucibles and reactors. The SHS charge, compacted in the form of a cylindrical briquette, was laid in the open air in a sand crater and evenly sprinkled with a standard copper thermite mixture from top to bottom. Ignition of the thermite mixture led to the formation of a copper melt, followed by ignition of the SHS charge to form a porous TiC skeleton, which was infiltrated by the copper melt due to the capillary effect. The content of the copper additive in the charge was 0-15 wt.%, the compacting pressure was 22-69 MPa. It has been established that highly porous composites with cracks and delaminations are formed without the addition of copper. Adding 5 wt.% Cu significantly increases the completeness of infiltration and uniformity of the structure. An increase in compacting pressure leads to a decrease in porosity, but at excessive values it contributes to the formation of cracks. Optimal synthesis conditions are achieved at a compacting pressure of 45 MPa, at which the maximum mass and density of the samples are observed. The highest density (~5.07 g/cm^3) is achieved at 10 wt.% Cu. The structure under these conditions is characterized by minimal defects. X–ray phase analysis showed that Ti-Cu intermetallides are formed without the addition of copper. With the introduction of 5 wt.% Cu they disappear, but free graphite appears and nonstoichiometric carbide TiC_x is formed. With an increase in the copper content to 10-15 wt.%, intermetallic compounds are being formed again. The maximum hardness up to 95 HB is achieved at 5-10 wt.% Cu and a pressure of 34 MPa, and at an optimal pressure of 45 MPa, the hardness is 88.5 HB at 15 wt.% Cu. Compressive strength increases with increasing copper content and reaches 390-414 MPa at 15 wt.% Cu. The optimal mode is 45 MPa and 5-10 wt.% Cu, which ensures the production of composites with high density, low defects and improved mechanical characteristics.

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Combustion in coupled processes of thermal metal reduction and self-propagating high-temperature synthesis for producing TiC-Cu cermet

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To increase the strength and wear resistance of copper and its alloys, composite materials are actively being developed in which the copper matrix is reinforced with hard and durable ceramic particles, including titanium carbide (TiC), which has high hardness and melting point values, as well as moderate electrical conductivity [1]. However, TiC particles are poorly wetted by the copper melt, for example, the contact wetting angle at 1200°C is 130° and decreases to 90° within 25 minutes. The high temperature and pressure required to produce TiC–Cu composites significantly complicate the manufacturing process using traditional methods of powder metallurgy and foundry production, making it energy-intensive and expensive. In this regard, the method proposed by the authors and based on the combustion phenomenon, which is a combination of a thermal reduction process for producing a copper melt and self–propagating high-temperature synthesis (SHS) of a porous titanium carbide skeleton with its infiltration by a copper melt, can become a promising basis for future energy-efficient technologies for manufacturing TiC-Cu composites [2-4].

In the first variant [2, 3] of a vertical two-crucible reactor made of graphite, a copper thermite mixture (2Al + 3CuO) in bulk is placed in the upper crucible, in which a thermite reaction (2Al +3CuO = Al2O3+ 3Cu) is triggered by local ignition, resulting in a copper melt with a very high temperature of more than 2000°C, which enters the lower chamber reactors under the influence of gravity. The copper melt ignites the SHS charge (Ti + C), the combustion reaction (Ti + C = TiC) begins, which results in the formation of porous TiC ceramics with an even higher temperature (up to 2800°C), which is spontaneously infiltrated with molten copper. The very high temperatures of the copper melt and the TiC skeleton ensure good mutual wetting and filling of the skeleton pores with molten copper. Then the metal-infiltrated skeleton cools down, thus forming a dense TiC-Cu cermet.

In the second simplified version [4], the reactor and crucibles are not used. The SHS charge, compressed in the form of a cylindrical briquette, is laid in the open air in a sand crater and evenly sprinkled with a copper thermite mixture from top to bottom. Ignition of the thermite mixture leads to the formation of a copper melt, followed by ignition of the SHS charge to form a porous TiC skeleton, which is infiltrated by the copper melt due to the capillary effect. As a final result of the synthesis and spontaneous infiltration of the copper melt into the TiC skeleton, after cooling down dense solid samples of TiC–Cu cermet are produced.

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The effect of mass discrimination in molecular beam time-of-flight mass spectrometry

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In the molecular beam time-of-flight mass spectrometry ion mass discrimination (MD) effects – different detection efficiencies for ions of different masses – may occur. This effect must be taken into account when analyzing experimental data.

In this study, mass discrimination effects were measured by recording signals for mixtures of gases with known ionization cross sections (NH_3, C_3H_6, C_4H_6, C_7H_8, CF_3I). The experimental setup comprises: an expansion vacuum chamber with piezo-electric pulse valve; a main vacuum chamber; and a time-of-flight mass spectrometer. The operating pressure in the main chamber was approximately 10^{-10} Torr, achieved by a pumping system consisting of turbomolecular and spiral pumps. The gas mixture entering the main vacuum chamber was sampled through a conical separating diaphragm (skimmer). The beam then entered the ionization region of a reflectron time-of-flight mass spectrometer where they were ionized by 118 nm laser pulses.

Based on the experimental data mass discrimination coefficients were extracted, and the sensitivity functions of the time-of-flight mass spectrometer were obtained for various backing pressures and carrier gasses.

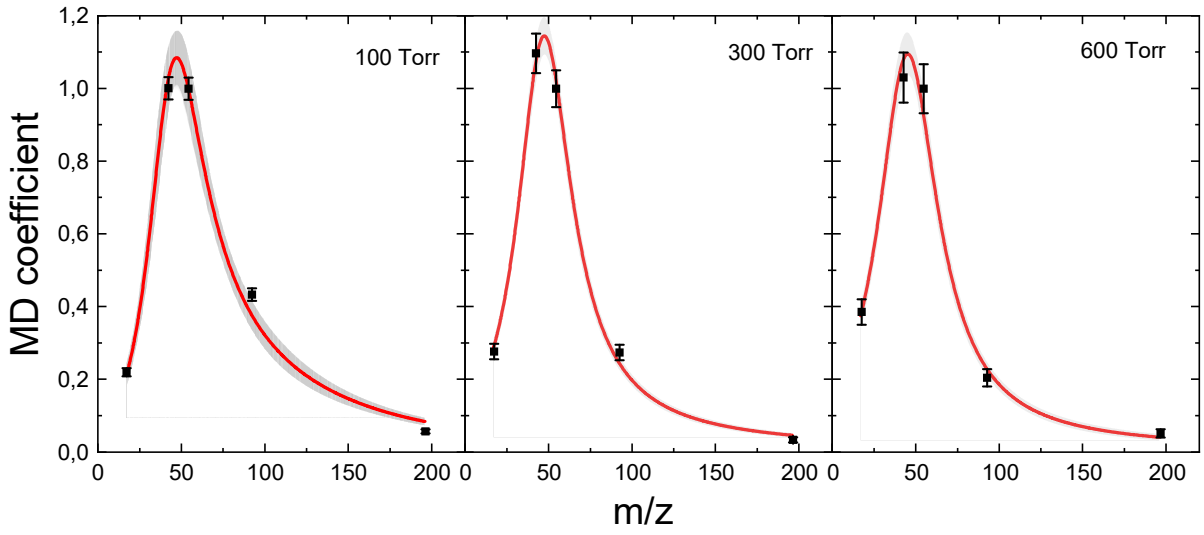

Figure 1. The mass discrimination coefficients at pressures of 100, 300, and 600 Torr, obtained by measuring the ion signal ratio for each of the target gases, are shown by symbols. The solid curve is a polynomial fit to the data.

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The effect of the oxidizer composition on sulfur absorption by calcium-containing additives during filtration combustion of sulfur fuels

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Steam-air gasification of various sulfur fuels was carried out, in which sulfur is mainly in the form of sulfides (brown coal), sulfates (charcoal with $CuSO_4$) and organic sulfur (rubber, acid tar, bitumen) with the addition of particles of non-combustible material. Particles of chemically inert sapphire and calcium carbonate capable of absorbing sulfur were used as a non-combustible material, the content of non-combustible material in the mixture was 50%.

Table 1

The elemental composition of fuels, % mass.

Type of fuel	C	H	N	S	O	Ash
Brown coal	42.6	3.8	0.8	2.7	23.1	27.0
Charcoal with $CuSO_4$	62.0	1.3	0.3	5.0	14.7	16.7
Rubber	83.6	7.5	0.3	1.6	2.1	4.9
Acid tar	84.1	9.4	0.9	5.6	--	--
Bitumen	85.1	9.8	0.7	4.4	--	--

Experiments have shown that the addition of water vapor to the oxidizer leads to a decrease of combustion temperature and an increase of the hydrogen content in gaseous products, which in some cases leads to a noticeable increase in their heat of combustion. At the same time, the proportion of sulfur absorbed by calcium carbonate when using a steam–air mixture as an oxidizer was two to three times lower than at air gasification (table 2).

Table 2

The part of sulfur absorbed by solid combustion products at the different types of oxidizer, %

Type of fuel	Air	Steam-air
Brown coal	82	33
Charcoal with $CuSO_4$	52.5	27
Rubber	40	19
Acid tar	83	30
Bitumen	90	26

The measurements of the elemental composition of the materials used and the combustion products were carried out using the equipment of FRC PCP MC RAS.

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Mass spectrometric study of the effect of dimethyl ether additives on the formation of carbon nanoparticles in ethylene/air flame

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Despite the global trend towards zero-carbon energy, hydrocarbons remain a vital energy source for human activities. A major challenge in hydrocarbon combustion is the formation and emission of carbonaceous species, including gaseous polycyclic aromatic hydrocarbons (PAHs) and condensed carbon phases such as organic carbon and soot. The addition of alternative fuels–oxygenates to conventional fuels is a perspective strategy for inhibition soot formation.

This paper presents an experimental and numerical investigation of the influence of dimethyl ether (DME) additives on soot formation in premixed laminar ethylene/air flame. A base ethylene/air mixture with an equivalence ratio $\varphi = 2.1$ was used. Two additional mixtures were prepared by replacing ethylene with 6% and 15% DME. Measurements were conducted at heights above the burner ranging from 2 to 6 mm, which correspond to the early stages of soot formation, where large PAHs grow and the transition from gas-phase molecules to condensed material occurs.

Temperature profiles were measured with B-type micro-thermocouple. Quadrupole mass spectrometry was used to study the chemical composition of flame. The components of the flame flow were sampled using a horizontally positioned stainless steel sampling tube. An orifice in the tube allowed combustion products to enter a flow of inert diluent gas, which rapidly diluted the sample and effectively stopped chemical reactions. Kinetic modeling was performed using the open-source Cantera software. Simulations were conducted with the detailed CRECK kinetic mechanism.

