

SAMARA,  
RUSSIAN FEDERATION,  
JULY 2-6, 2024

3d International Conference  
on Physics and Chemistry  
of Combustion and Processes  
in Extreme Environments  
**TECHNICAL PROGRAM**  
and  
**BOOK OF ABSTRACTS**



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  
dedicated to the 300th anniversary of the Russian Academy of Sciences  
(Samara, Russian Federation, July 2-6, 2024)

TECHNICAL PROGRAM  
AND  
BOOK OF ABSTRACTS

“Insoma-Press”

Samara, 2024

**УДК 544.45, 544.18, 539.186, 539.196**

**ББК 24.54, 22.317**

**A 35**

Edited by V.N. Azyazov & A.M. Mayorova

**A 35 International Conference on Physics and Chemistry of Combustion and Processes in Extreme Environments (Samara, Russia, 2-6 July 2024):**

Proceeding of the conference/ Edited by V.N. Azyazov and A.M. Mayorova/  
Lebedev Physical Institute, Samara Branch – Samara: Publishing OOO “Insoma-Press”, 2024 – 109 p.

**ISBN 978-5-4317-0560-1**

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'24) dedicated to the 300th anniversary of the Russian Academy of Sciences held at Samara on July 2-6, 2024. 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'24 is held in the "Univer Studia" of the Samara University.  
Address: 151, Molodogvardeyskaya str., Samara, 443001, Russia.

# **TECHNICAL PROGRAM**

Samara Time UTC +4	2 July Tuesday	Samara Time UTC +4	3 July Wednesday	Samara Time UTC +4	4 July Thursday	5 July Friday	Samara Time UTC +4	6 July Saturday
		09.15-9.40	Antonov (invited)	09.15-9.40	Kayazkov (invited)	Matveev (plenary)	09.15-9.40	<b>Excursion - Zhiguli, Volga</b> (is not included in the conference fee) <b>9.00-14.00</b>  <b>D E P A R T U R E</b>
09.30-10.00	Registration	09.40-10.20	Feldman (plenary)	09.40-10.20	Smirnov (plenary)	Prokofjevs (plenary)	09.40-10.20	
10.00-10.20	Opening remarks							
10.20-11.00	Shmakov (plenary)	10.20-10.45	Wiebe (invited)	10.20-11.00	Eremin (plenary)	Anyang Li (online) (invited)	10.20-10.45	
		10.45-11.10	Murga (invited)			Bykov (online) (invited)	10.45-11.10	
11.00-11.25	Gubernov (invited)	11.10-11.30	Coffee break	11.00-11.20	Coffee break	Coffee break	11.10-11.30	
11.25-11.45	Coffee break	11.30-11.55	Zinchenko (invited)	11.20-11.45	Fershtat (invited)	Abbasi	11.30-11.45	
11.45-12.00	Trubachev			11.45-12.00	Amosov	Stakhanov	11.45-12.00	
12.00-12.15	Sereschenko	11.55-12.10	Riashchikov	12.00-12.15	Titova	Shostov	12.00-12.15	
12.15-12.30	Kislov	12.10-12.25	Borshcheva	12.15-12.30	Shevchenko	Yakovlev	12.15-12.30	
12.30-12.45	Kasymov	12.25-12.40	Zavershinski	12.30-12.45	Salgansky	Sosnin	12.30-12.45	
12.45-13.00	Bolshova	12.40-12.55	Kuznetsov O.	12.45-13.00	Vershmina	Moroshkina	12.45-13.00	
13.00-13.15	Cherepanov	12.55-13.10	Dereev	13.00-13.15	Morar	Lunch	13.00-14.30	
13.15-14.45	Lunch	13.10-14.40	Lunch	13.15-14.45	Lunch			
14.45-15.10	Kiselev (invited)	14.40-15.20	Nakariakov (plenary) (online)	14.50	Departure to Samara University, Moskovskoe shosse	Kuznetsov A. (invited) online	14.30-15.10	
15.10-15.35	Osipova (invited)					Mebel (plenary) online	15.10-15.50	
15.35-15.50	Dorokhov	15.20-15.45	Fedoseev (online) (invited)		Excursion to the Aircraft Engine History Center (SSAU) + УНУ "Реакционная кинетика и динамика в экстремальных условиях"			
16.00	Departure to River Station	15.45-16.10	Vasyunin (invited)	15.30-17.30		Pershim	15.50-16.05	
16.30	Boarding 16-30	16.10-16.30	Coffee break			Gurakov	16.05-16.20	
	Ferry trip along the Volga River	16.45-18.40	Poster 16.45-18.40		15.30-18.30	Closing remarks	16.20-16.30	
17.00-21.00	Welcome Party			17.30	Conference Dinner (is not included in the conference fee)			

## 2 July, Tuesday (Samara time UTC +4)

### 10.00-10.20 Opening and Welcome Remarks

**Session 1.1 Chair:** Nicolay N. Smirnov (Lomonosov Moscow State University, FSC “Scientific Research Institute for System Analysis of RAS”)

**10.20-11.00** Andrey Shmakov<sup>1</sup>, D. Knyazkov<sup>1,2</sup>, T. Bolshova<sup>1</sup>, I. Gerasimov<sup>1</sup>, K. Osipova<sup>1,2</sup>, A. Dmitriev<sup>1,2</sup> (<sup>1</sup>Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, <sup>2</sup>Novosibirsk State University, Novosibirsk, Russia) **Study of the flame structure of CH<sub>4</sub>/H<sub>2</sub> mixtures at elevated pressure and development of reduced reaction mechanism** (*Plenary*)

**11.00-11.25** Vladimir Gubernov, (P.N. Lebedev Physical Institute of RAS, Moscow, Russia) **On the role of low temperature reactions in burner stabilized and propagating flames** (*Invited*)

### 11.25-11.45 Coffee Break

**Session 1.2 Chair:** Alexander Eremin (Joint Institute for High Temperatures of the RAS)

**11.45-12.00** Stanislav Trubachev<sup>1</sup>, O. Korobeinichev<sup>1</sup>, A. Karpov<sup>3</sup>, A. Paletsky<sup>1</sup>, E. Sosnin<sup>1,2</sup>, A. Shaklein<sup>3</sup>, I. Kulikov<sup>1</sup>, A. Sagitov<sup>1,2</sup>, A. Shmakov<sup>1</sup>, A. Chernov<sup>1</sup>, O. Tuzhikov<sup>4</sup>, Xin Wang<sup>5</sup> (<sup>1</sup>Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, <sup>2</sup>Novosibirsk State University, Novosibirsk; <sup>3</sup>Udmurt Federal Research Center, Izhevsk, <sup>4</sup>Volgograd State Technical University, Volgograd, Russia, <sup>5</sup> State Key Laboratory of Fire Science, USTC, P.R. China) **The influence of flame retardants on the combustion of fiber-reinforced epoxy resin**

**12.00-12.15** Evgenii Sereshchenko, V. Gubernov, S. Minaev (P.N. Lebedev Physical Institute of Russian Academy of Sciences, Moscow, Russia) **Dynamics of sporadic combustion waves and single ball-like flame in straight channels**

**12.15-12.30** Vladimir Kislov, M. Tsvetkov, Yu. Tsvetkova, M. Salganskaya, A. Zaichenko, E. Salgansky, D. Podlesniy (Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia) **Neutralization of sulfur compounds by calcium-based additives in the filtration combustion processes**

**12.30-12.45** Denis Kasymov<sup>1</sup>, V. Perminov<sup>2</sup>, E. Golubnichiy<sup>1</sup> (<sup>1</sup>Tomsk State University, <sup>2</sup>Tomsk Polytechnic University, Tomsk, Russia) **Firebrand Generation and Transport During Forest Fires: Experimental Approach**

**12.45-13.00** Tatyana Bolshova, V. Shvartsberg, A. Shmakov (Voevodsky Institute of Chemical Kinetics and Combustion, Novosibirsk, Russia) **Regularities of the combustion chemistry of PMMA in the oxidizer flow in microgravity**

**13.00-13.15** Andrey Cherepanov<sup>1,2</sup>, D. Knyazkov<sup>1,2</sup>, K. Osipova<sup>1,2</sup>, V. Kiselev<sup>1,2</sup>, A. Dmitriev<sup>1,2</sup>, A. Shmakov<sup>1,2</sup> (<sup>1</sup>Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, <sup>2</sup>Novosibirsk State University, Novosibirsk, Russia) **Ion chemistry in ammonia-hydrogen-oxygen flames**

**13.15-14.45** LUNCH



**Session 1.3 Chair:** Vladimir V. Gubernov (P.N. Lebedev Physical Institute of RAS, Moscow)

**14.45-15.10** Vitaly Kiselev,<sup>1,2,3</sup> M. Gorn,<sup>1,2</sup> Sh. Vaddypally,<sup>4</sup> M.J. Zdilla<sup>4</sup> (<sup>1</sup>Institute of Chemical Kinetics and Combustion SB RAS, <sup>2</sup>Novosibirsk State University, Novosibirsk, Russia, <sup>3</sup>Semenov Federal Research Center for Chemical Physics RAS, Moscow, Russia <sup>4</sup>Temple University, United States) **Thermal stability and unusual rearrangements of nitrogen-rich energetic compounds: New insights from predictive electronic structure calculations** (*invited*)

**15.10-15.35** Ksenia Osipova, A. Shmakov (Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk, Russia) **Kinetics of oxidation and combustion processes of ammonia-based fuel blends** (*invited*)

**15.35-15.50** Vadim Dorokhov, G. Nyashina, D. Romanov, K. Vershinina (Heat and Mass Transfer Laboratory, National Research Tomsk Polytechnic University, Tomsk, Russia) **Combustion of pellets from biomass and refused derived fuel**

### **3 July, Wednesday** (Samara time UTC +4)

**Session 2.1 Chair:** Valery N. Azyazov (Lebedev Physical Institute of RAS, Samara Branch)

**9.15-09.40** Ivan Antonov (Lebedev Physical Institute (Samara Branch), Samara National Research University, Samara, Russia) **Recent progress in the building of the Cryogenic Surface Processes apparatus: chemistry of interstellar methane ices** (*invited*)

**9.40-10.20** Vladimir Feldman (Lomonosov Moscow State University, Moscow, Russia) **Modeling of cold astrochemical processes through matrix isolation: extremely hot chemistry at extremely low temperatures** (*plenary*)

**10.20-10.45** Dmitri Wiebe (Institute of Astronomy of the RAS, Moscow, Russia) **Cosmic rays as an astrochemical factor** (*invited*)

**10.45-11.10** Maria Murga, (Institute of astronomy of Russian academy of sciences, Moscow, Russia) **Evolution of carbonaceous particles from AGB stars to planetary nebulae: observations and theory** (*invited*)

**11.10-11.30 Coffee Break**

**Session 2.2. Chair:** Vladimir I. Feldman (Lomonosov Moscow State University, Moscow)

**11.30-11.55** Igor I. Zinchenko (Federal Research Center A.V. Gaponov-Grekhov Institute of Applied Physics of RAS, Nizhny Novgorod, Russia) **Molecular inventory of the interstellar medium** (*invited*)

**11.55-12.10** Dmitry Riashchikov<sup>1,2</sup>, N. Molevich<sup>1,2</sup>, D. Zavershinskii<sup>1,2</sup>, E. Scoptsova<sup>1</sup> (<sup>1</sup>Samara National Research University, <sup>2</sup>Lebedev Physical Institute, Samara Branch, Samara, Russia) **Propagation features of acoustic-gravity waves in a medium with thermal misbalance**