Concentration profiles along flame height were obtained for various flame species, including water, oxygen, carbon dioxide, 1,3–butadiene (C_4H_6), benzene (C_6H_6) and compounds C_4H_8 and C_5H_{10}. For C_4H_8, C_5H_{10}, and C_6H_6 noticeable discrepancies were observed between the modeling results and experimental data. In the experiments benzene was completely consumed along the height above burner, whereas the model predicts a monotonic increase. Meanwhile, the addition of 6% and 15% DME had no significant effect on benzene formation. In addition, experimentally, as the DME fraction increased, the formation of C_4H_8 and C_5H_{10} also increased. These species are aliphatic structures and are believed to inhibit the soot formation process. However, the model predicts the opposite trend: with increasing DME addition, the formation of these species decreases. A detailed analysis of these discrepancies will require further investigation.

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Porous-microchannel burner with an optically open hot zone as an IR emitter

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A new design of a porous-microchannel burner is proposed. It represents the configuration considered in [1,2], truncated in half along the plane of symmetry, with a quartz output window installed in place of that plane. The latter enables efficient extraction of thermal IR radiation in the wavelength range from 1 to 5 μm. The operating regimes of this burner are studied as functions of the propane–air mixture flow rate and the diameter of the packed bed granules, which are zirconia spheres. It is found that the combustion front can stabilize: (a) inside or at the outlet of the feeding capillary; (b) at the outlet face of the porous matrix bounded by the quartz window; (c) inside the porous bed. The most efficient regime for radiation extraction is mode (b), which can be realized over a wide range of propane–air mixture flow rates. This allows the creation of a nearly uniformly heated outer layer of the packed bed spheres, emitting a heat flux with an intensity of up to 5 W/cm² at a distance of about 5 cm. The spectral characteristics of the radiation are investigated. It is shown that by focusing this radiation, a power of about 10 W can be achieved in a focal spot area of approximately 1 cm². A mathematical model of gas filtration combustion in the system under study is also developed. Within the framework of a single-step reaction mechanism, it describes the concentration and temperature fields of the fuel mixture, as well as the temperature of the porous matrix. Using numerical simulation, the regions of existence of various steady-state combustion regimes were determined, and the parameters maximizing the radiation flux through the output window were identified. Based on the obtained data, conclusions are drawn regarding the applicability of the system under study as an electrical power generator.

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Investigation of Isomerization and Cyclization Pathways in the Reaction of Naphthyl ($C_{10}H_7$) and Propargyl (C_3H_3) Radicals

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Polycyclic aromatic hydrocarbons (PAHs) represent one of the most abundant classes of organic molecules in the interstellar medium (ISM) and play a pivotal role in astrochemistry, atmospheric science, and materials research. Elucidating the molecular mechanisms underlying PAH growth is essential for interpreting interstellar infrared emission spectra and modeling the evolution of cosmic carbonaceous dust. A prominent hypothesis for PAH formation involves the sequential addition of small carbonaceous radicals to aromatic seed molecules. This study investigates the gas-phase reaction between the propargyl radical (C_3H_3), a well-established precursor in aromatic ring synthesis, and the 1-naphthyl radical ($C_{10}H_7$), which serves as a prototypical PAH growth nucleus.

Computed potential energy surface (PES) reveals that the reaction initiates via barrierless addition pathways, leading to the formation of four distinct covalently bound adducts. These intermediates correspond to different sites of propargyl attachment to the 1-naphthyl radical and exist as two pairs of rotational $C_{13}H_{10}$ isomers: i1min (-90.9 kcal/mol) and i1 (-90.8 kcal/mol) constitute one conformer pair, while i1_1min (-93.9 kcal/mol) and i1_1 (-93.0 kcal/mol) form the second pair. The surface features two primary channels leading to hydrogen-elimination products, designated p1 (phenalene) and p2 (benzoindene). Although the p1 channel yields a thermodynamically more stable product (-129.6 kcal/mol) compared to p2 (-125.1 kcal/mol), the overall reaction outcome is governed by kinetic accessibility rather than thermodynamic stability.

The formation of p2 proceeds through the intermediate p2x (-102.0 kcal/mol) and traverses the transition state of -87.3 kcal/mol. The effective barrier from p2x to the products is merely ~15 kcal/mol, rendering this channel highly accessible even at cryogenic temperatures. In contrast, the route leading to p1 necessitates surmounting a substantial energy barrier. Isomerization of i1_1min toward the p1-forming pathway requires passage through transition state ts2_1 (-28.0 kcal/mol), corresponding to an activation energy of approximately 66 kcal/mol relative to the preceding intermediate. This significant kinetic impediment effectively shuts down the p1 channel under typical interstellar conditions. Consequently, product p2 dominates the reaction flux, underscoring the critical importance of kinetic factors in astrochemical models of PAH growth, where systems rarely attain thermodynamic equilibrium due to the extreme environmental constraints of the ISM.

Gel combustion synthesis of a highly dispersed ZnO powder with a high photocatalytic activity for phenol decomposition

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Highly dispersed submicron and nanoscale zinc oxide powder (ZnO) exhibits significant photocatalytic activity during the decomposition of such toxic water pollutant as phenol (C_6H_5OH) under the influence of ultraviolet radiation and visible light, decomposing it and converting it into safe CO_2 and H_2O [1]. However, the existing gas-phase and solution methods for the synthesis of ZnO nanopowders are complex, implemented on expensive equipment, energy-intensive, and low-productivity, which prevents the organization of industrial production of ZnO nanostructured photocatalysts for wastewater treatment based on them. The process of solution self–propagating high-temperature synthesis of oxides in combustion mode (Solution Combustion Synthesis - SCS), which appeared relatively recently, differs markedly from these methods in its simplicity, energy saving and high productivity, which makes it attractive for the creation of industrial production technologies for various relatively inexpensive oxide nanomaterials of various applications [2]. The method of SCS is based on the combustion of a mixture of dissolved, most often in water, reagents of highly exothermic redox reactions. The method of Gel Combustion Synthesis (GCS) is even simpler. The gel of the reagent mixture is formed during the mixing of dry reagents, accompanied by their spontaneous humidification from the ambient air due to hygroscopicity [3]. The process of ZnO synthesis from the gel was studied by heating mixtures of zinc nitrate and glycine in an airy atmosphere in a metal vessel with a flat bottom on an electric stove with a temperature of the contact metal surface from 150 to 850°C. The results of the study showed that the characteristics and product of the GCS process, although similar, differ from the SCS process. Firstly, the GSC process is simpler and faster. In the case of using dry mixtures of reagents, combustion begins much faster (on average in 1.5 minutes) than in the case of dissolved reagents (on average 8 minutes), since in the latter case a lot of time is spent heating the solution to boiling water and evaporating water to form a gel. Secondly, the GCS product turns out to be smaller and cleaner in terms of the content of carbon impurities. Thirdly, the difference between the photocatalytic activity of the products of GCS and SCS in the decomposition of phenol is noticeable only at the initial stage of ultraviolet irradiation, then this difference disappears. The time and type of combustion, the color and consistency of the synthesized ZnO combustion product in the process of GCS remain close to the similar characteristics of the process and the product of SCS. Calcined products of GCS and SCS have almost the same high photocatalytic activity in the decomposition of phenol under the action of ultraviolet irradiation, leading to almost complete decomposition of phenol in 3.5–4.5 hours of ultraviolet irradiation.

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Solution combustion synthesis as a simple effective ZnO doping method for increasing photocatalytic activity

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The fundamental shortcomings of pure nanostructured ZnO as a photocatalyst for wastewater treatment are effectively overcome by doping with transition metals [1-3]. Various methods are employed for doping ZnO photocatalysts, such as sol-gel, hydrothermal, microwave-assisted deposition, and others. However, for the implementation of photocatalysis on an industrial scale, where treatment facilities with capacities of thousands of cubic meters of water per hour are required, the low-productivity and resource-intensive synthesis methods listed above appear unacceptable. A suitable approach that meets the requirements for the synthesis of both highly dispersed ZnO and its doping is synthesis via the combustion of reagent solutions with highly exothermic redox reactions (Solution Combustion Synthesis, SCS) [4, 5]. In the SCS method, zinc nitrate $Zn(NO_3)_2$ is used as an oxidizer, while urea $CO(NH_2)_2$, glycine $C_2H_5NO_2$, or citric acid $C_6H_8O_7$ are used as fuels, which are water-soluble, have low decomposition temperatures, and are readily available and inexpensive. The reaction equation for the synthesis of ZnO using, for example, glycine, is as follows:

$$Zn(NO_3)_2+\frac{10}{9}\varphi C_2H_5NO_2+\frac{5}{2}(\varphi-1)O_2=ZnO+\frac{25}{9}\varphi H_2O+\frac{20}{9}\varphi CO_2+(\frac{5}{9}\varphi+1)N_2, \quad (1)$$

where φ is the coefficient characterizing the fuel-to-oxidizer ratio in the initial reagent mixture. If doping of ZnO with an accessible and inexpensive metal (Fe, Co, Cu, or Mg) is required, a mixture of the nitrate of this metal with the fuel is prepared according to equation (1), replacing Zn with, for example, Mg, and this mixture is added in a small amount to the main mixture from equation (1). Combustion of an aqueous solution of these mixtures makes it possible to obtain ZnO doped with magnesium or another metal. If the pure nanostructured zinc oxide powder, synthesized by the SCS method after heat treatment of the combustion product, exhibits high photocatalytic activity in the phenol decomposition reaction under UV irradiation, then doping with 1 wt. % Mg further increases its photocatalytic activity, reducing the phenol decomposition time by more than half: from 3.75–5 h to 1.75–2.25 h.

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Calculation of thermodynamic functions for xylene and its radicals

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Para-, *ortho*-, and *meta*-xylene are aromatic hydrocarbons consisting of a benzene ring with two methyl substituents. Xylenes are widely used as solvents and as components of both biofuels and petroleum-derived fuels. Kinetic combustion models are employed for theoretical investigations of xylene and xylene-blend oxidation processes. Recent model developers have noted that the thermodynamic properties of xylenes and their radicals require refinement and have therefore supplemented their models with results from statistical thermodynamics calculations. However, due to differing methodological approaches, the resulting thermodynamic function values exhibited significant discrepancies. At the same time, relatively few experimental data have been published that could validate or refute any of these calculations.

In light of the above, the present study pursues several objectives:

1. to compare values of thermodynamic functions—heat capacity, enthalpy, and entropy—for xylenes and their radicals from various kinetic models against previously published calculations and experimental data;
2. to assess the impact of the identified discrepancies on the results of kinetic reactor modeling;
3. to determine updated values of thermodynamic functions based on high-accuracy quantum-chemical G4 calculations and statistical thermodynamics methods implemented in the GoodVibes program.

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Influence of a dielectric barrier discharge on the combustion of lean methane-air mixtures

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It is known that dielectric barrier discharge (DBD) is used in combustion processes to suppress soot formation [1] and to enhance the burning rate of lean fuel-air mixtures [2]. The aim of this work was to experimentally investigate the effect of DBD on the combustion stability of a methane-air mixture.