**12.10-12.25** Ekaterina Borshcheva<sup>1</sup>, A. Vasyunin<sup>2</sup> (<sup>1</sup> Institute of Astronomy of RAS, Moscow, Russia, <sup>2</sup> Ural Federal University, Yekaterinburg, Russia) **Formation of complex organic molecules in prestellar cores: the role of non-diffusive grain chemistry**

**12.25-12.40** Dmitry Zavershinskii<sup>1,2</sup>; N. Molevich <sup>1,2</sup>; D. Riashchikov; S. Belov<sup>2</sup> (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia) **Dynamics of slow magnetoacoustic and entropy modes in flaring coronal loops**

**12.40-12.55** Oleg Kuznetsov, M. Evseev, V. Azyazov (Lebedev Physical Institute, Samara Branch, Samara, Russia) **Experimental investigation of naphthalene growth via HACA mechanism**

**12.55-13.10** Sergey Derteev, M. Sapraliev, N. Shividov, B. Mikhalyaev (Kalmyk state university named after B.B. Gorodovikov, Elista, Russia) **Quasi-periodic pulsations in active regions of the solar corona**

**13.10-14.40** LUNCH

**Session 2.3 Chair:** Maria Murga (Institute of Astronomy of the RAS, Moscow)

14.40-15.20 Valery Nakariakov (University of Warwick, Coventry, United Kingdom) **Solar corona as active MHD media (plenary) (online)**

**15.20-15.45** Gleb Fedoseev<sup>1,2</sup> (<sup>1</sup> Xinjiang Astronomical Observatory, Chinese Academy of Sciences, <sup>2</sup> Xinjiang Key Laboratory of Radio Astrophysics, Urumqi, China) **Laboratory investigation of interstellar ice analogues in view of the newest open data from JWST observatory (invited) (online)**

**15.45-16.10** Anton Vasyunin<sup>1</sup>, Ekaterina Borscheva<sup>2,1</sup>, Alexey Mozhegorov<sup>1,3</sup>, Anna Punanova, Maxim Ozhiganov<sup>1</sup>, Mikhail Medvedev<sup>1</sup>, Varvara Karteeva<sup>1</sup>, Ruslan Nakibov<sup>1</sup> (<sup>1</sup> Ural Federal Institute, Yekaterinburg, <sup>2</sup>Institute of Astronomy of the RAS, Moscow, Ekaterinburg Theological Seminary, Yekaterinburg, Russia) **Modeling the Composition of Interstellar Ices observed with the James Webb Space Telescope (invited)**

**16.10-16.30** Coffee Break

**16.30-18.30** Poster Session

P1. Nikita Bystrov, A. Emelianov, A. Eremin, P. Yatsenko (Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia) **Measurements of the oxygen dissociation rate constant with verification of modern models of hydrocarbon combustion**

P2. Artëm Dmitriev, D. Knyazkov, A. Shmakov (Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, <sup>2</sup>Novosibirsk State University, Novosibirsk, Russia) **Chemical structure of laminar hydrogen flames with the addition of tetraethoxysilane**

P3. A. Eremin, Egor Khodyko, R. Kolotushkin, (Joint Institute for High Temperatures of the RAS, Moscow, Russia) **Investigation of the soot growth process in a flame by the 2D-LII method**

- P4. A.V. Eremin<sup>1</sup>, M. R. Korshunova<sup>1</sup>, E. Yu. Mikheyeva<sup>1</sup>, V.N. Zolotarev<sup>1,2</sup> (<sup>1</sup> Joint Institute for High Temperatures of the RAS, <sup>2</sup> Moscow Institute of Physics and Technologies, Moscow, Russia) **Investigation of soot and PAHs formation during hydrocarbons pyrolysis with kinetic modeling and optical density measurements in UV-VIS range**
- P5. Alina Ponomareva<sup>1,2</sup>, A. Moroshkina<sup>1</sup>, E. Sereshchenko<sup>1</sup>, V. Mislavskii<sup>1</sup>, V. Gubernov<sup>1</sup> (<sup>1</sup>Lebedev Physical Institute of RAS, Moscow, <sup>2</sup>ITMO University, Saint Petersburg) **Activation energy of lean methane-hydrogen-air mixtures**
- P6. Eugene Salgansky, A. Zaichenko, D. Podlesniy, M. Salganskaya, M. Tsvetkov, Yu. Tsvetkova (Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia) **Thermodynamic assessment of the composition of mixed solid fuel for the gas generator of a high-speed flying vehicle**
- P7. M. Tsvetkov<sup>1</sup>, D. Podlesniy<sup>1</sup>, M. Salganskaya<sup>1</sup>, Yu. Tsvetkova<sup>1</sup>, A. Glukhov<sup>1</sup>, E. Latkovskaya<sup>2</sup>, A. Zaichenko<sup>1</sup>, Eugene Salgansky<sup>1</sup> (Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia, <sup>2</sup>Sakhalin State University, Yuzhno-Sakhalinsk, Russia) **Characteristics of algae biomass-derived biochars**
- P8. Vladimir Kislov, M. Tsvetkov, Yu. Tsvetkova, M. Salganskaya, A. Zaichenko, E. Salgansky, D. Podlesniy (Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia) **Thermal decomposition of sulfur brown coal at different heating rates**
- P9. Vladimir Kislov, M. Tsvetkov, Yu. Tsvetkova, M. Salganskaya, A. Zaichenko, E. Salgansky, D. Podlesniy (Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia) **The dynamics of sulfur compounds release investigation at combustion and its absorption by the calcium-based additives**
- P10. Raphael Kryev, A.M. Korobkov, E.G. Belov, S.V. Mikhailov, A.A. Yagofarov (Kazan National Research Technological University, Kazan, Russia) **Energy-saturated materials based on silicon and halogen-containing polymers**
- P11. V. Arkhipov<sup>1</sup>, Nikolay Zolotarev<sup>1,2</sup> (<sup>1</sup> National Research Tomsk State University, Tomsk, Russia, <sup>2</sup> Kutateladze Institute of Thermophysics of the Siberian Branch of the RAS, Novosibirsk, Russia) **Influence of aluminum powder additives on the acoustic conductivity of the burning surface of solid propellant**
- P12. Denis Davydov, E. Umerov, V. Novikov (Samara State Technical University, Samara, Russia) **Preparation of Ti<sub>3</sub>SiC<sub>2</sub> and Ti<sub>3</sub>AlC<sub>2</sub> MAX phases from TiSi<sub>2</sub>-C and TiAl-C by SHS in river sand shield**
- P13. Denis Davydov, A. Amosov (Samara State Technical University, Samara, Russia) **Synthesis of porous MAX phases Ti<sub>3</sub>SiC<sub>2</sub> and Ti<sub>3</sub>AlC<sub>2</sub> by combustion in air and river sand**
- P14. V. Perminov<sup>1</sup> Denis Kasymov<sup>2</sup> (<sup>1</sup>Tomsk Polytechnic University, <sup>2</sup>Tomsk State University, Tomsk, Russia) **Mathematical and physical modeling of forest fire spread in the presence of firebreaks**
- P15. Alexey Chichinin (Institute of Chemical Kinetics and Combustion, Siberian Branch RAS, Novosibirsk, Russia) **Astropolarimetry: reduced form of statistical equilibrium equations**
- P16. Ivan Pomelnikov<sup>1,2</sup>, D. Riashchikov<sup>1,2</sup>, N. Molevich<sup>1,2</sup> (<sup>1</sup> Lebedev Physical Institute, Samara Branch, <sup>2</sup> Samara National Research University, Samara, Russia) **Study of clumps in atomic zones of photodissociation regions**

- P17. Elizaveta Scoptsova<sup>1</sup>, D. Riashchikov<sup>1,2</sup>, D. Zavershinskii<sup>1,2</sup> (<sup>1</sup>Samara National Research University, <sup>2</sup>Lebedev Physical Institute, Samara Branch, Samara, Russia) **Impact of non-adiabatic heating and cooling on the gravitational stratification of the solar atmosphere**
- P18. Maksim Ozhiganov, U. Sapunova, M. Medvedev, V. Karteeva, R. Nakibov, A. Vasyunin (Ural Federal University, Yekaterinburg, Russia) **The effect of N<sub>2</sub> presence on the interstellar ice analogs infrared spectra**
- P19. Anna Astashova<sup>1,2</sup>, M. Evseev<sup>1</sup>, E. Bashkirov<sup>2</sup> (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia) **Synthesis of the simplest alcohols and nitrogen-substituted PAHs in the interstellar medium**
- P20. Mikhail Evseev<sup>1</sup>, A. Astashova<sup>1,2</sup> (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia) **Radical substitution reactions between light alkanes and their radicals**
- P21. Anatoliy Nikolayev<sup>1,2</sup>, V. Azyazov<sup>1,2</sup>, A. Mebel<sup>2,3</sup> (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia, <sup>3</sup>Florida International University, Miami, Florida, USA) **Gas-phase synthesis of phenylacetylene in the reaction of 1,3-butadiene with the butadiynyl radical**
- P22. Vladislav Krasnoukhov<sup>1</sup>, A. Mebel<sup>2,3</sup> (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia, <sup>3</sup>Florida International University, Miami, Florida, USA) **Gas-phase Formation of Phenanthrene and Dibenzofulvene via the Reaction of Fluorenyl and Methyl Radicals**
- P23. Sergey Tuchin, E. Batrakova, D. Trufanov, I. Antonov (Lebedev Physical Institute, Samara Branch, Samara National Research University, Samara, Russia) **Experimental optimization of the time-of-flight mass spectrometer of the cryogenic surface processes: mass spectrum of butadiene**
- P24. Evgeniya Batrakova, S. Tuchin, D. Trufanov, I. Antonov (Lebedev Physical Institute, Samara Branch, Samara National Research University, Samara, Russia) **Reactions in cryogenic methane films initiated by ultraviolet vacuum radiation**
- P25. Danila Trufanov, E. Batrakova, S. Tuchin, I. Antonov (Lebedev Physical Institute, Samara Branch, Samara National Research University, Samara, Russia) **Numerical simulation of the time-of-flight mass spectrometer of the cryogenic surface processes apparatus: influence of the inhomogeneity of the source region field**
- P26. Alina Kuznetsova, D. Porfiriev, V. Azyazov (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia) **Theoretical study of 1-acenaphthyl oxidation with molecular oxygen**
- P27. Lubov Krikunova, D. Porfirev, V. Azyazov (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia) **The Acetobenzene with methyldiyne potential energy surface**
- P28. Mehdi Abbasi, A. Nateghi (University of Tehran, Tehran, I.R. Iran) **Further Development of Multi-component Diesel Surrogate Model on Naphthanes for High Temperature Combustion**
- P29. Aleksei Torbin<sup>1,2</sup>, A. Chernyshov<sup>1</sup>, P. Mikheyev<sup>1</sup> (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup>Samara National Research University, Samara, Russia) **NO<sub>2</sub> production in a dielectric barrier discharge in air-CH<sub>4</sub> mixtures**

- P30. Ruslan Kuramshin<sup>1,2</sup>, A. Torbin<sup>1,2</sup>, A. Chernyshov<sup>1</sup> (<sup>1</sup>Lebedev Physical Institute, Samara Branch, <sup>2</sup> Samara National Research University, Samara, Russia) **Measuring gas temperature in Ar-He plasma using diode laser absorption spectroscopy**
- P31. Ekaterina Sidorova<sup>1</sup>, A. Shtyrlov<sup>1</sup>, P. Strizhak<sup>2</sup>, D. Antonov<sup>2</sup>, I. Zubrilin<sup>1</sup> (<sup>1</sup> Samara National Research University, Samara, <sup>2</sup> Energy Engineering School, National Research Tomsk Polytechnic University, Tomsk, Russia) **Methodology for plotting a distillation curve for multicomponent fuels with the addition of ethers**
- P32. Andrey Golenko<sup>1</sup>, A. Savchenkova<sup>1</sup>, I. Chechet<sup>1</sup>, S. Matveev<sup>1</sup>, A. Konnov<sup>2</sup>, A. Mebel<sup>1,3</sup> (<sup>1</sup>Samara National Research University, Samara, Russia, <sup>2</sup>Lund University, Lund, Sweden, <sup>3</sup>Florida International University; Miami, USA) **Rate constants for the interaction of para-pyridyl with O<sub>2</sub>: Theoretical study**
- P33. Anna S. Savchenkova, A. M. Golenko, I.V. Chechet, S.G. Matveev, A.A. Konnov, A.M. Mebel (Samara National Research University, Samara, Russia) **Interaction of pyridine radicals with molecular oxygen: Theoretical study**
- P34. Aleksandr Semenikhin, A. Savchenkova, S. Matveev, A. Mebel (Samara National Research University, Samara, Russia) **Singlet potential energy surface of C<sub>3</sub>H<sub>2</sub>+O<sub>2</sub> interaction**
- P35. Vladislav Anisimov, I. Chechet, O. Kolomzarov, M. Anisimov, D. Bobkova (Samara National Research University, Samara, Russia) **The efficiency of combustor perforated plate**
- P36. Nikita Gurakov, A. Popov, S. Matveev, S. Matveev, D. Idrisov, S. Gilyazova (Samara National Research University, Samara, Russia) **Calculation method for lean flame blowout limit of CH<sub>4</sub>/H<sub>2</sub>/air combustion considering laminar flame speed values**
- P37. Sergey Matveev, D. Idrisov, N. Gurakov, A. Litarova, R. Ivanov (Samara National Research University, Samara, Russia) **Numerical and experimental study of NO<sub>x</sub> formation during hydrogen combustion in a model combustion chamber with a cluster microflame burner device**
- P38. Dmitry Idrisov, S. Matveev, V. Abrashkin, S. Lukachev, A. Litarova, D. Kutcher (Samara National Research University, Samara, Russia) **Development of a method for determining the flashback limits when using methane-hydrogen fuel in the combustion chambers of gas turbine engines**
- P39. Maksim Labaev, I. Platonov, I. Muhanova, A. Saltanova (Samara National Research University, Samara, Russia) **Solid-phase extraction of synthetic dyes from wastewater and their analysis by HPLC**
- P40. Aleksandr Bryksin, I. Platonov (Samara National Research University, Samara, Russia) **Testing of monolithic chromato-desorption systems with organic solvents under extreme conditions**
- P41. Igor Liskov, B. Aduiev, D. Nurmukhametov (The Federal Research Center of Coal and Coal-Chemistry of Siberian Branch of the RAS, Kemerovo, Russia) **Ignition of carbon microparticles by continuous laser radiation of various wavelengths**
- P42. Denis Nurmukhametov, B. Aduiev, G. Belokurov (The Federal Research Center of Coal and Coal-Chemistry of Siberian Branch of the RAS, Kemerovo, Russia) **Ignition of microparticles of coals of different ash content by laser pulses**

P43. Boris P. Aduiev, D.R. Nurmukhametov, I.Y. Liskov (The Federal Research Center of Coal and Coal-Chemistry of Siberian Branch of the Russian Academy of Sciences, Kemerovo, Russia)  
**Features of laser ignition of carbon particles by laser radiation (overview)**

## **4 July, Thursday** (Samara time UTC +4)

### **Session 3.1**

**Chair:** Andrey G. Shmakov (Voevodsky Institute of Chemical Kinetics and Combustion SB RAS)

**09.15-09.40** Denis Knyazkov, A. Cherepanov, V. Kiselev, A. Dmitriev, A. Shmakov, (Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, Novosibirsk, Russia) **A comprehensive chemical kinetic model for the evolution of charged species naturally occurring in non-sooting flames of hydrocarbons** (*Invited*)

**09.40-10.20** Nickolay N. Smirnov (Moscow Lomonosov State University, Federal Science Center “Scientific Research Institute for System Analysis of Russian Academy of Sciences”, Moscow, Russia) **Control of detonation propagation by chemical physics methods** (*Plenary*)

**10.20-11.00** Alexander Eremin (Joint Institute for High Temperatures of the Russian Academy of Sciences, Moscow, Russia) **Passive and active laser methods for studying the kinetics of high-temperature reactions in shock tubes** (*Plenary*)

**11.00-11.20** **Coffee Break**

### **Session 3.2**

**Chair:** Denis A. Knyazkov (Voevodsky Institute of Chemical Kinetics and Combustion SB RAS)

**11.20-11.45** Leonid L. Fershtat<sup>1</sup>, Nikita V. Muravyev<sup>2</sup> (<sup>1</sup> N.D. Zelinsky Institute of Organic Chemistry, <sup>2</sup> N.N. Semenov Federal Research Centre for Chemical Physics, Russian Academy of Sciences, Moscow, Russia) **Polynitrogen Heterocycle-based Energetic Materials: Synthesis and Properties** (*Invited*)

**11.45-12.00** Aleksandr P. Amosov, I. Uvarova, Yu. Titova (Samara State Technical University, Samara, Russia) **Combustion synthesis of highly dispersed powder composition AlN-SiC using sodium azide and polytetrafluoroethylene**

**12.00-12.15** Yulia Titova, G. Belova, A. Yakubova (Samara State Technical University, Samara, Russia) **Application of combustion of Ti-Si-Na<sub>3</sub>N<sub>3</sub>-Na<sub>2</sub>SiF<sub>6</sub>-C powder mixture for the synthesis of highly dispersed Si<sub>3</sub>N<sub>4</sub>-TiC ceramic composition**

**12.15-12.30** Alexander Shevchenko<sup>1,2</sup>, M. Frolov<sup>2</sup>, V. Blatov<sup>2</sup> (<sup>1</sup> Lebedev Physical Institute, Samara Branch, <sup>2</sup> Samara State Technical University, Samara, Russia) **Crystallochemical approach to high-throughput screening of potential ionic electrides**



**12.30-12.45** Eugene Salgansky, A. Zaichenko, D. Podlesniy, M. Salganskaya, M. Tsvetkov, Yu. Tsvetkova (Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS, Chernogolovka, Russia) **Experimental study of low-temperature gasification of urotropine at different flux of filtering gas with obtaining combustible gaseous products**

**12.45-13.00** D. Romanov<sup>1,2</sup>, P. Strizhak<sup>1,2</sup>, Ksenia Vershinina<sup>1</sup>, K. Kartashova<sup>1</sup> (<sup>1</sup>National Research Tomsk Polytechnic University, <sup>2</sup>Kutateladze Institute of Thermophysics SB RAS, Novosibirsk, Russia) **Ignition, combustion, and emission performance of composite fuels from fossil and biomass derived components**

**13.00-13.15** Gabriela Morar, A. Karpov, A. Shaklein (Udmurt Federal Research Center Ural Branch Russian Academy of Science, Izhevsk, Russia) **Numerical Study of the Thermal Structure of Turbulent Diffusion Flame on PMMA surface**

**13.15-14.45** LUNCH

## **5 July, Friday** (Samara time UTC +4)

**Session 4.1 Chair:** Ivan O. Antonov (Lebedev Physical Institute of RAS, Samara Branch)

**09.15-09.40** Sergey G. Matveev, S. Matveev, N. Gurakov (Samara National Research University, Samara, Russia) **Issues of process modelling in aircraft gas turbine engines' combustion chambers** (*Plenary*)

**09.40-10.20** Aleksandrs Prokofjevs (North Carolina Agricultural and Technical State University, Greensboro, USA) **Organic Chemists' Journey into 2D Materials** (*Plenary*)

**10.20-10.45** Anyang Li (College of Chemistry and Materials Science, Northwest University, Xi'an, P. R. China) **Effects of submerged barrier on rate coefficients and microscopic mechanisms of ion-molecule reactions** (*Invited*) (*Online*)

**10.45-11.10** Viatcheslav Bykov, (Karlsruhe Institute of Technology, Institute of Technical Thermodynamics, Karlsruhe, Germany,) **Model reduction of mechanisms of chemical kinetics and the problem of estimation of reaction rate constants** (*Invited*) (*Online*)

**11.10-11.30** **Coffee Break**

**Session 4.2 Chair:** Leonid L. Fershtat (N.D. Zelinsky Institute of Organic Chemistry)

**11.30-11.45** Mehdi Abbasi<sup>1</sup>, Ali Chaibakhsh Langroudi<sup>2</sup>, Amirreza P. Shirazi<sup>1</sup> (<sup>1</sup> University of Tehran, Tehran, I.R. Iran, <sup>2</sup> University of Guilan, Rasht, I.R. Iran) **Rearrangement of Combustion Control System of Gas Turbine, Based on the Diesel Surrogate Model**

**11.45-12.00** Vyacheslav Stakhanov, O. Shults, A. Ryakin, I. Sharapov, A. Ushkov (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin», Snezhinsk, Russia) **Experimental investigation of combustion limits of hydrogen/ methane/carbon monoxide/air/water vapor mixtures**

**12.00-12.15** Artyom Shostov, K. Fedotova (Bauman Moscow State Technical University, Moscow, Russia) **Numerical simulation of waveguide elements of an experimental microwave setup to determine the burning rate of energy condensed systems**

**12.15-12.30** Savva Yakovlev, E. Bezgodov, S. Pasyukov, A. Tarakanov, M. Nikiforov (FSUE «RFNC – VNIITF named after Academ. E. I. Zababakhin», Snezhinsk, Russia) **Combustion of non-uniformly hydrogen-air mixtures in partially obstructed closed volume**

**12.30-12.45** Egor Sosnin<sup>1,2</sup>, S. Trubachev<sup>1,2</sup>, O. Korobeinichev<sup>1</sup>, A. Karpov<sup>3</sup>, A. Paletsky<sup>1</sup>, A. Shaklein<sup>3</sup>, I. Kulikov<sup>1</sup>, A. Sagitov<sup>1,2</sup>, A. Shmakov<sup>1</sup>, A. Chernov<sup>1</sup>, O. Tuzhikov<sup>4</sup> (<sup>1</sup>Voevodsky Institute of Chemical Kinetics and Combustion SB RAS, <sup>2</sup>Novosibirsk State University, <sup>3</sup>Udmurt Federal Research Center., Izhevsk, <sup>4</sup>Volgograd State Technical University, Russia) **Experimental study of flame spread over flame retardant glass fiber-reinforced epoxy resin in opposed oxidizer flow**