The experimental setup for DBD generation is detailed in [3]. A premixed methane-air mixture was supplied into the discharge zone through the side walls of the central electrode. Two rubber rings secured the central Al_2O_3-coated aluminum electrode inside a quartz tube (inner diameter 16 mm, wall thickness 2 mm). The outer electrode consisted of a fine steel mesh ring providing a diffuse DBD. At an air flow rate of 4 $L \cdot min^{-1}$ and an equivalence ratio $\varphi = 0.62$, combustion without discharge was unstable, with periodic flame detachment. This φ value (φ_{ext}) was taken as the minimum sustaining combustion under our conditions. With the discharge operated at 30 W, the flame became stable at the same φ, with optimal stability at 50–60 W (Table 1).

After stable flame ignition, the methane flow rate was gradually reduced until flame extinction, at which φ_{ext} was recorded. The procedure was repeated at various discharge powers. Increasing discharge power markedly reduced φ_{ext}. At 85 W φ_{ext} decreased by 28% compared to the no-discharge condition (Figure 1).

Table 1. Appearance of the flames at different discharge powers

ϕ\ W	0 W	30 W	60 W
0.62			

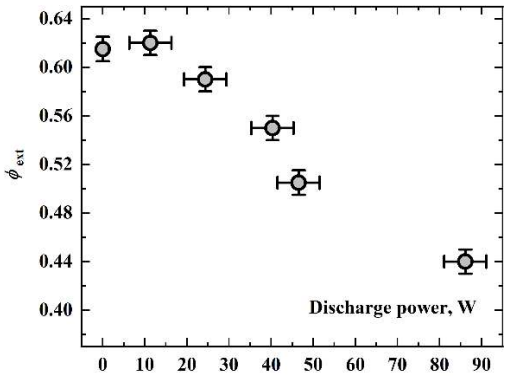

Fig 1. Dependence of ϕ_{ext} on the discharge power

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A comprehensive study of diethyl ether high temperature oxidation

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Diethyl ether (DEE, $C_2H_5OC_2H_5$) is being considered as a promising additive for diesel fuel and non-carbon ammonia fuel due to its exceptionally high cetane number. Nevertheless, combustion kinetics of even pure DEE still remains insufficiently studied, which makes it difficult to introduce it industrially. Several scientific groups all over the world are developing their own kinetic mechanisms of DEE combustion, but this works are based predominantly on calculated data, so, new experimental results are still urgently needed to make further significant model improvements.

Thus, this work is aimed at a comprehensive study of the kinetics of high temperature diethyl ether oxidation. An experimental part was carried out behind reflected shock waves in a high vacuum kinetic shock tube in highly argon diluted mixtures via the precise method of the atomic resonance absorption spectrometry (ARAS) in the vacuum UV region of the spectrum at the resonant line of the oxygen atom 130.5 nm. O_2 and N_2O were chosen as oxidizing agents to study both molecular and atomic oxygen channels of primary interaction with the fuel. Overall experimental conditions implemented in this work are temperatures from 900 to 3400 K, pressure 1,7−3,4 bar, mixtures of 5 ppm DEE + 30 ppm O_2 and 5 ppm DEE + 15 ppm N_2O in Ar. Time-resolved absorption profiles of oxygen atoms in the ground electronic state $O(^3P)$ obtained in the experiment, then, were transformed into the corresponding concentration profiles using inhouse calibration and special parasitic absorption accounting technique.

Along with the experimental measurements, a detailed kinetic analysis with a simulation of oxidation processes was performed using the Cantera v.3.1.0 software and modern kinetic mechanisms. The data obtained during a comprehensive study provide new valuable information on the features of the interaction of diethyl ether with molecular and atomic oxygen at high temperatures, which can help both to validate existing models and to create new reliable kinetic schemes over a wide range of temperatures and pressures.

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Theoretical study of reactions of boron trihydride with molecular oxygen

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Boranes, or boron compounds, possess outstanding energetic properties, but their use as fuels is limited by the physical and chemical properties of the boranes themselves and their combustion products. However, the development of a new generation of hypergolic (capable of spontaneous combustion upon contact with an oxidizer) propellants for spacecraft engines based on boron-containing ionic liquids has renewed interest in the chemical processes that occur during the ignition and combustion of boranes. In particular, the ignition mechanism of the simplest borane, BH_3, upon contact with molecular oxygen has remained virtually unstudied using modern quantum chemical computational methods. This reaction plays a fundamental role in the oxidation mechanisms of boranes, as high-molecular boron molecules decompose upon heating, and BH_3 is one of the simplest and highly reactive products of their thermolysis.

This paper presents the results of a theoretical study of the reaction of boron with BH_3 and molecular oxygen in the singlet $O_2(a^1\Delta_g)$ and triplet $O_2(X^3\Sigma_g^-)$ states. First, the geometries and molecular parameters were found for local minima and second-order saddle points at the ωb97X-D/6-311g(d,p) level. Then, the energies were refined using the explicitly correlated coupled-cluster method with single and double excitations ccsd(t)-f12 and the correlation-consistent cc-pvtz-f12 basis set. It was found that the reaction of borane with triplet molecular oxygen BH_3 + $O_2(X^3\Sigma_g^-)$ includes only one channel leading to the formation of products BH_2 + OH with a relative energy of -28 kcal/mol, and is accompanied by overcoming a barrier with a height of 33 kcal/mol. The reaction of borane with molecular oxygen in the singlet state BH_3 + $O_2(a^1\Delta_g)$ begins with the barrier-free formation of a reactant complex with an energy of 11 kcal/mol relative to the chosen zero. Then, as a result of the combination of molecules of the complex, the reaction can proceed along four main pathways leading to three different products: P1 (O_2BH + H_2) with an energy relative to zero equal to 10 kcal/mol, P2 (BHO_2 + H_2) with an energy of -50 kcal/mol, and P3 (HBO + H_2O) with an energy of -125 kcal/mol.

The barriers calculated on the singlet and triplet surfaces indicate an insignificant reaction rate of BH_3 with molecular oxygen under normal conditions, which is in good agreement with experimental estimates of the upper limit of the reaction rate constant of ~10-16 cm^3/s [1].

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Chemical evolution of aromatic compounds in circumstellar envelopes of AGB stars

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Understanding the formation mechanisms of complex organic molecules, including polycyclic aromatic hydrocarbons (PAHs), in the interstellar medium (ISM) remains one of the key problems in modern astrochemistry. Evolved stars, particularly carbon-rich asymptotic giant branch (AGB) stars with C/O > 1, are considered the primary sources of PAHs. The synthesis of PAHs and the nucleation of carbonaceous dust occur in circumstellar envelopes under conditions of elevated temperature and pressure that favorable for active chemical processing.

PAHs (e.g., naphthalene $C_{10}H_8$, biphenyl $C_{12}H_{10}$, coronene $C_{24}H_{12}$) are important precursors of carbon dust. Their presence in the ISM is supported by broad emission features observed in the 3-20 μm range, attributed to their vibrational transitions.

Despite the general understanding of organic synthesis in the envelopes of carbon-rich stars, the detailed underlying mechanisms remain insufficiently constrained. The modeling of chemical evolution is based on the numerical integration of systems of kinetic differential equations using reaction networks that include elementary reactions and associated rate coefficients. Existing models of AGB envelopes remain limited in both chemical complexity and reaction coverage [1, 2]. Notably, the physical conditions in circumstellar envelopes show similarities to those in pyrolysis and combustion chemistry, allowing the use of data from these fields to constrain reaction kinetics.

In this work, we construct an extended and systematically organized chemical reaction network that integrates previous models [2, 3] and incorporates up-to-date kinetic data. Using the Presta and Brahma codes, we simulate the chemical evolution in AGB circumstellar envelopes. The main pathways of transformation from simple hydrocarbons to PAHs, up to pyrene ($C_{16}H_{10}$), are identified. We also demonstrate the significant role of surface acetylene cyclotrimerization in enhancing PAHs formation yields.

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Cosmic ray irradiation of interstellar grain icy mantles

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One of the key tasks of modern astrochemistry is to determine the role of cosmic rays (CRs) in the synthesis of complex organic molecules (COMs) in the icy mantles of interstellar dust grains. This synthesis is extensively studied under laboratory conditions, and experimental results are usually presented as an radiochemical yield, i.e., the number of synthesized molecules per certain amount of deposited energy. So, to use experimental results in astrochemical models, it is necessary to estimate the energy absorbed by typical interstellar dust grains as a result of CR bombardment.

Previously, in work [1], estimates of the absorbed energy were obtained for two model CR spectra (H and L [2]) and a dust grain consisting of a refractory core and an icy mantle of fixed sizes. However, the evolution of the mantle thickness can significantly affect the accumulated dose. Furthermore, in recent years, refined data on the CR spectrum in molecular clouds [3] have appeared, which must be taken into account in calculations. In this regard, the aim of this work was to calculate radiation doses of icy mantles of dust particles irradiated by CRs, taking into account the variation of the mantle thickness during the chemical evolution of the environment and the recently proposed CR spectrum, in order to assess the contribution of this mechanism to the synthesis of complex organic molecules.

The dust grain model is similar to [1]: a spherically symmetric silicate core of fixed radius (10^{-5} cm and 10^{-6} cm) surrounded by an icy mantle whose thickness varies with time.

Three variants of the model CR spectrum were used in the work: H and L spectra from [2] and the LD spectrum proposed in [3], which takes into account a significant suppression of low-energy CRs at the periphery of molecular clouds.

Energy losses of particles in the dust grain material were calculated using the SRIM program [4]. Both primary particles (H, He, Fe, C, O, N, Co, e^-) and secondary electrons were taken into account. The doses accumulated from different primary particles were summed.

The dependence of the accumulated dose on the type of CR spectrum, the position of the dust grain inside the molecular cloud, and its parameters was analyzed. It is shown that over the characteristic time of the molecular cloud evolution (about 1 million years), the accumulated dose is sufficiently large for radiochemical processes to affect the COM abundance.

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Numerical and Experimental Investigation of the Combustion Processes of Methane–Hydrogen Mixtures and Hydrogen in a Cluster Microflame Burner

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The growth of global energy consumption, still largely driven by hydrocarbon fuels, is accompanied by rising pollutant emissions and increasing climate risks. In these conditions, the role of technologies aimed at reducing emissions and improving the environmental efficiency of energy systems is becoming more important, since stricter requirements for exhaust composition directly affect the competitiveness of industrial developments.

One of the most promising directions in low-emission combustion is the expansion of stable combustion limits for lean fuel–air mixtures and the intensification of ignition processes. Of particular interest in this context is the use of hydrogen as an additive to hydrocarbon fuels, since hydrogen can significantly increase mixture reactivity, accelerate flame propagation, and help reduce the carbon footprint. At the same time, the transition to hydrogen-containing fuels requires new approaches to burner design, because at high hydrogen fractions traditional schemes no longer provide the required stability and controllability of the combustion process.

Given the high cost of full-scale testing and the limited informativeness of individual experimental measurements, numerical modeling methods are playing an increasingly important role, making it possible to jointly analyze gas dynamics, heat transfer, and chemical kinetics in combustion chambers. For hydrogen-containing fuels, models that can correctly describe the thin flame front, high reaction rate, and changes in turbulent combustion characteristics with hydrogen addition are especially important.