**12.45-13.00** Anastasia Moroshkina, A. Ponomareva, E. Sereshchenko, V. Mislavskii, V. Gubernov (P.N. Lebedev Physical Institute of Russian Academy of Sciences, Moscow, Russia) **Investigation of critical phenomena of the methane-air flames at normal and elevated pressure**

**13.00-14.30** LUNCH

**Session 4.3** Chair: Valery N. Azyazov (Lebedev Physical Institute, Samara Branch)

**14.30-15.10** Aleksey Kuznetsov (Universidad Técnica Federico Santa María, Vitacura, Chile) **Graphene composites with various partner species: porphyrinoids, organometallic compounds, metal clusters, etc. (Invited), (online)**

**15.10-15.50** A. Nikolayev,<sup>1</sup> M. Evseev,<sup>1</sup> V. Krasnoukhov<sup>1</sup>, A. Kuznetsova,<sup>1</sup> P. Pivovarov,<sup>1</sup> D. Porfiriev,<sup>1</sup> Alexander M. Mebel,<sup>2</sup> and R. Kaiser<sup>3</sup> (<sup>1</sup>Samara National Research University, Samara, Russia, <sup>2</sup>Florida International University, Miami, USA, <sup>3</sup>University of Hawaii at Manoa, Honolulu, USA) **Functionalization of pyrimidine and purine to RNA bases in water/ammonia ices via radical substitution reactions (Plenary), (online)**

**15.50-16.05** Andrey Pershin, S. Miroshnichenko (Samara University, Samara Branch of LPI RAS) **Inelastic cross sections for Ar\*-He complex**

**16.05-16.20** Nikita Gurakov, A. Popov, R. Ivanov, O. Kolomzarov, A. Semenikhin (Samara National Research University, Samara, Russia) **Study of the Initial Air-Fuel Mixture Temperature Effect on Ethane Flame Heat Release Rate Pulsation**

**16.20-16.30** Closing remarks



# **BOOK OF ABSTRACTS**

## **PLENARY AND INVITED TALKS**

# **Recent progress in the building of the Cryogenic Surface Processes apparatus: chemistry of interstellar methane ices**

Ivan Antonov

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An experimental facility for the study of cryogenic surface processes (CSP) was created in the Samara branch of Lebedev Physical Institute under the Megagrant No. 075-15-2021-597 from June 2, 2021. The apparatus allows reproducing the conditions of the interstellar medium (ultra-high vacuum, cryogenic temperatures and ionizing radiation) to obtain ice films analogues of the interstellar ices and study the non-equilibrium chemical processes occurring in them.

The report will present the design, principles of operation, current status and future directions of development of the new apparatus. Preliminary experiments to study chemical processes in methane ice films initiated by vacuum ultraviolet radiation and future research plans will be discussed.

# Model reduction of mechanisms of chemical kinetics and the problem of estimation of reaction rate constants

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The problem of parameter estimation of models of chemical kinetics plays an important role and attracts attention nowadays because of increasing usage of computational tools, see e.g. [1] where the problem for laminar flame velocity as one of most important property of the flame predictions is revised. At present, existing conventional methods to cope with this problem led to constant increase of complexity and dimension of corresponding models [1]. The problem requires both revision of the estimation process with respect to experiments by enriching the experimental evidences for independent estimation of the key rate limiting parameters [2]. This can be used to access the key reactions (via e.g., sensitivity analysis) that control the combustion systems behaviour in the special dynamics regimes – as e.g. relaxation oscillations [3]. In this study a combination of some standard techniques (i.e. sensitivity, time scale, entropy production etc. analyses) and model reduction approach is suggested. The approach is illustrated by the problem of the Michaelis-Menten type kinetics. The model of enzyme paraoxonase 1 (PON1) is used as an illustrative example, which naturally occurs in mammalian blood. PON1 plays an anti-oxidative role in the bloodstream, presumably via the breakdown of oxidized lipids [4].

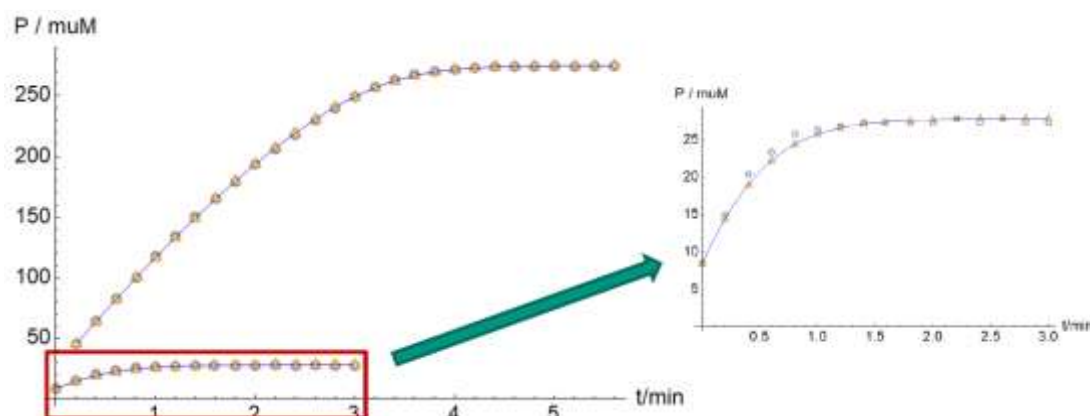


Fig.1. Original data – for two different initial substrate concentrations ( $\sim 30 \mu\text{M}$  and  $\sim 300 \mu\text{M}$ ) shown by blue circles [4], the model performance with the suggested approach by using the reduced model representation are shown by blue line with the triangles.

By the suggested combination of brut-force, recursive-iterative optimization procedure to fit the systems parameters of the toy exmample of the model in [4] is treated. The comparison of the product formation of the reconstructed network and experimental data is presented in Fig. 1. This figure shows the accuracy of model with estimated parameters and illustrate loos of accuracy for lower initial substrate concentrations especially in the transient stage ( $\sim 0.5$ - $1.5$  min).

## References

1. A. A. Konnov, et al. *Progress in Energy and Combustion Science* **2018** 68: 197-267.
2. A. Moroshkina, et al. *Fuel* **2023** 332(2) 125754.
3. D. Volkov, et al. *Combustion and Flame*, **2024** 259: 113141.
4. B. Petrič, M. Goličnik, A. Bavec, *Molecule* **2022** 27(4): 1306. doi: 10.3390/molecules27041306.

# **Passive and active laser methods for studying the kinetics of high-temperature reactions in shock tubes.**

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The shock tube is one of the most versatile and precision instruments for studying the kinetics of high-temperature reactions in gaseous and heterogeneous media. The simplicity of varying over a wide range and reliable control of temperature, pressure and mixture composition makes it possible to study a wide variety of classes of nonequilibrium processes, ranging from relaxation of the internal degrees of freedom of molecules to chemical and plasma reactions, including the processes of formation and transformation of condensed nanoparticles.

Of course, the possibilities of a detailed analysis of nonequilibrium processes occurring behind shock waves are completely determined by the use of a diversity of modern diagnostic methods. Among such methods, various laser methods occupy a special place. As laser technology develops, their capabilities expand significantly and, accordingly, new methods of their application are developed. In this review, we tried to present the possibilities and specifics of using various laser methods to study the kinetics of nonequilibrium processes behind shock waves. Wherein, we divided all existing laser methods into passive and active. We classified as passive methods those methods in which changes in the parameters of the laser beam itself when passing through the studied mixture are recorded, and changes in the parameters of this mixture under the influence of laser radiation can be neglected. In turn, active methods are those in which laser exposure changes the parameters of the medium under study and the change in these parameters that occurs as a result of laser exposure that is recorded. Both methods provide the ability to monitor changes in both integral parameters of the medium, such as temperature, density or volume fraction of the condensed phase, and detailed characteristics of the medium - concentrations of separate components (molecules, radicals, or even populations of separate states), sizes, optical and thermodynamic properties of condensed particles, etc.

The review provides examples of the use of various laser methods, illustrating the wide possibilities and rich prospects for studying complex nonequilibrium processes that open up when a shock tube is combined with modern laser technique.

# Laboratory investigation of interstellar ice analogues in view of the newest open data from JWST observatory

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Star systems similar to our Solar systems are formed from the interstellar clouds of gas in dust. Prior to the formation of a protostar the temperature in the densest region of such cloud drops to as low as 10 K. The depletion of atoms and simple species from the gas-phase onto the dust surface results in rich chemistry triggered by various reactions between the accreting species. This process results in formation of ~10-20 nm thick ice mantles on the surface of dust grains referred as “interstellar ices”. These icy covered dust grains provide the initial material for the formation of various celestial bodies during the later stages of star formation. The James Webb Space Telescope (JWST) provides new mid-IR spectroscopic data with an unprecedented sensitivity and resolution toward star-forming regions. These data reveal new information about ice composition in quiescent dark clouds, protostars, protostar envelopes and protoplanetary disks including a plausible presence of Complex Organic Molecules (COMs) [1,2,3].

A key condition behind the correct interpretation of these spectroscopic data is the availability of reference laboratory spectra and laboratory verified formation routes resulting in the formation of the identified molecules in the ice. These laboratory data are acquired using specialized ultra-high vacuum (UHV) cryogenic setups where interstellar ice analogues are “grown” under the conditions closely resembling physical and chemical conditions found in the ISM.

In this talk a brief overview of recent JWST observations towards dark clouds, protostars and protoplanetary disks will be presented. Then some recent results obtained at the Laboratory for Astrophysics at Leiden Observatory and the Research Laboratory for Astrochemistry at Ural Federal University will be discussed. The talk will be completed with a presentation of ongoing research work performed at Xinjiang Astronomical Observatory of Chinese Academy of Sciences. Particular attention will be paid to the formation of COMs starting from HCCH and HCCCH<sub>3</sub>. These molecules are the simplest representatives of “carbon chains”, a class of chemical compounds ubiquitous in the ISM and described by the general formulas  $-(C\equiv C)_n-$  and  $C-(C\equiv C)_n-$  with  $n \geq 1$  [4,5,6,7].

The research work performed at the Research Laboratory for Astrochemistry at Ural Federal University was benefited from the financial support of the Russian Ministry of Science and Higher Education via the State Assignment Contract FEUZ-2020-0038 and the Russian Science Foundation via RNF 23-12-00315 agreement.

## References

1. Y.-L. Yang, J. D. Green, K. M. Pontoppidan et al., *The Astrophysical Journal Letters* **2022**, 941, L13
2. M. McClure, W. Rocha, K. M. Pontoppidan et al., *Nature Astronomy* **2023**, 7, 431.
3. P. Nazari, W. R. M. Rocha, A. E. Rubinstein et al., *Astronomy & Astrophysics* **2024**, in press
4. D. Qasim, G. Fedoseev, K.-J. Chuang et al., *Astronomy & Astrophysics* **2019**, 627, A1
5. D. Qasim, G. Fedoseev, T. Lamberts et al., *ACS Earth and Space Chemistry* **2020**, 3, 986
6. K.-J. Chuang, G. Fedoseev, D. Qasim et al., *Astronomy & Astrophysics* **2020**, 635, A199
7. K.-J. Chuang, G. Fedoseev, C. Scirè et al., *Astronomy & Astrophysics* **2021**, 650, A85

# Modeling of cold astrochemical processes through matrix isolation: extremely hot chemistry at extremely low temperatures

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The chemical evolution of molecules in space is induced by solar and galactic radiation, which make it possible to initiate the reactions in cold astrochemical media, including diffuse interstellar molecular clouds, cometary and planetary ices. Matrix isolation is a useful tool to simulate reaction channels and to elucidate the mechanism of molecular assembling occurring under the conditions of completely frozen diffusion mobility. The current state and new applications of this technique to the laboratory astrochemistry are presented in a recent review [1]. This lecture gives an overview of recent results of the matrix isolation studies on the radiation-induced transformations of astrochemically important molecules and their complexes obtained in our laboratory.