The aim of this work is to improve the efficiency of designing promising multifuels microflame burner devices by developing and validating a computer modeling method for combustion processes. Within the framework of the study, a computational and experimental investigation of methane–hydrogen mixture combustion and pure hydrogen combustion in a cluster burner device was carried out, the levels of nitrogen oxide formation were evaluated, and a mathematical model for numerical simulation of hydrogen combustion was developed and verified.

The obtained results are intended to support the development of scientifically grounded approaches to the creation of low-emission burner systems of a new generation and may be used in the design of combustion chambers operating on fuels with an increased hydrogen content.

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Effect of Hydrogen Addition on the Lean Blowout Limit in a Premixed Swirl Burner

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This work is devoted to an experimental investigation of lean blowout during combustion of methane–hydrogen mixtures in a model premixed swirl burner, which is of interest for the development of low-emission combustion chambers for gas turbine units operating on hydrogen-enriched fuels. The relevance of the study is associated with the fact that hydrogen addition to methane expands the stable combustion region, while simultaneously modifying the flame stabilization mechanism in a swirling flow and affecting the burner operating limits.

The experiments were carried out using a model swirl burner with a quartz flame tube at atmospheric pressure and an inlet air temperature of 423 K. The hydrogen volume fraction in the fuel was varied from 0 to 50%, while the burner operating condition was changed by varying the pressure drop across the burner in the range of 2–5%. The lean blowout limit was determined by a quasi-steady mixture-leaning procedure with registration of the critical excess air ratio, α_{LBO} at the moment of complete flame extinction.

It was shown that increasing the hydrogen fraction leads to a monotonic shift of the blowout limit toward leaner mixtures. In particular, for the operating condition with a 3% pressure drop, the addition of 40% hydrogen increases the critical value of α_{LBO} from 1.87 to 2.43, i.e., by approximately 30%. At the same time, an increase in air flow rate shifts the blowout limits for all fuel compositions toward richer mixtures; however, the presence of hydrogen partially compensates for the destabilizing effect of the increased flow velocity.

Flame visualization showed that hydrogen addition changes the flame macrostructure: the reaction zone becomes more compact and the flame front shifts closer to the burner outlet. Even under extremely lean conditions, unattainable for pure methane, the flame retains a stable V-shaped structure anchored near the flame root. A comparison of the experimental lean blowout limits with the calculated laminar flame speed values revealed a nonlinear relationship, indicating the combined influence of chemical kinetics, turbulent mixing, and swirling-flow aerodynamics on the flame stabilization mechanism.

The obtained results expand the experimental database on the stability of methane–hydrogen combustion in swirl burners and can be used for CFD model validation as well as for the design of advanced low-emission combustion chambers for power-generation and aviation gas turbine applications.

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From detailed mechanism to skeletal model: MBMS study of TS-1 kerosene and its SU4 surrogate in lean and stoichiometric flames

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Increased attention to the climate agenda and the tightening of ICAO environmental standards are driving the development and optimization of advanced low-emission gas turbine engines. A critical tool in the design of gas turbine engines is computational modeling. A primary requirement for such modeling is the availability of a reliable kinetic combustion scheme for a kerosene surrogate, validated under conditions representative of those found in gas turbine engine combustors.

In this work, the thermal and chemical structure of laminar premixed flames of lean (φ = 0.8) and stoichiometric (φ = 1.0) mixtures of aviation kerosene TS-1 with O_2/Ar and its four-component surrogate (n-decane, isocetane, methylcyclohexane, tetralin) SU4 with O_2/Ar was experimentally and numerically investigated for the first time at atmospheric pressure. Using molecular beam mass spectrometry, concentration profiles for more than 20 species were obtained, including C_0–C_4 intermediates and radicals (O, OH, HO_2, CH_3). SU4 showed good agreement with TS-1 in the mole fraction profiles of most intermediates but underpredicted the C_6H_6 concentration by more than a factor of 2. This agreement confirms the fundamental applicability of SU4 for modeling TS-1 combustion without accounting for soot formation processes. Based on the experimental data, the CRECK_2003_TOT_HT mechanism was validated, and the validation revealed the main discrepancies between the model and experiment in the peak concentrations of typical soot precursors. Through sequential reduction of the detailed CRECK_2003_TOT_HT mechanism using the DRG and CSP methods, a skeletal mechanism, named KCPsur, was developed. This reduction decreased the number of species from 368 to 85 and the number of reactions from 14412 to 183. The KCPsur mechanism provides predictive capability comparable to the detailed mechanism while significantly reducing computational costs and has prospects for use in CFD modeling of combustion processes in gas turbine engine combustors, particularly for simulations where soot formation is not the primary focus.

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Kinetic Mechanisms of Ammonia/Hydrogen Combustion: A Comparative Study

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At present, the global trend toward decarbonization has stimulated the search for alternative low-carbon or carbon-free fuels for gas turbine applications. Hydrogen and ammonia, as carbon-free fuels, are considered among the promising solutions to eliminate carbon emissions. Ammonia can serve as an energy carrier because it liquefies easily, contains a high hydrogen density, and can use existing infrastructure for storage and transportation. However, its direct use in high-intensity combustion systems is limited by a low laminar burning velocity, high ignition energy, and narrow flammability limits. To overcome these challenges, ammonia can be partially cracked to hydrogen and nitrogen, enhancing reactivity and improving flame stability. Hence, It is essential to understand the chemical pathways of the combustion of these blends to control emissions while maintaining combustion performance.

This study aims to evaluate ten promising kinetic mechanisms from the literature for NH3/H2 blends using CHEMKIN-Pro software. The chosen mechanisms are: C3MechV4.0-2025, Glarborg-2024, Tsinghua-2024, KAUST-2023, POLIMI-2023, Otomo-2018, Han-2020, Mei_2021, NUIG-2024, and W.Zhu 2024. The mechanisms have been validated against experimental data for ignition delay time, flame speed, and species concentrations across a wide range of operating conditions to identify the best-performing models and provide a validated framework for the design of low-emission NH3/H2-fueled gas turbines. The performance of each combustion mechanism was evaluated quantitatively using the error function E by Turanyi et al. Measurement standard deviations were estimated using both the experimental uncertainty and the scatter error of the datasets determined by the Minimal Spline Fit code.

The models NUIG-2024, C3MechV4.0-2025, and Tsinghua-2024 demonstrated the best performance. However, even these mechanisms cannot reproduce the experimental data within their 3σ uncertainty limits. Additionally, the prediction quality of each mechanism varies depending on the specific operating conditions and the evaluated data types. To address these discrepancies, in future work, we will conduct a sensitivity analysis to define the critical reactions that control the predictions of ignition delay times, flame propagation, and NOx emission pathways under gas turbine-relevant conditions.

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Acid-base reactions of aniline at low temperatures

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Gaseous aromatic molecules containing one to four rings have been detected in the interstellar medium (ISM). In cold dense regions – such as molecular clouds, protostellar envelopes, and the inner parts of protoplanetary disks – most of these molecules are expected to be in the condensed phase as a part of interstellar icy mantles. Amino-substituted arenes are organic bases and, as we assume in this study, can react with acids in astronomical ices in a manner analogous to ammonia (NH_3). The resulting ammonia salts represent semi-refractory organic material with sublimation temperatures higher than those of the major ice components (e.g., H_2O). Consequently, these salts significantly influence the desorption kinetics of nitrogen-bearing molecules bound within them and potentially impacting the formation of complex organic species and their subsequent delivery to forming planets, similar to early Earth. Despite its importance, such acid-base chemistry has not yet been explored for any type of amine in astronomical ices.

Among arenes, aniline ($C_6H_5NH_2$) is particularly notable as the simplest amino-substituted arene and a derivative of benzene (C_6H_6), a key building block for more complex aromatic molecules. It is also a direct precursor of interstellar indole, an important structural fragment of proteins and other biochemically relevant compounds [1].

In this work, we experimentally investigate aniline using ultra-high vacuum Ice Spectroscopy Experimental Aggregate (ISEAge). Specifically, we: (1) determine its thermal desorption kinetics; (2) assess the feasibility of its solid-phase reactions with ISM-relevant organic acids (HCOOH, CH_3COOH, HNCO, HCN) and the resulting effects on its desorption behavior; and (3) evaluate how a realistic multi-component ice composition influences both the reactivity and thermal desorption of aniline, particularly when it competes with NH_3 in acid–base reactions. Our results demonstrate that amines, including aromatic amines, can be presented in interstellar and cometary ices in form of salts.

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Airy propagator method for calculation of cross sections for inelastic atomic scattering

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Optically pumped metastable rare gas lasers (OPRGLs) require accurate collisional data for Ar*–He, especially for high-pressure operation [1,2].

Close-coupling (CC) equations in diabatic representation are solved with an Airy propagator using previously calculated potential energy curves and spin-orbit matrix elements [3,4].

For transitions $2p_9 \rightarrow 2p_{10}$ and $2p_8 \rightarrow 2p_{10}$, the CC cross sections exceed the exponential Born distorted wave approximation (EBDW) by factors of 5–100, revealing shape and Feshbach resonances not seen in EBDW. For $2p_8 \rightarrow 2p_9$, the CC cross section shows clear Stueckelberg oscillations from an avoided crossing, while EBDW is larger above 200 cm^{-1}. The $2p_6 \rightarrow 2p_7$ transition exhibits a dramatic discrepancy: the CC cross section is three orders of magnitude smaller than EBDW and remarkably smooth. For the $1s_4 \rightarrow 1s_5$ transition (fine-structure relaxation), CC captures shape resonances and oscillatory structures; EBDW underestimates by 10 times, approximately.

The CC-derived rate constants agree well with the experimental results of Torbin et al. [5] at 375–600 K, whereas EBDW values deviate by orders of magnitude. This study validates previously calculated potential energy curves and matrix elements, providing reliable data for modeling high-power OPRGLs [3,4].

This endeavor would not have been possible without Alexander P. Palov, PhD, Senior Researcher at Skobeltsyn Institute of Nuclear Physics (Lomonosov Moscow State University), who generously provided knowledge and expertise of this work.

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Investigation of the mechanism of formation of fluoranthene and pyrene in the reaction of benzyl and indenyl recombination

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One of the main environmental pollutants is soot, or polycyclic aromatic hydrocarbons (PAHs). The mechanisms of their growth are still poorly understood, which does not allow the environmental factor to be adequately taken into account when designing systems. The reaction C_7H_7 + C_9H_7 studied in this work is one of the possible steps of 'fast' PAH growth. The increase in atomic mass upon benzyl addition is 91 amu, which agrees better with experimental data on PAH growth rates than, for example, the HACA mechanism (26 amu).

The aim of this work is to construct a potential energy surface (PES) diagram for the reaction C_7H_7 + C_9H_7. Geometries and vibrational frequencies of reactants, barriers, intermediates, and products were calculated using density functional theory with the WB97XD/6-311G** method. IRC calculations were also performed at the same level of theory. Energies were refined using the CASPT2(5e,5o)/cc-pVDZ//CCSD(T)/6-311G** scheme for rotational transitions with strong multiconfigurational character, and using the composite G3(MP2,CC)//WB97XD scheme for the remaining states. WB97XD calculations were carried out in the GAUSSIAN software package, while MP2, CCSD(T), and CASPT2 were performed in the MOLPRO package.

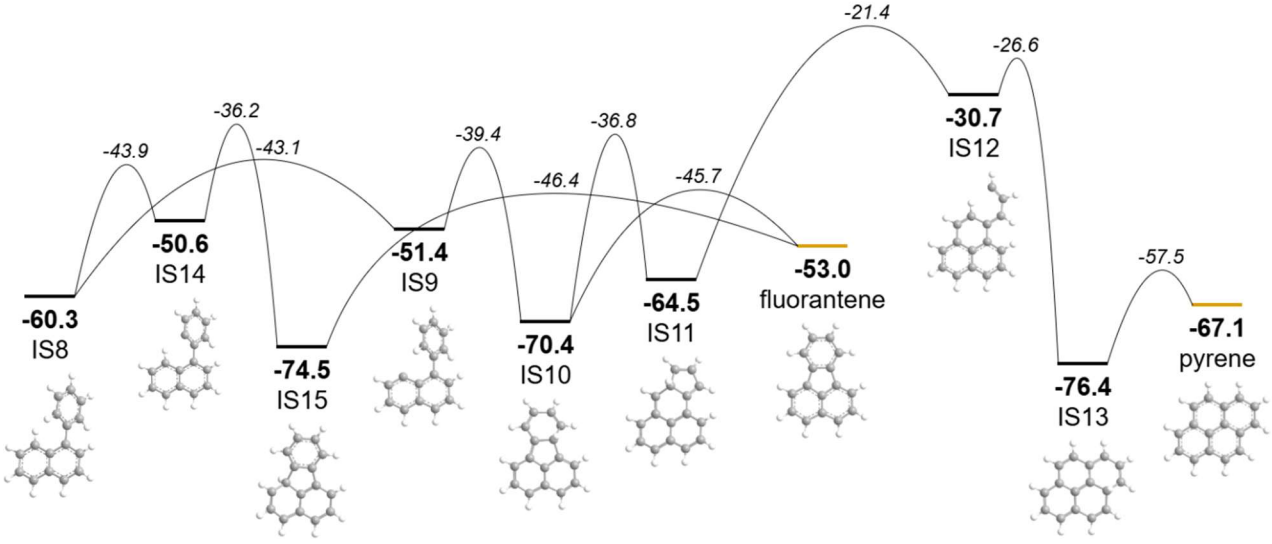

Fig. 1 — One of the possible channels to products starting after the incorporation of the terminal carbon of benzyl into the five-membered indole ring (intermediate IS8). Energies are given relative to the reactants (dashed line) in kcal/mol.

The work was carried out within the framework of the state assignment "Oxidation and Formation of Simple Polycyclic Aromatic Hydrocarbons in Flames of Synthetic Hydrocarbon Fuels" No. FSSS-2026-0010.

Combustion characteristics of gel fuel in a hypergolic system

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Hypergolic fuel components are widely used in a variety of applications, including boosters, emergency launch systems, and propulsion systems that require near-instantaneous ignition of the fuel without an external energy source [1]. The study of ignition and combustion mechanisms of hypergolic fuels is becoming increasingly relevant due to the growing demand for their efficient utilization in various fields such as aerospace and aviation industries. However, the lack of experimental data on the combustion characteristics of various compositions limits the possibilities of efficient use of such fuels. Therefore, the aim of this work is to establish, based on the results of experimental studies, the main patterns and characteristics of the combustion process of a fuel particle in a hypergolic system.

Hypergolic fuel consists of the following components: gel fuel is tetramethylethylenediamine $C_6H_{16}N_2$; liquid oxidizer is highly concentrated nitric acid HNO_3. The fuel thickening process was carried out by adding 5% silicon dioxide and mixing in an ultrasonic bath. The study of the main patterns and characteristics of the combustion process was carried out using a proven experimental technique and an experimental setup consisting of a high-speed video camera, a spotlight, a fuel supply system, and a laptop [2]. During the experiments, the following parameters were recorded: ignition delay time, burnout area, fragment movement velocities, and flame temperatures.

It was found that with an increase in the fall height of a fuel particle from 5 to 20 cm (the particle speed upon contact with the oxidizer is 0.89–1.78 m/s), the ignition delay time is reduced by 69%, and the burnout time is reduced by 56%. The higher the fall height of a fuel particle, the larger its average burnout area. The maximum average flame temperature was approximately 1168 °C. Component burnout was stable, but accompanied by average temperature fluctuations within the confidence interval of 1123–1134 °C. A dispersion process was detected in a quarter of the experiments. This may contribute to improved fuel performance by intensifying fuel combustion. A hypothesis was formulated about the combustion mechanisms of components (gel fuel and liquid oxidizer) of hypergolic fuel system.

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On the evolution of an isochorically unstable medium

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According to [1] the process of 'catastrophic cooling' is usually associated with the presence of isochoric thermal instability. This type of instability always implies additional isobaric and (or) isentropic ones. Our aim is to investigate disturbance evolution in the medium with the isochoric and isobaric instabilities. To study perturbation evolution in detail we constructed model heat-loss function $L\,(P,V)$ (see Fig 1a), which allow us to control types of realized instabilities in the whole steady state curve and particularly in the state of interest $(ln\,P_0, ln\,V_0) = (0,0)$ (see Fig 2b).

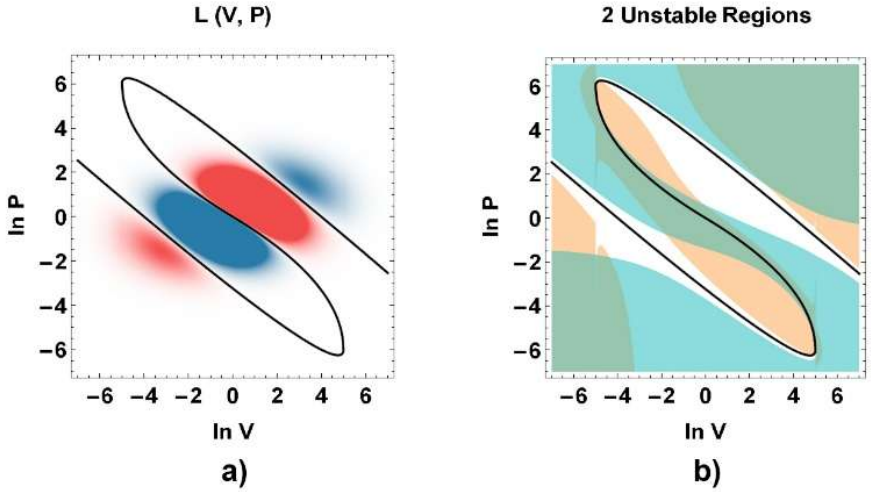

Fig. 1. **a):** The PV-diagram of heat-loss function, red regions indicate heating, blue regions indicate cooling. **b):** The PV-diagram showing isochoric (cyan) and isobaric (orange) unstable regions; mixed color indicates the coexistence of both instabilities, and white denotes stable region. In both diagrams the black S-curve represents the solution of the equation $L\,(P,V) = 0$.

We conducted numerical simulations of perturbations evolution including both Gaussian and noise-induced disturbances. The simulation demonstrates that the evolution of an isochorically unstable medium results in a shift towards a new steady state through heating or cooling depending on the type of initial condition. Additionally, we found that supplementary presence of isobaric instability leads to dense isobaric structures formation during the transition.

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Supramolecular Double Spin-Flip Transition in van der Waals Complexes of Isoprene with Oxygen as a Source of Singlet Oxygen $O_2(^1\Delta_g)$

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Singlet oxygen is the lowest excited state of the oxygen molecule with an energy of 0.98 eV, which is successfully used in applications such as photodynamic therapy [1]. However, due to the high symmetry of oxygen, optical transitions from the molecular ground state are forbidden, including the transition to the singlet $O_2(^1\Delta_g)$ state.

It is known that the presence of a weakly bound molecular environment near the oxygen molecule breaks this symmetry and makes the transition partially allowed. Consequently, the absorption cross-section of the transition can increase by orders of magnitude [2]. For instance, photoexcitation of a weakly bound complex M-O_2 (where M is an environmental molecule) can trigger a spin-allowed "double spin-flip" process:

$$^3\,(^1M{-}^3O_2\ X^3\Sigma_g^-) + h\nu \rightarrow {}^3\,(^3M{-}^1O_2\ a^1\Delta_g) \rightarrow\ ^3M + {}^1O_2.$$

This process has been established for a number of van der Waals complexes with various X under excitation at wavelengths shorter than 300 nm [3]. To investigate the nature of this process, we studied the formation of singlet oxygen upon photoexcitation of van der Waals complexes C_5H_8-O_2 as a model system for collisional complexes in the atmosphere.

The complexes C_5H_8-O_2 were generated in a pulsed molecular beam. The formation of singlet oxygen was confirmed by the appearance of an ion signal when isoprene was added to the oxygen in the molecular beam. A (2+1) Resonance-Enhanced Multiphoton Ionization (REMPI) spectrum was recorded. Additionally, the photoexcitation spectrum of singlet oxygen from isoprene-oxygen complexes was obtained in the 282–322 nm range. The band maximum coincides with the theoretically predicted value for a vertical transition. Using the velocity map imaging (VMI) technique, the velocity distribution of photofragments was recorded, revealing two components with temperatures of 120 and 493 K.

The results of this study have been published in *The Journal of Physical Chemistry A* 2025, 129 (23), 5092-5097, DOI: 10.1021/acs.jpca.5c02445.

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A method for constructing the solar coronal heating function in a gravitationally stratified atmosphere

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The problem of solar coronal heating remains one of the key challenges in modern solar physics. The functional dependence of coronal heating on plasma parameters remains unknown. In this work, we assume that the heating rate is a function of local density and temperature $Q(\rho, T)$, whose specific form is unknown [1]. A practically important task is to construct a heating function $Q(\rho, T)$ that, considering the thermal balance between heating and radiative cooling, sustains a long-lived gravitationally stratified atmosphere with a realistic temperature profile. Such a heating function would enable numerical modeling that simultaneously accounts for gravity, stratification, and thermal misbalance effects.

In this work, we propose a method for constructing the heating function that ensures a balance between heating and radiative cooling in a stationary gravitationally stratified atmosphere. The coronal heating function is approximated by a piecewise power-law dependence

$Q(\rho, T) = Q^* \left(\frac{\rho}{\rho_0}\right)^a \left(\frac{T}{T_0}\right)^b$ [1]. Under the assumption that the exponents a and b are constant within a certain range of temperatures and densities, they can be determined from the hydrostatic equilibrium equation, the ideal gas law, and the thermal balance condition applied at different heights.