The experimental approach is based on X-ray irradiation of deposited solid-noble gas films doped with small amounts of target compounds at 4 - 6 K, while the product formation is monitored by a combination of FTIR and EPR spectroscopy. In this way we have extensively characterized the mechanism of radiation-induced decomposition of a number of key astrochemically relevant molecules [2 - 7]. An important finding is that physical properties of inert matrix have strong effect on the degradation efficiency and pathways because of primary significance of the excess energy relaxation. To a certain extent, the observed chemistry may look quite “hot” in conventional terms, even though the medium temperature is quite low.

Another direction is concerned with the radiation chemistry of isolated intermolecular complexes. In fact, this approach implies a concept of “building blocks”, which may provide an important insight into the mechanism of cold astrochemical synthesis. In this way, we have directly observed elementary steps of the low-temperature reactions, which may be responsible for formation of intermediates and molecules detected in interstellar media, including both prebiotic species and polycyclic aromatic hydrocarbons (PAHs) [8-12]. New intriguing results and implications for astrochemistry are discussed.

The work was supported in part by the Russian Science Foundation (project no. 21-13-00195).

## References

1. V.I. Feldman, S.V. Ryazantsev, S.V. Kameneva, *Russ. Chem. Rev.* **2021**, 90, 1142.
2. S.V. Ryazantsev, V.I. Feldman, *Phys. Chem. Chem. Phys.* **2015**, 17, 30648.
3. E.V. Saenko, V.I. Feldman, *Phys. Chem. Chem. Phys.* **2016**, 18, 32503.
4. M.A. Lukianova, E.V. Sanochkina, V.I. Feldman, *J. Phys. Chem. A* **2019**, 123, 5199.
5. A.D. Volosatova, S.V. Kameneva, V.I. Feldman, *Phys. Chem. Chem. Phys.* **2019**, 21, 13014.
6. P.V. Zasimov, E.V. Sanochkina, V.I. Feldman, *Phys. Chem. Chem. Phys.* **2022**, 24, 419.
7. P.V. Zasimov, E.V. Sanochkina, D.A. Tyurin, V.I. Feldman, *Phys. Chem. Chem. Phys.* **2023**, 25, 21883.
8. P.V. Zasimov, S.V. Ryazantsev, D.A. Tyurin, V.I. Feldman, *MNRAS* **2021**, 506, 3499.
9. P.V. Zasimov, D.A. Tyurin, S.V. Ryazantsev, V.I. Feldman, *J. Am. Chem. Soc.* **2022**, 144, 8115.
10. A.D. Volosatova, M.A. Lukianova, P.V. Zasimov, V.I. Feldman, *Phys. Chem. Chem. Phys.*, **2021**, 23, 18449.
11. M.A. Lukianova, V.I. Feldman, *Rad. Phys. Chem.* **2022**, 191, 109847.
12. V.Z. Drabkin, A.D. Volosatova, V.I. Feldman, *MNRAS* **2023**, 518, 1744.



# Polynitrogen Heterocycle-based Energetic Materials: Synthesis and Properties

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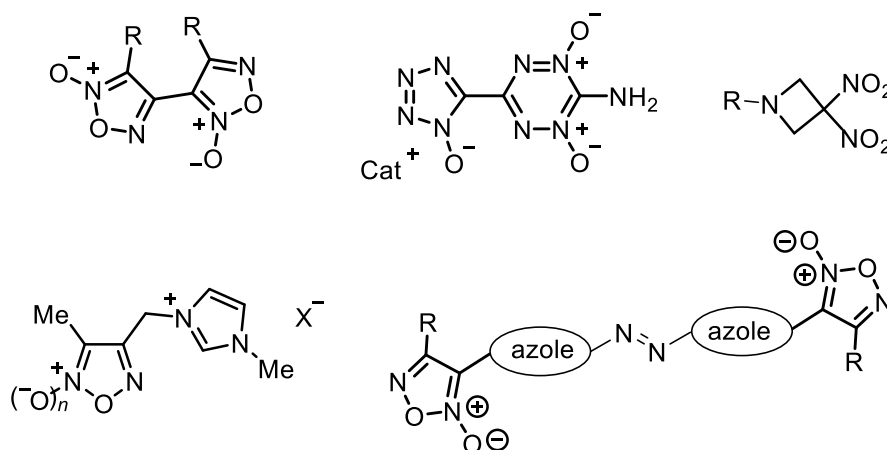
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The current stage of development of science and technology necessitates a constant search for new organic materials with improved applied properties. From the point of view of the molecular structure of such organic materials, one of the most promising classes of compounds are conjugated polyheteroatom heterocyclic systems. As a rule, such structures have a number of advantages, including high thermal stability and balanced physicochemical and photophysical properties. Such a vast potential of organic molecular systems built on the basis of nitrogen heterocycles explains their multipurpose use in various advanced applications. Therefore, the development of new approaches to the target design of polynitrogen heterocyclic systems remains highly relevant.

Herein, we present the latest achievements of our scientific group in the development of new methods for the synthesis of polynitrogen heterocyclic structures for various purposes. Over the past 5 years, we created promising synthetic strategies for an assembly of a wide variety of heterocyclic systems, including 1,2,5-oxadiazoles and their *N*-oxides (furazans and furoxans), 1,2,3-triazoles, tetrazines, 1,3,4-thiadiazoles, etc.



This work was supported by the Russian Science Foundation (grant 23-43-00090).

## References

1. I.D. Deltsov, I.V. Ananyev, D.B. Meerov, L.L. Fershtat, *J. Org. Chem.* **2024**, 89, 174.
2. N.V. Muravyev, L.L. Fershtat, Q. Zhang, *Chem. Eng. J.* **2024**, 486, 150410.
3. A.A. Larin, D.D. Degtyarev, I.V. Ananyev, A.N. Pivkina, L.L. Fershtat, *Chem. Eng. J.* **2023**, 470, 144144.
4. A.V. Shaferov, S.T. Arakelov, F.E. Teslenko, A.N. Pivkina, N.V. Muravyev, L.L. Fershtat, *Chem. Eur. J.* **2023**, 29, e202300948.
5. M.A. Epishina, A.S. Kulikov, I.V. Ananyev, A.A. Anisimov, K.A. Monogarov, L.L. Fershtat, *Dalton Trans.* **2023**, 52, 7673.
6. E. S. Zhilin, A. N. Pivkina, I. V. Ananyev, L. L. Fershtat, *Dalton Trans.* **2022**, 51, 14088.

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

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In this presentation we overview our recent findings in the analysis of the role of the low-temperature reactions in the dynamics of combustion fronts. Two configurations are considered: burner-stabilized methane-air flames at atmospheric pressure and hydrogen-air freely propagating flames at elevated pressure. In the former case, we focus on the investigation of the dynamics of diffusion-thermal oscillations which are studied analytically, numerically and experimentally. We have found that in the case of small and moderately relaxational flame oscillations the flame structure remains similar to that observed in freely propagating combustion waves, while the flame structure completely breaks in the regime of highly relaxational oscillations. The combustion front separates in two zones which can be associated with high- and low-temperature reaction zones. They are shown to be highly and weakly sensitive to the diffusive-thermal pulsations. The high temperature reaction zone drifts downstream and extinguishes during the flame pulsation and the low temperature zone stays near the burner and initiates reignition of the combustion front.

The concept of interacting low- and high-temperature reaction zones is then used to describe the formation of spiral waves at the background of the propagating rich hydrogen-air flames at elevated pressure. The emergence of spiral waves is observed in experiments with spherically expanding combustion waves, however, the mechanism of their formation is not explained until now. The detailed reaction mechanism for planar deflagration in rich hydrogen-air mixture is considered to obtain a reduced reaction mechanism taking into consideration the low- and high temperature reaction regions. The distribution of reaction species, the laminar burning velocity and the onset of diffusive-thermal instabilities are shown to be well simulated by the reduced mechanism. This mechanism is further reduced to derive the model for the dynamics of temperature and HO<sub>2</sub> concentration in thin two dimensional layer at the leading edge of the propagating (or expanding) combustion front located in front of main reaction front governed by high temperature kinetics. The reaction-diffusion system obtained in this way is studied theoretically and numerically and it is shown that with the increase of pressure this system becomes excitable and can generate spiral waves as it is described in experiments. The time and length scales of the spirals agree by the order in magnitude with the values reported in experiments. Thus in terms of qualitative analysis, it is demonstrated that the formation of spiral waves is due to the low temperature oxidation processes.

# Thermal stability and unusual rearrangements of nitrogen-rich energetic compounds: New insights from predictive electronic structure calculations

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The derivatives of high-N heterocycles, e.g., tetrazole and triazole, containing long catenated nitrogen atom chains, are of great interest as promising green energetic materials. However, these compounds often exhibit poor thermal stability and high impact sensitivity. Kinetics and mechanism of the primary decomposition reactions are directly related to these issues. Due to the natural experimental problems arising from the energetic nature of these species, modern predictive quantum chemical calculations very often complement experiment in a very efficient way. Apart from this, the computations are very useful in elucidating the reaction mechanisms and synthetic pathways of nitrogen-rich heterocycles. However, due to the prohibitive computational cost, high-level *ab initio* calculations had been impractical for a large number of important high-N energetic materials of medium size. The widely used DFT calculations very often could not provide the uniform “chemical accuracy” (~1 kcal/mol) and, ultimately, the convincing mechanistic evidence on the decomposition pathways of important EMs.

In the present work, with the aid of highly accurate CCSD(T)-F12 and DLPNO-CCSD(T) quantum chemical calculations, we considered two instructive examples. Firstly, we obtained reliable bond dissociation energies and activation barriers of thermolysis reactions for a number of N-rich heterocycles with long catenated chains of nitrogen atoms. We studied all existing 1,1'-azobistetrazoles containing an N<sub>10</sub> chain, their counterparts with the 5,5'-bridging pattern, and the species with hydrazo- and azoxy-bridges, which are often present energetic moieties. The insights into the mechanism of primary decomposition reactions and related kinetics and sensitivity issues will be discussed in detail.

As a second example, we considered the unusual rearrangements of cyanuric triazide and 2-amino-4,6-diazido-1,3,5-triazine to an asymmetric bitetrazolate involving cleavage of the six-membered aromatic ring. These reactions occur both as a transition-metal-mediated reduction and a metal free process. The calculations effectively complement the experimental findings with mechanistic evidence.