The algorithm is implemented in Wolfram Mathematica. A tabulated heating function is constructed based on the obtained values of a and b along the parametric curve $(\rho(z), T(z))$. The resulting table is then exported to a format compatible with the MPI-AMRVAC software package, where the heating rate for arbitrary plasma parameters is recovered via bilinear interpolation. Numerical simulation of the solar atmosphere using the constructed heating function demonstrated the feasibility of the proposed method.

The proposed method allows constructing a coronal heating function that provides local thermal balance in the gravitationally stratified solar atmosphere. The results can be used for realistic MHD modeling of wave propagation in the solar corona accounting for gravitational stratification and thermal misbalance.

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Methods for approximating longitudinal compressional waves in the magnetic structures of the solar corona

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This work compares different approaches to approximating longitudinal compression waves in magnetic structures of the solar corona, obtained from the SDO database, analytical solution of the evolutionary equation for MHD waves in coronal loops . The effectiveness of several methods is compared using observational data. The sound speed, temperature, and thermal conductivity of the plasma are estimated for the minima of different error functions.

Intensity variations observed in magnetic structures of the solar corona (coronal loops, spicules) are often interpreted as magnetohydrodynamic (MHD) waves propagating in the medium. In the general case, the perturbations of these waves are a superposition of magnetoacoustic and entropy modes.

To correctly estimate plasma parameters (sound speed, temperature, thermal conductivity), it is necessary to use the full solution of the evolutionary equation describing all the eigenmodes of the system, rather than considering only the fundamental harmonic.

In this study, observations of compressional waves in hot coronal loops, obtained from the SDO (Solar Dynamics Observatory) database, served as initial data. The work presents a comparative analysis of several methods for approximating these observations using solutions to evolutionary equation, achieved by introducing different error functions and locating their minima. Key plasma parameters such as temperature and thermal conductivity coefficient were estimated and compared with theoretical models.

The obtained estimates of plasma parameters enable refinement of existing models of thermal transport in plasma. This represents a significant advance toward improved modeling of solar activity (in particular, solar flares) and better prediction of space weather.

Detection of solid CN^- in the protostellar envelopes using the JWST data

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Salts – the chemical compounds consist of acids and bases residuals – are the significant compound of the interstellar ices. For example, ammonium cation (NH_4^+) abundance could reach up to 23 % relative to solid water. Such an abundant positive ion should have adjacent counterions – various anions, such as cyanate (OCN^-), hydrosulfide (HS^-), formate ($HCOO^-$), acetate (CH_3COO^-) and cyanide (CN^-). While the existence of OCN^- in interstellar ices is beyond doubt, and the other mentioned anions have been tentatively detected, the search for the CN^- has still not received sufficient attention. The only work that includes the determination of cyanide anion upper limits in the icy mantles is limited to the fitting with Gaussian profile of the band at 4.78 μm attributed to the vibrations of the –C≡N group and ^{13}CO.

Determining the amount of CN^- in interstellar ice is important for several reasons. First, accurate estimates of charged species will help address the current issue of charge disbalance. Second, the cyanide anion in the form of $NH_4^+CN^-$ is a product of the reaction between ammonia (NH_3) and hydrogen cyanide (HCN), and during the sublimation process it dissociates back into the parent molecules. HCN, in turn, is a key intermediate in reaction chains leading to the formation of complex organic molecules in the interstellar medium, including nucleobases – the building blocks of DNA.

In this work, we fitted the 4.78 μm band in observational data obtained with the JWST toward the protostars HOPS91 and B335. The significantly overlapping contributions of ^{13}CO and CN^- were separated, allowing us to report the detection of the cyanide anion in condensed phase at abundances of (0.40±0.05) and (0.21±0.05) % relative to solid H_2O for these two sources, respectively.

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Methods for determining of PAHs concentration in hydrocarbon fuel emissions

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The combustion of hydrocarbon fuels, particularly kerosene, gasoline, and biofuels, can produce soot particles and their precursors, polycyclic aromatic hydrocarbons (PAHs). These substances are carcinogenic, so their presence in hydrocarbon fuel emissions has a negative impact on the environment and human health. Furthermore, soot particles reduce the service life of combustion systems. However, experimental determination of PAH content in emissions has fraught with a number of difficulties, and the accuracy of the results is often insufficient.

The main difficulties arise in collecting and preparing PAH samples for analysis, because PAHs and soot particles can stick to the walls of equipment and samplers and are poorly soluble in most solvents, which complicate their transfer to the liquid phase for further analysis. PAH sample analysis itself is most often performed using gas (or sometimes liquid) chromatography-mass spectrometry. However, despite all the advantages of this method, a mass spectrometer is a complex and expensive instrument to maintain, which is not always feasible to install in industrial laboratories. Therefore, developing an accurate and accessible method for determining PAHs content in hydrocarbon fuel emissions remains a pressing issue.

In this paper, we reviewed the main global methods for sample preparation and experimental determination of PAH concentrations in hydrocarbon fuel emissions, identified their advantages and disadvantages, identified the most accurate and easily implemented methods, and proposed optimal conditions for the experimental determination of PAH content in hydrocarbon fuel emissions.

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Theoretical study of the mechanism and kinetics of the reaction of the benzyl radical with hydroxyl

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The benzyl radical C_7H_7 is a key intermediate in the pyrolysis and oxidation of toluene, a monocyclic aromatic hydrocarbon widely used in the chemical industry and present in fuel blends at concentrations up to 15%. Due to resonance stabilization, the benzyl radical exhibits enhanced chemical stability, which leads to its accumulation in combustion processes and makes it an important species in the mechanisms of soot and polycyclic aromatic hydrocarbon (PAH) formation. Combustion processes involving PAHs and soot result in emissions of carcinogenic and toxic substances; therefore, a deep understanding of reactions involving the benzyl radical is essential for the development of cleaner fuel combustion technologies and the creation of accurate kinetic models.

Most studies to date have focused on the reactions of the benzyl radical with molecular oxygen O_2. The interaction with the hydroxyl radical OH, which has high reactivity, has been studied to a much lesser extent. Nevertheless, this reaction is important for understanding combustion processes as well as the atmospheric oxidation of benzyl alcohol $C_6H_5CH_2OH$, a substance widely used in industry.

In this work, a quantum chemical study of the potential energy surface (PES) of the C_7H_7 + OH reaction was performed using Gaussian 09. Optimized geometries of the stationary points on the PES were obtained using the b3lyp functional and the 6-311G(d,p) basis set. Relative energies were refined using the composite G3(MP2,CC) scheme in the Molpro 15 software package. Achieving chemical accuracy is necessary for subsequent calculations of rate constants and relative product yields.

The reaction is characterized by the barrierless initial addition of OH to form stabilized adducts. This is followed by competing channels of isomerization, hydrogen atom migration, and elimination of small stable molecules. Under high-pressure and relatively low-temperature conditions, the stabilization of benzyl alcohol dominates. Under conditions typical of flames (high temperatures, reduced pressure), isomerization channels followed by the elimination of water H_2O, carbon monoxide CO, and formaldehyde CH_2O prevail.

The obtained data on the structure of the PES provide the basis for further kinetic modeling. The results of this study may be useful in the development of cleaner hydrocarbon fuel combustion technologies, the reduction of PAH emissions, as well as in the creation of more accurate combustion models for internal combustion engines and power generation systems.

The Effect of Thermal Conductivity and Thermal Misbalance on the Properties and Dynamics of Magnetoacoustic and Entropy Waves in Coronal Loops

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Both thermal misbalance and thermal conduction can be significant in closed (coronal loops) and open (spicules) coronal structures. We study the longitudinal waves induced in coronal loops, taking these effects into account simultaneously. Not only propagating magnetoacoustic (MA) waves but also non-propagating entropy waves are excited in the plasma structures. These effects determine the dispersive properties (attenuation/growth rate and phase speed) of entropy and magnetoacoustic modes and the energy distribution between the modes.

In the current work, we consider the linear dynamics of slow MA and entropy waves under the approximation of an infinitely strong magnetic field. Under these assumptions, we obtain an evolutionary equation describing the properties and evolution of MA and entropy waves. We then analytically solve the Cauchy problem for this equation.

The properties of waves and their evolution in the presence of thermal misbalance and thermal conduction alone have been studied previously. It has been shown that in presence of thermal misbalance there can be only eight regimes with qualitively different behavior of dispersion curves. These regimes imply that entropy and slow MA waves can separately grow or decay. Moreover, slow MA can become non-propagating through the influence of thermal misbalance and their properties can become mixed with entropy modes. In turn, thermal conductivity implies only one possible behavior which is damping of all eigenmodes.

Using the exact solution of the evolutionary equation, we show that the behavior of the modes for the induced harmonics may be significantly complex when both non-adiabatic processes are taken into account. The phase velocities and increments/decrements can be non-monotonic with respect to the wavenumber because thermal conduction restricts the range of amplified harmonics. Moreover, under certain conditions zero, one, or even two ranges of non-propagating magnetoacoustic harmonics can appear within the spectrum. In other words the number of regimes with qualitively different behavior significantly increases.

In our study, we classify the main regimes, including cases with or without non-propagating bands, mixed properties and growth of modes. The results have direct implications for interpreting observations. This investigation is useful for plasma analysis and can be used for modeling MHD perturbations in coronal loops under the combined effect of thermal conduction and misbalance. The study was funded by the state assignment of the Ministry of Science and Higher Education of the Russian Federation, project code FSSS-2026-0010.

Theoretical study of the *i*-C_4H_5 + O_2 reaction

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The resonantly stabilized *i*-C_4H_5 radical (CH_2=C$^{\bullet}$–CH=CH_2) plays a key role in the combustion of unsaturated hydrocarbons and the formation of polycyclic aromatic hydrocarbons (PAHs). Understanding its reaction with O_2 is essential for optimizing combustion processes and minimizing soot formation. The potential energy surface was mapped at the ωB97XD/6-311G(d,p) level, with energies refined via CCSD(T)-F12/cc-pVTZ-f12. Temperature- and pressure-dependent rate constants were computed using MESS (RRKM-ME), including asymmetric Eckart tunneling. Lennard–Jones parameters for $C_4H_5O_2$ (σ=5.18 Å, ε=285.2 cm^{-1}) and N_2 (bath gas; σ=3.610 Å, ε=68.0 cm^{-1}) were used, with collisional energy transfer modeled by the "exponential down" approach (n=0.7, a_{300}=333 cm^{-1}).

The reaction begins with O_2 addition to two distinct radical sites in *i*-C_4H_5. Addition to the vinylic site proceeds with a barrier of 0.9 kcal/mol, directly forming the 1,3-divinyl-2-peroxy radical adduct. Addition to the allenic site has a barrier of 4.9 kcal/mol and yields the allenemethylperoxy adduct, which subsequently isomerizes to the same 1,3-divinyl-2-peroxy species. These two adducts serve as key intermediates connecting the entrance channel to multiple product pathways. Importantly, a new intermediate was discovered on the pathway from cyclic adduct to the vinoxy radical + ketene products. Contrary to the original mechanism proposed by Rutz et al. [1], which assumed direct dissociation via TS11 (dissociation barrier of -1.2 kcal/mol), our calculations reveal a two-step process: $C_4H_5O_2$ → new intermediate → C_2H_3O + C_2H_2O. This stationary point on the $C_4H_5O_2$ PES was not identified in previous work. The refined PES and updated kinetic scheme provide a reliable basis for modeling hydrocarbon combustion and PAH formation.