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

# A comprehensive chemical kinetic model for the evolution of charged species naturally occurring in non-sooting flames of hydrocarbons

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Chemiiionization reactions proceeding in flames initialize a generation of numerous charged species in the flame reaction zone. Although the concentration of ions in the combustion zone is low ( $10^8$ – $10^{12}$  cm<sup>-3</sup>), the so-called “ionic wind” occurs in the flame, when an external electric field is applied. This can have a significant effect (depending on a strength of a field) on the combustion process due to momentum transfer from charged species to neutrals. This feature lies at the heart of an electric field assisted combustion technology, which exhibits a great promise for improving flame stabilization, intensifying combustion (due to the formation of excited molecules as a result of collisions with ions), reducing soot formation, etc. Monitoring the current of ions formed during combustion allows one to control and analyse the process in combustion devices. Therefore, the development of computational models for the prediction of ion currents and behaviour of electrified flames is of great practical importance. The proper ion chemistry should be incorporated into these models to render a reliable description of the relevant processes.

This work reports recent findings from the laboratory of combustion kinetics ICKC SB RAS for the development of a predictive kinetic model for ion chemistry in the flames of hydrocarbons. Flame sampling molecular beam mass spectrometry is used in this study to measure spatial distributions of cations in premixed burner-stabilized flames fueled by different C<sub>1</sub>–C<sub>7</sub> hydrocarbons. Apart from major flame cations (H<sub>3</sub>O<sup>+</sup>, C<sub>2</sub>H<sub>3</sub>O<sup>+</sup>, C<sub>3</sub>H<sub>3</sub><sup>+</sup>), many C<sub>x</sub>H<sub>y</sub><sup>+</sup> cations were experimentally detected in the reaction zone of the fuel-rich flames, whereas only hydronium and acetyl cation are found to be dominant in the stoichiometric and fuel-lean conditions. The experimental data on the profiles of relative mole fractions of the cations are used to validate an updated mechanism of ion chemistry. In addition to the reactions between cations (HCO<sup>+</sup>, H<sub>3</sub>O<sup>+</sup>, C<sub>2</sub>H<sub>3</sub>O<sup>+</sup>, CH<sub>5</sub>O<sup>+</sup>, CH<sub>3</sub><sup>+</sup>), electrons, and 6 anions (O<sub>2</sub><sup>-</sup>, OH<sup>-</sup>, O<sup>-</sup>, CHO<sub>2</sub><sup>-</sup>, CHO<sub>3</sub><sup>-</sup>, CO<sub>3</sub><sup>-</sup>), the mechanism includes an updated reaction subset for C<sub>3</sub>H<sub>3</sub><sup>+</sup> and the reactions involving several dominant C<sub>x</sub>H<sub>y</sub><sup>+</sup> cations (C<sub>4</sub>H<sub>5</sub><sup>+</sup>, C<sub>5</sub>H<sub>3</sub><sup>+</sup>, C<sub>5</sub>H<sub>5</sub><sup>+</sup> и C<sub>5</sub>H<sub>7</sub><sup>+</sup>). The highly accurate W2-F12 quantum chemical calculations are used to obtain the reliable formation enthalpies of the cations. Saturation ion current is measured in premixed ethylene flames in a wide range of equivalence ratios and dilution ratios by argon. These experimental data are used to figure out a total rate of chemiiionization in different conditions and to refine the rate constant of this process. The kinetic mechanism for the ion chemistry is combined with detailed reaction mechanisms for neutral species to describe combustion chemistry of methane, ethylene ethane, propane, n-butane, n-heptane, isooctane, and toluene flames. The cationic flame structures are modelled with Cantera software solving the problem for 1D premixed laminar flames. The mechanism presented in this work is demonstrated to quite adequately reproduce the experimental data. The major reaction pathways of formation of different cations in the flames and the ways for further refinement of the mechanism are discussed.

This work is supported by Russian Science Foundation (Project No: 23-23-00521).

## **Graphene composites with various partner species: porphyrinoids, organometallic compounds, metal clusters, etc.**

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Carbon is known to exist in numerous allotropic (nano)forms which include graphene, carbon nanotubes, carbon onions, graphdiyne, carbon nanotori, fullerenes, etc. Since its discovery by Geim and Novoselov in 2004, graphene has received a lot of researchers' attention because of its unusual nanostructure and intriguing characteristics, such as high thermal conductivity, relatively low manufacturing costs, large specific surface area, good pliability, high chemical stability, high porosity, outstanding electron-transport properties, etc. This makes graphene an extremely promising material for uses in various fields, such as for batteries, supercapacitors, fuel cells, organic light-emitting devices and solar cells, catalysis, in various composites, etc. Furthermore, the intense research on graphene and its derivatives, graphene oxide (GO) and reduced graphene oxide (rGO), successfully led to the development of efficient catalysts which were successfully employed in organic chemistry, photochemistry, and electrochemistry.

Nowadays, the studies of numerous composites formed by graphene with various partner species, such as porphyrinoids, metal atoms and clusters, organometallic complexes, etc., have become a very important, promising, and quickly developing area of research. Thus, the detailed understanding and both theoretical and experimental predictions of structures, properties, and adsorption behavior of single metal atoms/ions or metal nanoparticles (NPs) on graphene (both pristine and defect-containing) and graphene derivatives, including polyaromatic hydrocarbons (PAHs), is of paramount importance for many advanced technologies, since it opens a way to fine-tune electronic, magnetic, catalytic, and other properties of the nanomaterials obtained. Furthermore, donor-acceptor complexes of biomimetic compounds such as porphyrins and phthalocyanines with graphene are currently an outstanding scientific frontier as well. The composites made by these compounds anchored on the surface of graphene and their widespread applications have gained ever-increasing interest in the last decade. Graphene can also form hybrids via covalent or non-covalent interactions with different metal complexes of carboxylates, amines, polypyridine compounds, a host of N, O-containing ligands, carbonyls, cyclopentadienyls, pyrene-containing moieties, and other aromatic structures. The composites obtained are very interesting for applications in catalysis, energy storage, and corrosion inhibition and present possibilities of modulating the electronic structure of graphene.

Thus, this talk reviews recent experimental and, most importantly, theoretical studies of numerous versatile composites formed by graphene with different partner species, such as porphyrinoids, organometallic compounds, metal atoms and clusters, and so on. State-of-the-art and perspectives of these studies are highlighted.

# Effects of submerged barrier on rate coefficients and microscopic mechanisms of ion-molecule reactions

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In a chemical reaction, a submerged barrier is a saddle point on the potential energy surface, with a barrier height lower than the entrance channel of the reaction, connecting two lower energy local potential wells. Although the submerged barrier does not dominate the progress of the reaction like the transition state substantial barrier, it is a bottleneck in the reaction, playing a complex role in reaction dynamics, which may lead to non-traditional reaction pathways and dynamics properties. Due to the long-range electrostatic attraction between the charge of ions and the multipole moment of molecules, the rate coefficients of ion-molecule reactions can be described by a simple capture model theory. However, the presence of submerged barriers can cause significant deviations between capture rates and reaction rates. For three important reactions ( $\text{Be}^+/\text{C}^+/\text{Si}^+ + \text{H}_2\text{O}$ ) in astrochemistry and atmospheric chemistry, the accurate potential energy surfaces are constructed, reaction rates are calculated by quasi-classical trajectory, and important new reaction mechanisms for these reactions are revealed by quantitative classification of trajectories.



# Issues of process modelling in aircraft gas turbine engines' combustion chambers

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Major trends in aircraft engine development include increasing efficiency, environmental friendliness and reducing design and development time. The most effective methods for the design and development of gas turbine engines (GTE) and its individual components are computational fluid dynamics (CFD) methods.

There are a number of processes occurring simultaneously in the combustion chamber (CC) of a GTE, namely: turbulent flow in the combustion zone, fuel atomization by nozzles, vaporization of liquid fuel droplets, gaseous fuel mixing with air, ignition of the fuel-air mixture, combustion with subsequent formation of pollutants and combustion products. Each of these phenomena is modelled sequentially and there is a different set of mathematical models for each of them. The approach based on the solution of the Navier-Stokes differential equation system and the corresponding closure equations is used for modelling turbulent flows in the combustion chamber. At present, the most efficient method is the Large Eddy Simulation (LES) method, but it is necessary to develop, on the basis of the existing ones, turbulence scale criteria to determine the sufficiency of discrete (grid) model resolution of the combustion chamber computational domain for the correct use of this method. The Lagrangian approach is the most appropriate for modelling atomization and droplet evaporation, but the fuel atomization characteristics of the nozzles must be obtained to use it. This problem has been partially solved for pressure swirl atomizers by using a combination of numerical volume-of-fluid (VOF) methods combined with semi-empirical techniques to determine droplet diameters. At the same time, the issue of numerical determination of atomization characteristics of spray atomizers has not been solved at the moment. Models considering turbulent-chemical interaction (Zimont, Peters models) are primarily used for turbulent combustion modelling, but the issues related to the constants used in these models have not been fully resolved, as they are selected for methane combustion and are not suitable for combustion of other fuels, including alternative fuels. The issue of accounting for the heat exchange of turbulent reacting flow with the flame tube wall also remains unsolved, since a gas temperature decrease in the near-wall region can lead to additional CO formation. In addition, sufficiently detailed kinetic mechanisms, which involve the use of a model reference fuel composed of a finite number of known hydrocarbons - a surrogate similar in physicochemical properties to real kerosene, are required to correctly determine the main combustion products concentration (H<sub>2</sub>O, CO<sub>2</sub>) as well as the emission of pollutants such as NO<sub>x</sub>, CO, HC, PAHs and soot. Specific kinetic mechanisms must be used in modelling the combustion process of alternative fuels such as biofuels and hydrogen. Also, one of the problems of modern combustion chambers with lean homogeneous mixtures combustion technology is oscillatory combustion caused by heat release pulsations in the flame front. To predict this phenomenon, computational and experimental studies are currently being carried out to determine the pressure pulsations in the CC caused by heat release pulsations, as well as to determine the natural frequencies of the CC volume and their effect on the pulsations in the flame front.



# Functionalization of pyrimidine and purine to RNA bases in water/ammonia ices via radical substitution reactions

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Pyrimidine and purine represent immediate precursors of the four RNA bases, cytosine, uracil, adenine, and guanine. Those can be, in principle, synthesized by replacing hydrogen atoms in given positions in pyrimidine and purine by NH<sub>2</sub> and/or OH substituents with subsequent H atom migrations from OH to the neighboring “bare” N atom in the ring creating the carbonyl moiety. Electronic structure calculations of the potential energy profiles for these functionalization reactions show that they are plausible and involve moderate barriers for the radical addition and H atom elimination steps. The OH-for-H substitution reaction steps are the most facile and have lower barriers on purine (~4 kJ mol<sup>-1</sup> submerged) than on pyrimidine (10-19 kJ mol<sup>-1</sup>). The NH<sub>2</sub>-for-H substitution reactions are more energetically demanding, with their barriers ranging between 33 and 54 kJ mol<sup>-1</sup> and no significant differences have been found between pyrimidine and purine. In the gas phase, the critical reaction step is the H shift following the OH-for-H substitution with barriers as high as 126-154 kJ mol<sup>-1</sup> but these barriers can be greatly reduced with the direct involvement of 1-2 protic solvent molecules (e.g., H<sub>2</sub>O, methanol, and NH<sub>3</sub>) in ices, to only ~30-50 kJ mol<sup>-1</sup>, thus making the H migrations comparable in terms of the energy demands with the NH<sub>2</sub>-for-H substitution reaction steps. The minimal barriers have been found with participation of two solvent molecules in the H transfer process. The barriers with involvement of only one solvent molecule are slightly higher than with two and the increase of the number of solvent molecules directly taking part in the reaction to three and four raise the barriers significantly. For the reactions in water ice, the H transfer transition state structures feature a central role of transient hydronium (H<sub>3</sub>O<sup>+</sup>) and Zündel (H<sub>5</sub>O<sub>2</sub><sup>+</sup>) ions in the hydrogen migration process. The presence of explicit solvent (dielectric continuum) does not significantly affect the reaction energetics and barrier heights for radical substitutions but slightly reduce the H shift barriers, where this effect is found to be most pronounced (up to ~20 kJ mol<sup>-1</sup>) inside ammonia ice.

# **Evolution of carbonaceous particles from AGB stars to planetary nebulae: observations and theory**

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The review of studies devoted to the evolution of carbonaceous grains at stages from the shells of asymptotic giant branch stars to planetary nebulae will be presented. This topic will be covered from several sides: observational data are summarized; the conditions for the formation of dust in the shells of stars and the conditions under which dust evolves further in protoplanetary and planetary nebulae are described; the results of experiments on creating analogues of interstellar dust and an analysis of their characteristics are presented; the mechanisms of formation of aromatic molecules and their clustering are considered; and finally, possible evolutionary scenarios for carbon particles are presented. Particular attention is paid to fullerene molecules, since they play an important role in constructing a whole picture of evolution. Their presence and heterogeneous distribution indicate that, depending on conditions, dust formation can proceed along two branches: through planar and non-planar aromatic molecules.

The work was supported by the Russian Science Foundation (project 24-22-20104).

# Kinetics of oxidation and combustion processes of ammonia-based fuel blends

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The continuously growing demand for energy resources causes the depletion of fossil fuel sources and increases in the emissions concentration. In this regard, one of the most important problems is the search for new low-carbon fuels. From this point of view, hydrogen is the most attractive, since the only product of its combustion is water, and emissions of carbon-containing compounds are completely absent. However, the use of pure hydrogen as fuel for modern engines has a number of limitations, primarily related to fire and explosion safety. Ammonia is a promising chemical carrier of hydrogen, as well as a carbon-free fuel. Unlike hydrogen, ammonia has a well-developed infrastructure for its use, storage and transportation. However, pure ammonia is also unsuitable for use as a fuel. This is due to its poor combustion properties. The use of ammonia/methane blends could be the first step towards the transition to low-carbon fuels. Methane is also widely used nowadays, in particular for transportation needs. The presence of methane in the mixture could improve ammonia combustion characteristics, while higher ammonia content will lead to lower emissions of carbon-containing compounds.

The experiments on flame structure were performed using the molecular beam mass-spectrometric setup with a soft electron-impact ionization. The structure of  $\text{CH}_4/\text{NH}_3/\text{O}_2/\text{Ar}$  flames ( $\varphi=0.8, 1.0$  and  $1.2$ ) was measured at 1, 3 and 5 atm. In the experiments flames were stabilized on a flat Botha-Spalding type burner. The temperature of the burner was 368K throughout the experiments. In experiments at 3 and 5 atm the burner was placed in a high-pressure chamber pressurized with nitrogen. Temperature profiles were measured with the thin S-type thermocouples of 0.05 mm in diameter. Flame structure simulation was performed using the PREMIX code from the CHEMKIN package. We used several published detailed chemical-kinetic models, which include reactions of ammonia and hydrocarbons oxidation. Experimentally measured and simulated mole fraction profiles of reactants, main combustion products and intermediates were obtained in this work. The comparison of the measured and simulated results enabled to assess the predictive capability of the published models. We also analyzed the effect of the fuel/oxidized ratio and pressure on the concentration of the key species, which form during ammonia/methane blends oxidation.

This research was funded by Russian Science Foundation, grant number 24-19-00165.

# Organic Chemists' Journey into 2D Materials

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We seek to improve the existing approaches for the synthesis of 2D materials by making extensive use of organic and inorganic synthesis techniques. Thus, we are working to develop a toolbox of methods for achieving atomic-level structural control in the synthesis of B, N-doped graphenes by using custom precursors. In this pursuit, we target small-molecule “tile” precursors that could be used to grow continuous, precision-doped 2D sheets under CVD or related conditions via dehydrogenative chemistry. Another area of our research deals with the bottom-up assembly of the molecular 2D BCN nanosheets using conventional organic/inorganic synthesis techniques. The intent here is to understand the effects of the B and N dopant placement onto the electronic properties of the resulting nanosheet in comparison with the parent all-carbon structure. Furthermore, we seek to improve conventional 2D material handling methodology by developing new substrates and techniques that enable faster and cleaner transfers of the delicate 2D materials.

## References

1. O. O. Ayodele, S. Pourianejad, A. Trofe, A. Prokofjevs, T. Ignatova, *ACS Omega* **2022**, *7*, 7297.

# Study of the flame structure of CH<sub>4</sub>/H<sub>2</sub> mixtures at elevated pressure and development of reduced reaction mechanism

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Understanding and controlling the combustion of clean and efficient fuel blends, like methane + hydrogen, is essential for optimizing energy production processes and minimizing environmental impacts. To extend the available experimental database on CH<sub>4</sub>+H<sub>2</sub> flame speciation, the novel measurement data for chemical speciation and thermal structure of laminar premixed burner-stabilized CH<sub>4</sub>/H<sub>2</sub>/O<sub>2</sub>/Ar flames at different equivalence ratios ( $\phi=0.8$  and  $\phi=1.2$ ), hydrogen contents in the CH<sub>4</sub>/H<sub>2</sub> blend ( $X_{H_2}=25\%$ , 50% and 75%) and pressures (1, 3 and 5 atm) was obtained. The flame-sampling molecular-beam mass spectrometry (MBMS) technique was used to detect reactants, major products, and several combustion intermediates, including major flame radicals. The mole fraction profiles of the some key intermediates (H, OH, CH<sub>3</sub>, HO<sub>2</sub>, H<sub>2</sub>O<sub>2</sub>, formaldehyde, acetylene, ethylene and ethane) were measured. The experimental data presented in this work extend the available experimental database for the chemical speciation of flames fueled by CH<sub>4</sub>/H<sub>2</sub> mixtures at elevated pressures and can be used for the validation of relevant chemical kinetic models.

The experimental profiles of the species mole fractions were utilized to validate the detailed chemical kinetic mechanism AramcoMech 2.0 and reduced kinetic mechanisms RMech1 (30 species and 70 reactions) was developed employing a combination of several methods (DRG, ROP and CSP) and using ignition delays, maximum temperature and concentrations of important intermediates as targets. The even compact kinetic mechanism RMech2 (21 species and 31 reactions) was obtained starting with RMech1 and using ROP and sensitivity analyses. Both mechanisms were demonstrated to reasonably capture numerous literature data for the laminar burning velocity values and ignition delays of methane/hydrogen fuel blends, and demonstrated a good predictive ability of the structure of fuel-lean flames ( $\phi=0.8$ ), which is close to the desirable gas-turbine conditions. This suggests that these mechanisms have good prospects to be used for the CFD calculations of processes in realistic combustion devices.

This work is supported by the Ministry of Science and Higher Education of the Russian Federation (Agreement dated April 24, 2024 No. 075-15-2024-543).

# Control of detonation propagation by chemical physics methods

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Hydrogen and synthesis gas mixtures with air are very sensitive to ignition and explosion. Synthesis gas, actually, presents a mixture of hydrogen and carbon monoxide. Those mixtures can be ignited even from static electricity, and the flame propagation rate is very high, which can lead to onset of detonation. This process got the name of deflagration to detonation transition. Most often, physical barriers are used to prevent an explosion during the interaction of hydrogen with oxygen. Recently, more and more researchers aimed their studies at chemical methods for controlling different combustion regimes. Scientists, including authors, have shown the effectiveness of using inhibitors to control the combustion of hydrogen-air mixtures.

Most often detonation is simulated based on a model of a one-step reaction, although this approach does not explain the reasons for the occurrence of extremely high rates of chemical transformations and their strong temperature dependence, which are the main characteristics of detonation processes. Also, the temperature dependence of the reaction rate is usually represented by the Arrhenius formula, although the Arrhenius law refers not to the reaction rate, but to the rate constant, and does not describe the observed sharp acceleration of the process during a thermal explosion and detonation. Thus, in order to obtain reliable simulation results, as well as agreement with experimental data, it is necessary to correctly simulate chemical processes.

Cellular structure of detonation waves plays a decisive role in establishing propagation regime of detonation wave, its onset and decay. For many years, it was considered that chemical kinetics does not play a role in determining velocity of detonation wave, only energy release is of importance. However, this concept being valid for a steady state detonation wave propagation becomes less grounded for transient modes of detonation. In the present paper, we'll perform analysis of detonation cellular structure being affected by the inhibiting additives. It will be demonstrated that chemical kinetic chain branching mechanism essentially affects the onset and degeneration of a detonation wave. The method for braking the reaction chains is to reduce the concentration of atomic hydrogen by adding these radicals to an unsaturated hydrocarbon with the elimination of the double bond between carbon atoms. The resulting alkane radical is much less active than atomic hydrogen. Numerical simulations testified the effect of the present inhibitor on suppressing the detonation wave and splitting it into a shock wave and lagging behind flame zone.

Authors wish to acknowledge financial support from Russian science foundation (Project Nr 23-11-00117).

# Modeling the Composition of Interstellar Ices observed with the James Webb Space Telescope

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Infrared observations with ground-based and space telescopes such as NASA Infrared Telescope Facility (NASA IRTF) and James Webb Space Telescope (JWST) provide information on chemical composition and physical structure of interstellar ices. It is well established observationally that ices include water, carbon monoxide and dioxide, methanol, methane and ammonia. Numerical modeling of interstellar gas-grain chemistry along with laboratory experiments with interstellar ice analogues suggest that interstellar ices shall also consist of other species in addition to mentioned above. The set of predicted ice species include at least one major yet infrared-inactive molecule N<sub>2</sub>, and a zoo of less abundant complex organic molecules some of which have prebiotic importance. In the scope of IceAge Early Science Release (ERS) program carried out with James Webb Space Telescope, the ice composition towards the field stars NIR38 and J110621 has been recently observed. As a result, solid water, carbon monoxide and dioxide, ammonia, methanol and methane were unambiguously detected on the lines of sight towards the both stars.

Using a well-established MONACO code [1] with added treatment of non-diffusive chemical processes we modeled chemical composition of interstellar icy mantles towards NIR38 and J110621. We adopted time-dependent physical conditions following the 0D description of evolution of a parcel of gas and dust during the collapse of a prestellar cloud starting at translucent phase and until the phase of a prestellar cloud. A grid of nine models was explored for both stars: with three final gas densities of collapse ( $10^4$ ,  $10^5$  and  $10^6$  cm<sup>-3</sup>) and three collapse times ( $10^4$ ,  $10^5$  and  $10^6$  years). We found that the modeled composition of interstellar ices depends strongly on the collapse time. The closest agreement between the observed ice composition towards both field stars and modeling results is found for the models with collapse times of  $10^5$  and  $10^6$  years and the final gas densities equal to  $10^5$  and  $10^6$  cm<sup>-3</sup>. Interestingly, the fraction of CO<sub>2</sub> ice was overestimated in all models in comparison to the results of observations. The inconsistency between the modeling results and observed data may probably be related to the values of the band strengths of molecules presented in [2]. However, other explanations are also possible.