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Experimental and Theoretical Raman Spectroscopy Study of Novel Energetic Ionic Liquids

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Owing to a combination of properties such as thermal stability, low volatility, and hypergolicity (the ability to self-ignite upon contact with an oxidizer), ionic liquids (ILs) are considered a promising alternative to toxic hydrazine derivatives in liquid rocket fuel formulations. It is well known that the presence of a nitrogen-containing heterocycle in the cation structure of ILs significantly affects their ignition characteristics. Furthermore, the introduction of a 1,2,5-oxadiazole fragment into the cationic moiety facilitates the production of energetic materials with enhanced density and improved performance characteristics.

The aim of this work is to present an experimental and theoretical study of the Raman spectra of novel energetic ILs synthesized at the N. D. Zelinsky Institute of Organic Chemistry [1], for the subsequent identification of reactive species during real-time IR/Raman monitoring of the reaction of these ILs with an oxidizer.

The objects of the study are three ILs differing in the anion (NO_3^-, $N(NO_2)_2^-$) and in the type of heterocyclic fragment of the cation – a substituted furazan (Fur) or furoxan (Fur-O) linked by a methylene bridge to a 3-methylimidazolium ring. The experimental Raman spectra are compared with calculated vibrational frequencies; the assignment of bands is performed using literature data and visualization of vibrational modes via the GaussView 6 graphical interface (Gaussian software package).

The analysis and comparison of experimental and calculated vibrational modes provide a foundation for the accurate interpretation of data from future in situ spectroscopic monitoring of the reaction of novel hypergolic ILs with an oxidizer, and for investigating the proposed mechanism of their combustion.

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A method for acoustic potential manipulation in a bichromatic levitator for controlled droplet coalescence

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Various approaches exist for controlled droplet coalescence in acoustic levitators. In conventional emitter-reflector systems, coalescence is typically realized either by horizontal focusing of trap points or by vertical signal modulation. Horizontal focusing requires complex positioning control, while vertical modulation suffers from low reproducibility due to the risk of droplet fragmentation or escape from the acoustic trap. Here, we propose a method based on a bichromatic acoustic field that enables deterministic coalescence through manipulation of the acoustic potential.

A one-dimensional model consisting of two parallel planar emitters was first investigated. Analytical expressions for the pressure distribution and Gor'kov potential along the vertical axis were derived. Calculations showed that superposition of two frequencies (40 and 25 kHz) leads to redistribution of potential wells: in some regions the well depth increases, while in others it decreases. This effect served as the foundation for controlled vertical coalescence. The investigation was extended to the hemispherical transducer array configuration of the BigLev levitator. Based on the one-dimensional results, the optimal spatial arrangement of dual-frequency transducers was determined. By calculating two-dimensional distributions of acoustic pressure and Gor'kov potential, a hybrid design was selected: 40 kHz transducers in the inner and outer rings, and 25 kHz transducers in the middle ring. Initially, only the 40 kHz field is active, trapping two droplets in adjacent pressure nodes. When the 25 kHz field is activated, the contributions from both frequencies add near the lower droplet, deepening its potential well and enhancing trapping. Near the upper droplet, the low-frequency contribution opposes the primary trapping potential, reducing the well depth and causing the droplet to destabilize and fall onto the lower one. The obtained plots confirmed this behavior: the lower well deepens upon activation of the low-frequency field, while the upper well becomes shallower.

Based on these results, the configuration was implemented experimentally. The setup uses the BigLev levitator with 48 transducers operating at 40 kHz and 24 at 25 kHz, controlled by a Teensy 4.1 microcontroller. The process was recorded using a high-speed camera. Experiments with 4 μL water droplets demonstrated a 95% successful coalescence rate without sample loss. The method enables reliable initiation of coalescence via acoustic potential manipulation for conducting contactless chemical reactions in the liquid phase.

This study was supported by the Russian Science Foundation, project no. 25-69-00068.

Preparation of Highly Dispersed TiN–TiC Nitride–Carbide Composites by the Azide SHS Method during Combustion of the Ti–NaN_3–C–C_2F_4–N_2 System

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Titanium nitride (TiN) and titanium carbide (TiC) are among the most important refractory inorganic compounds widely used in modern technical ceramics and powder metallurgy. Ultrafine TiN–TiC powder composites combine the advantages of both components and find application in areas requiring high wear resistance, thermal stability, and resistance to aggressive environments. TiC is an ultra-high-temperature ceramic with high hardness, elastic modulus, and corrosion resistance, while TiN is a material with high hardness, thermal stability, and wear resistance. It is known that adding 5% TiN to TiC can increase the relative density of the material by approximately 1.5%, the Vickers hardness up to 2750 HV, and the flexural strength up to 450 MPa [1].

The application areas of TiN–TiC composites cover several directions. First of all, this material is considered for wear-resistant components of petrochemical equipment, bearing bushings, flanges, valve seats, spray chamber nozzles, sandblasting units, drilling jigs, and aluminum alloy modifiers.

The TiN–TiC composite can be produced by several methods, depending on the required material properties and application area. The main approaches include self-propagating high-temperature synthesis (SHS) for powder materials and gas-phase deposition methods for thin films and coatings [2].

In the present work, the combustion of the "Ti–NaN_3–C–C_2F_4–N_2" system was studied to obtain ultrafine TiN–TiC nitride-carbide composites by the Azide SHS-method, with the actual content of the synthesized target phases in each composite corresponding to the specified theoretical content while minimizing impurities. Instead of technical carbon and halide salts, polytetrafluoroethylene was used as the initial carbidizing and activating reagent, which promotes the formation of silicon carbide in large quantities [2]. The initial reaction equations for the synthesis of target TiN–TiC composites with a molar phase ratio ranging from 1:4 to 4:1 were as follows in this case:

$$5Ti+0,2NaN3+0,9C+0,05C2F4+1,7N2= 4TiN+TiC+0,2NaF \quad (1)$$

$$3Ti+0,2NaN3+0,9C+0,05C2F4+0,7N2= 2TiN+TiC+0,2NaF \quad (2)$$

$$2Ti+0,2NaN3+0,9C+0,05C2F4+0,2N2= TiN+TiC+0,2NaF \quad (3)$$

$$3Ti+0,4NaN3+1,8C+0,1C2F4= TiN+2TiC+0,4NaF+0,1N2 \quad (4)$$

$$5Ti+0,8NaN_3+3,6C+0,2C_2F_4= TiN+4TiC+0,8NaF+0,7N_2 \quad (5)$$

The results of thermodynamic calculations of these reactions are presented, according to which the adiabatic temperatures (3220–4106 K) are sufficient for the combustion regime to occur, and the composition of the reaction products is close to the right-hand sides of equations (1)–(5). The experimental study was carried out by combusting the initial powder mixtures in loose form and in pressed form in an SHS reactor under a gaseous nitrogen atmosphere at a pressure of 3 MPa. The study showed that the synthesized composites are powder agglomerates consisting of submicron particles ranging in size from 100 to 700 nm, whose phase composition includes only the target phases of titanium nitride (TiN) and titanium carbide (TiC).

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Thermodynamic evaluation of possibility of extracting industrial metals combined with downdraft gasification of metal-containing waste

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A comprehensive thermodynamic analysis of the recovery of industrial metals (Fe, Cu, Zn, Sn, Pb) from their oxides during the gasification of industrial waste in a downdraft gasification within the temperature range of 500–1500 K was presented. The methodology is based on the minimization of the Gibbs free energy, which allows for the prediction of the equilibrium composition of the reaction products and the determination of the most favorable temperature regimes for the extraction of pure metals. The study identifies the optimal temperature ranges for metal extraction: 840–1000 K for lead, copper, and tin; and above 1000 K for iron and zinc. The results show that metal recovery occurs under high-temperature conditions in a reducing environment predominantly consisting of CO and H_2, which facilitates the selective extraction of metals in metallic or gaseous form. Thermodynamic modeling confirms the feasibility of efficient and environmentally safe processing of industrial waste for the extraction of industrial metals and the production of combustible gases for energy needs. The data obtained enable optimization of process parameters, increasing process efficiency and reducing environmental impact. Overall, the study highlights the potential of integrating gasification and metal extraction processes, facilitating the development of waste management technologies and resource recycling.

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Formamide ($HCONH_2$) formation in $CO:NH_3$ interstellar ice analogs

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Formamide ($HCONH_2$) is the simplest molecule with a peptide bond and an important precursor in the abiotic synthesis of amino acids and nucleotides. The aim of this work is an experimental study of formamide synthesis in model NH_3:CO ices under VUV radiation using photoionization time-of-flight mass spectrometry. The experiment was conducted using the "Cryogenic Surface Processes" setup. A 50 nm thick film of NH_3:CO (3:2) was deposited onto a silver substrate at 10 K. Under ultrahigh vacuum conditions (10^{-10} Torr), the film was irradiated with vacuum ultraviolet light (115–400 nm, peaks at 124 and 160 nm) for 6 hours with a photon flux of 1.7×10^{13} $s^{-1}cm^{-2}$ (dose — 30.6 eV/molecule). Product analysis was performed using temperature-programmed desorption and time-of-flight mass spectrometry with photoionization at 10.5 eV. In the mass spectrum of the irradiated sample, at a desorption onset temperature of about 180 K [1] (maximum at 200 K), a signal at m/z = 45 was detected, corresponding to the $HCONH_2^+$ cation. Additionally, signals at m/z = 32 and 58 were detected with an intensity an order of magnitude lower, identified as hydrazine (N_2H_4) and glyoxal ($(CHO)_2$). The detection of formamide together with alternative radical recombination products confirms the previously proposed radical mechanism [2]. However, an alternative direct pathway —insertion of an excited CO molecule (in the lower triplet state $a^3\Pi$ with an energy of 6 eV) into the N–H bond of ammonia — cannot be ruled out. Further experiments with different $CO:NH_3$ ratios are required to determine the contributions of the various mechanisms.

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Unified Description of Propagating and Non-Propagating Modes in Thermally Active Plasma and Broad-Area VCSELs

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This study presents a comparative analysis of two seemingly disparate classes of phenomena: thermal instabilities in thermally active plasma and spatiotemporal optical instabilities in broad-area vertical-cavity surface-emitting lasers (VCSELs).

The theoretical framework for the plasma component focuses on the evolution of gas-dynamic perturbations, specifically slow magnetoacoustic and entropy waves [1, 2]. These modes are analyzed under the approximation of an infinitely strong magnetic field, with thermal conductivity incorporated as a key dissipative mechanism. For the laser component, optical instabilities in broad-area VCSELs are modeled using the Maxwell-Bloch equations [3]. A central finding of this investigation is the discovery of an identical mathematical structure in the dispersion relations governing both systems. Despite the distinct physical origins the dispersion relations are both cubic in frequency ω and quadratic in the wavenumber k. In each case, the spectrum consists of three distinct types of modes: two propagating modes characterized by a non-zero real frequency and a finite growth or decay rate, and one non-propagating mode with a zero real frequency that can nonetheless experience amplification or damping. This shared structure suggests a deeper underlying analogy between the wave dynamics in plasma and laser systems.

Further linear analysis reveals specific correspondences between the types of instabilities observed. It is established that isobaric thermal instability in gas-dynamic systems is directly analogous to modulation instability in VCSELs. Conversely, isochoric thermal instability closely resembles plane wave instability in the laser system.

Beyond the immediate results, this work has broader implications for astrophysics and plasma physics. Studying the development of laser instabilities under controlled laboratory conditions may provide valuable insights into the patterns and processes governing energy dissipation in astrophysical plasmas.

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Detection of quasi-periodic pulsations in stellar flare light curves using a convolutional neural network from Kepler telescope data

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Quasi-periodic pulsations (QPP) are quasi-periodic brightness oscillations detected by space observatories in the light curves of solar and stellar flares, containing important information about plasma dynamics. With the advent of the Kepler and TESS space missions, the volume of data on stellar flares has reached scales at which traditional analysis methods become labor-intensive, while the application of deep learning is constrained by the lack of labeled data.

For automatic QPP detection, this study employs a fully convolutional neural network (FCN). The network architecture includes three convolutional blocks with batch normalization, ReLU activation function, and average pooling after each block, as well as a two-channel input: the first channel contains the original light curve, the second – the signal with the trend removed using the Savitzky-Golay filter. Model training is performed on a synthetic dataset generated using three parametric flare profile models (Davenport, Gryciuk, Two Half-Gaussians), exponentially decaying QPP oscillations, and combined noise components. Accuracy evaluation is conducted on a synthetic test set and on real Kepler telescope data.

This study investigates the influence of FCN hyperparameters on QPP detection accuracy. A series of computational experiments is conducted, varying training parameters (learning rate, weight decay, batch size), signal preprocessing parameters (Savitzky-Golay filter), and considering various architectural choices.

The experiments analyze the influence of selected hyperparameters on final classification accuracy, model robustness to overfitting, and generalization ability to real data. Particular attention is paid to finding an optimal configuration that balances QPP detection completeness with minimizing false positives on noisy signals.

Application of trained models to real Kepler telescope data allows assessment of the practical applicability of the proposed approach for automated analysis of large-scale astrophysical datasets.

Further work involves extending the parametric study, exploring alternative architectures, and adapting the approach for data from other observatories.

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A Modified Kinetic Mechanism for the Combustion of Methane-Hydrogen Mixtures

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Currently, there is growing interest in methane-hydrogen fuels for gas turbine systems; such mixtures combine the advantages of natural gas and hydrogen, yet the resulting changes in combustion kinetics and flame front stability necessitate more precise models for the design and safe operation of combustion chambers. The normal flame propagation speed is a critical parameter influencing flame stability, flashback risk, and overall combustion efficiency; therefore, an accurate description of elementary reactions and their rate constants is particularly vital when varying the H_2 content in the fuel.

As part of this study, a step-by-step analysis of the Wang2018 mechanism was conducted. A sensitivity analysis was performed for a stoichiometric H_2/air mixture at P_0 = 1 atm and T_0 = 300 K, identifying the nine most significant reactions that determine the normal flame speed (S_L) under these conditions. For these reactions, the authors reviewed current statistical estimates and results from quantum-chemical calculations, and compared rate constant expressions derived from various sources. Based on this comparative analysis, a revision of the reaction rate constants is proposed; in several instances, averaged values or more up-to-date expressions from the cited literature were adopted. In most cases, these adjustments result in an increased calculated S_L while preserving the original structural framework of the Wang2018 mechanism.

A key outcome of this work is the identification and correction of a systematic error stemming from the absence – in the original mechanism – of a specific set of trimolecular reactions of the form H + O2 + M → products, which exert a significant influence on the calculated SL. The modified mechanism incorporates these trimolecular reactions, along with a series of refined elementary transformations featuring coefficients derived primarily from the Konnov2019 mechanism and the statistical analysis by Yang2021, as well as utilizing contemporary data from Sutherland and Hong for specific individual reactions. Incorporating these additions results in a reduction of calculated SL values by approximately 4–10% compared to the version of the mechanism utilizing only updated constants, thereby significantly improving agreement with experimental data.

The practical significance lies in the fact that the refined mechanism provides a more plausible prediction of laminar flame speed for methane-hydrogen mixtures and can be utilized in the modeling of combustion within gas turbine combustion chambers to assess flame stability and optimize operating conditions. The authors emphasize the need for further validation of the model across mixtures with varying hydrogen fractions in the fuel, as the influence of H_2 on kinetics and transport properties requires additional experimental and numerical investigation.

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Enhancing the efficiency of gas turbine engine combustor component design through machine learning models

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Modern aviation industry faces stringent requirements of the International Civil Aviation Organization (ICAO) regarding the reduction of harmful emissions. The primary regulated substances are nitrogen oxides (NO_x) and carbon monoxide (CO), the formation of which is governed by combustion processes within the gas turbine engine (GTE) combustor. Experience in combustor development demonstrates that fuel combustion efficiency, flame stability, temperature field uniformity at the turbine inlet, and other parameters depend on its geometry and aerodynamics. Under these conditions, the task of optimizing the combustor configuration with due regard for environmental requirements acquires paramount importance for the development of advanced aero-engines.

The processes in the combustion liner are dependent on the flow pattern from the combustor inlet to its outlet. Of particular significance is the diffuser — the component providing deceleration of the airflow delivered from the compressor and generating a uniform velocity field upstream of the combustion zone. Non-uniformity of the velocity profile at the diffuser exit, the presence of separation zones and secondary flows directly affect: ignition and combustion stability; formation of local high-temperature regions (hot spots) causing increased NO_x emissions; combustion completeness and, consequently, CO emission levels; total pressure losses, which reduce the overall engine efficiency. Thus, the diffuser serves as a critical connecting link between the compressor and the combustion liner. Total pressure losses across the diffuser account for approximately 30% of the overall combustor losses. Therefore, its optimization is a prerequisite for enhancing the environmental and economic efficiency of GTEs.

Currently, the application of intelligent data analysis methods for diffuser optimization appears particularly promising, given that its geometry is characterized by a multi-parameter space and complex non-linear relationships between structural features and aerodynamic performance indicators. The use of ML models enables: approximation of the total pressure loss function based on a limited number of numerical experiments; rapid screening of design variants without full-scale CFD analysis; identification of hidden correlations between geometric parameters and integral flow characteristics.

As a result of the optimization calculation, a database was generated containing information on geometric parameters of various diffuser configurations and corresponding total pressure loss values at the exit. Three machine learning models were trained on this dataset: LSTM, CatBoost, and MLP.

The obtained results demonstrate the feasibility of applying intelligent data analysis methods at the preliminary design stage of GTE combustor configuration, which allows reducing the volume of computational experiments and improving the accuracy of total pressure loss prediction when varying geometric parameters of the diffuser and combustion liner to within 12%.

Temporal and spectral measurements of LIF during pyrolysis of hydrocarbons of various chemical structures behind shock waves

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The transition from gas-phase polyaromatic hydrocarbons (PAH) to condensed incipient soot particles remains one of the most challenging stages of soot formation to study [1, 2]. This work presents in situ laser-induced fluorescence (LIF) measurements during shock-wave pyrolysis of methane, ethane, ethylene, diethyl ether, acetylene, and benzene, conducted in a standard shock tube behind reflected shock waves.

Fluorescence was excited by a 75 ps Nd:YAG laser pulse at 266 nm. Time-resolved signals were acquired at 340±20 nm and 430±20 nm, corresponding to PAHs of 2-3 and 4+ aromatic rings respectively [3]. LIF decay times of 2-9 ns were measured during pyrolysis of ethane, ethylene, DEE, and acetylene - longer than expected for gas-phase PAHs at high temperatures [4], but shorter than laser-induced incandescence (LII) from mature soot particles. This intermediate behavior is attributed to condensed aromatic structures within incipient soot particles, with aromatic islands on average smaller than pyrene. Incipient particles were detected at reaction times as short as 125 μs in ethylene, DEE, and acetylene mixtures.

Clear fuel-dependent trends were observed. Methane and benzene pyrolysis produced only PAH LIF signals under the investigated conditions. Acetylene showed a uniquely different spectral evolution with no PAH spectral shift and rapid transition to blackbody-like emission, suggesting a distinct nucleation pathway. Kinetic modeling using the CRECK mechanism [5] confirmed faster intermediate species formation in ethane, ethylene, and DEE relative to methane, consistent with earlier particle appearance. However, modeling significantly underestimates PAH and particle yields during acetylene pyrolysis, indicating that additional nucleation pathways remain unaccounted for.

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Thermal Misbalance Signatures in Wavelet Spectrograms of Coronal Slow Magnetoacoustic Wave Trains

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Slow magnetoacoustic (MA) wave trains are among the key wave modes in the solar corona and serve as diagnostic tools of coronal seismology [1]. Thermal misbalance with characteristic timescales τ_1 and τ_2 makes the coronal plasma response frequency-dependent: a passing wave induces periodic deviations in pressure, density, and temperature, resulting in frequency-dependent damping/amplification and dispersion of MA waves, which can excite quasi-periodic slow MA wave trains even in homogeneous plasma [2]. The present study focuses on the wavelet signatures of the thermal misbalance and their distinction from the classic "tadpole" and "boomerang" wave train patterns caused by geometric (waveguide) dispersion of MA waves due to the transverse density structuring [3].

A Python package was developed, comprising an analytical solver for the third-order linear evolutionary MHD equation [4] and a wavelet analysis module implementing the continuous wavelet transform with three mother wavelets: Morlet ($\omega_0 = 6$), Paul ($m = 4$) and the derivative of Gaussian (DOG, $m = 2$); in the amplification regime, time series from numerical MHD simulations performed with the Athena++ MHD code were additionally used. In the damping regime ($\tau_1 > \tau_2$), high-frequency harmonics propagate with higher phase velocity and simultaneously decay faster, so they arrive at the observation point first (head) while low-frequency components arrive later (extended tail), producing a "reverse tadpole" pattern. This is opposite to the geometrically dispersive case, where lower-frequency components travel faster. In the amplification regime ($\tau_1 < \tau_2$), nonlinear effects generate a sequence of growing pulses, each mapped to a separate power region on the spectrogram, forming an "orange slice" pattern. Both patterns are reproduced in all three wavelet bases, ruling out artefact interpretations and confirming their physical origin.

The results provide a basis for diagnosing τ_1 and τ_2 from wavelet spectrograms of SDO/AIA and Solar Orbiter data and for incorporating the developed toolkit into coronal seismology [1].

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