The work is partially supported by the Russian Science Foundation via the Project 23-12-00315.

## References

1. A.I. Vasyunin et al., *Astrophys J.* **2017**, 842, 33V.
2. M. McClure et al., *Nat. Astron.* **2023**, 7, 431–443



# Cosmic rays as an astrochemical factor

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The existence of some external ionizing factor in the Earth atmosphere, which has been lately coined cosmic rays (CR), had been firmly established in 1912. By the 1930s it became clear that cosmic rays are positively charged particles; in the early 1940s it turned out that they are mostly protons. Later, nuclei of other chemical elements, along with electrons, were added to the components of cosmic rays.

Understanding the true nature of cosmic rays has made them an important tool for exploring the world of elementary particles. At the same time, it turned out that cosmic rays not only open the door to the microcosm. They are an important macroscopic factor that significantly influences and sometimes even determines the physical and chemical state of interstellar matter (ISM).

Cosmic rays mainly comprise nuclei of chemical elements (plus a small number of electrons, positrons and antiprotons). By some process (or processes) they are accelerated to near-light speeds. In relation to elements heavier than helium, cosmic rays generally retain the ISM composition with significant differences only for Li, Be, and B. Cosmic ray particles with kinetic energies from several hundred MeV to  $10^{21}$  eV are observed on Earth and in its environments. Over almost all this range, their spectrum is described by a power law with an exponent of about  $-2.6$ , but the shape of the CR spectrum below this lower limit is highly uncertain, which is unlucky as those are these particles that are the most important astrochemical factor.

From an astrochemical point of view, the most interesting is the effect of CR on the matter of molecular clouds. The propagation of cosmic rays in the clouds leads to several significant consequences. Cosmic rays ionize the cloud material, which is important for chemical processes, for thermal balance, and for the interaction of the material with the magnetic field. Thanks to cosmic rays, weak ultraviolet (UV) radiation is always present in dark regions of molecular clouds shielded from interstellar UV radiation, stimulating important photoreactions. Finally, the penetration of cosmic ray particles into the icy mantles of dust grains leads to their partial evaporation and initiates organic synthesis in these mantles.

I will present a review of our current understanding of the CR spectrum evolution in molecular clouds, especially at low energies, inaccessible to direct measurement, their heating effect on the interstellar gas, and their role in the chemical evolution of both the gas phase and the solid phase of the ISM.

# Molecular inventory of the interstellar medium

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As of April 2024, more than 300 molecules have been detected in the interstellar medium (ISM) or circumstellar shells [1]. The largest molecules detected by radio spectroscopy contain 19 atoms. ISM plays a huge role in the lifecycle of galaxies. It consists of several constituents: neutral atomic gas, ionized gas, and molecular gas. Dense interstellar clouds serve as cradles of newborn stars. Since the main constituent of cold dense interstellar clouds, molecular hydrogen, is unobservable there, spectral lines of these molecules, atoms and ions represent the main source of information about the chemical composition as well as physical conditions and processes in these objects (e.g. [2]).

Radio spectroscopy is the most important and, in many cases, unique instrument for studies of the ISM. These studies are performed with various facilities, operating in a wide frequency range from the lowest observable frequencies to the far-infrared band. One of the most advanced instruments is the Atacama Large Millimeter/submillimeter Array (ALMA) located at a very dry high-altitude site in Chile. Observations at higher frequencies are performed with spaceborne and airborne telescopes.

Spectral line observations make it possible to determine the main physical parameters of the clouds. For example, symmetric top molecules are good “thermometers” [3], because relative population of their K-ladders is governed by collisions. The relative abundance of the isomers  $\text{H}^{13}\text{CN}$  and  $\text{HN}^{13}\text{C}$  is also a temperature indicator [4]. The gas density and temperature can be derived from observations of several transitions of a molecule based on non-LTE excitation analysis. An optically thin emission of the molecules with a known abundance (e.g.,  $\text{C}^{18}\text{O}$ ) gives information on the total gas column density and mass (e.g., [5]). Investigation of the line Doppler shifts and line profiles provide an information on the cloud kinematics. For example, broad non-Gaussian line wings indicate high-velocity flows. An asymmetric dip on the line profile can be an indicator of collapse. Special opportunities for studies of the physical parameters and processes in interstellar clouds provide cosmic masers (e.g., [6]). The relative abundances of some molecules can serve as a chemical clock, indicating age of the cloud.

Detailed studies of the kinematics of cold clouds require accurate laboratory frequencies of some molecules. For this purpose, a Lamb-dip spectrometer was developed at the IAP RAS [7].

This work has been supported by the Russian Science Foundation (grant 24-12-00153).

## References

1. <https://cdms.astro.uni-koeln.de/classic/molecules>
2. I.I. Zinchenko. Radiophysics and Quantum Electronics, 46, 577-593 (2003)
3. S.Yu. Malafeev, I.I. Zinchenko, L.E. Pirogov, L.E.B. Johansson. Astronomy Letters 31, 239-244 (2005)
4. A.G. Pazukhin, I.I. Zinchenko, E.A. Trofimova, C. Henkel. Astronomy Reports 66, 1302-1310 (2022)
5. O.L. Ryabukhina, I.I. Zinchenko. MNRAS 505, 726-737 (2021)
6. S.V. Saliu, I.I. Zinchenko, S.-Y. Liu, A.M. Sobolev, A. Aberfelds, Y.-N. Su. MNRAS 512, 3215-3229 (2022)
7. G.Yu. Golubiatnikov, S.P. Belov, I.I. Leonov, A.F. Andriyanov, I.I. Zinchenko, A.V. Lapinov, V.N. Markov, A.P. Shkaev, A. Guarnieri. Radiophysics and Quantum Electronics 56, 599-609 (2014)

# **ORAL TALKS**

# Rearrangement of Combustion Control System of Gas Turbine, Based on the Diesel Surrogate Model

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The Gasoil fuel is widely used in the power plant industry worldwide, particularly in the gas turbine system. Despite its particular importance, the number of existing multi-component surrogate models, remained limited. This issue became the topic of recent researches of us. The recently published diesel surrogate model by the authors consists of a semi-detailed kinetic model and three surrogate formulas, including four components, namely: n-dodecane, iso-octane, toluene and cyclohexane, with various mole fractions [1]. As found in this research, the high-temperature reactions of cyclohexane, as the simplest naphthene molecule available, play important roles in determination of the high-temperature combustion behavior of the surrogate blends, specifically the cascading dehydrogenation of cyclohexane pathways in prediction of ignition delay time data, and formation of the poly aromatic hydrocarbons. This mechanism has been recently undated at high temperatures, replacing cyclohexane with propyl-cyclohexane, which is a more complex naphthene. The surrogate modeling iterative procedure was carried to reach the final composition [2]. The output of both kinetic models are used to provide the require inputs for mathematical model of a gas turbine unit. This mathematical model was previously published, aimed to fault diagnosis of power plant gas turbine, through an adaptive threshold method (Fig 1). At the end, the overall daily power generation will be simulated using the new parameters and the emission level will be extracted.

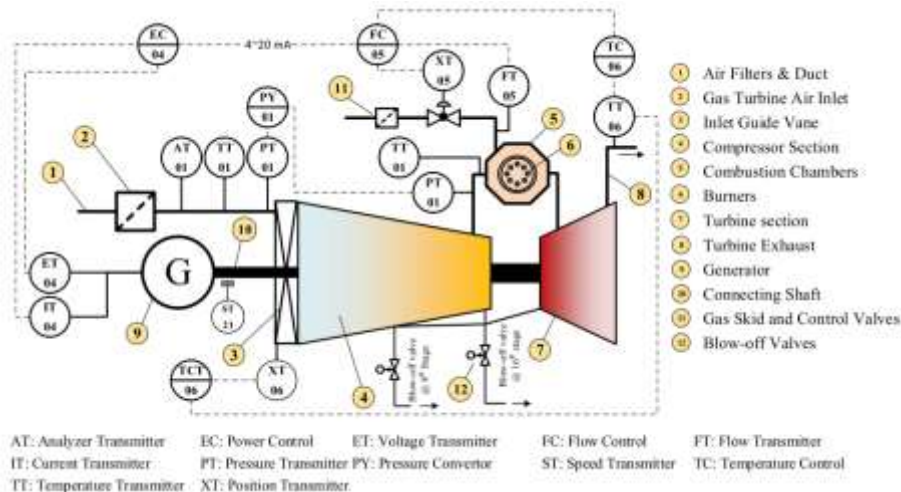


Fig 1. Schematic of a gas turbine unit and generator, with the corresponding control system [3].

## References

- [1] Abbasi, M., Slavinskaya, N., "Development of a 4-Component Surrogate Model for Combustion of Gasoil, including investigation of PAH Formation," in 10th INTERNATIONAL SEMINAR ON FLAME STRUCTURE, Novosibirsk, Russian Federation, 2023.
- [2] Abbasi, M., Nateghi, A., "Development of a Multi-component Surrogate Model for Diesel Combustion at High Temperatures via Extension of the Naphthene Model," in HiSST: 3rd International Conference on High-Speed Vehicle Science Technology, Busan, Korea, 2024.
- [3] Amirkhani, S., Chaibakhsh, A., Ghaffari, A., "Nonlinear robust fault diagnosis of power plant gas turbine using Monte Carlo-based adaptive threshold approach," ISA Transactions, vol. 100, pp. 171-184, May 2020.

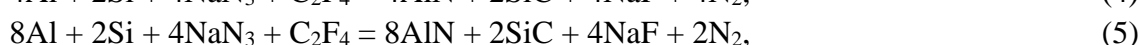
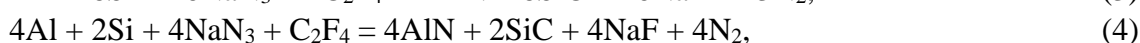
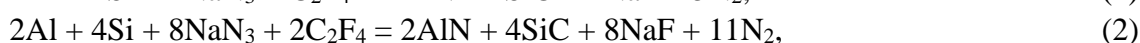
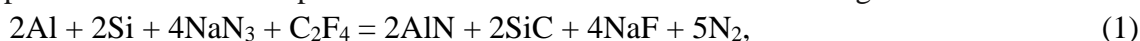
# Combustion synthesis of highly dispersed powder composition AlN-SiC using sodium azide and polytetrafluoroethylene

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Highly dispersed (less than 1 micron) ceramic powders AlN and SiC are promising for the creation of new composite materials AlN-SiC with a complex of properties such as high strength, thermal stability, chemical resistance. The use of a simple energy-saving method of self-propagating high-temperature synthesis (SHS) of the AlN-SiC composition in the combustion mode of mixtures of inexpensive reagents attracts great attention of researchers [1]. The process of azide SHS, in which sodium azide powder  $\text{NaN}_3$  as nitriding agent and halide salts are used, provides great opportunities to regulate the dispersion and structure of synthesized ceramic powders, bringing them to the nanoscale level. The application of azide SHS with halide salt  $(\text{NH}_4)_2\text{SiF}_6$  and carbon black made it possible to synthesize highly dispersed AlN—SiC powder compositions with different ratios of nitride and carbide phases, however, the amount of SiC phase synthesized in experiments (up to 5.9 wt. %) turned out to be significantly lower than the expected theoretical amount (up to 79.6%) [1]. At the same time, combustion products contained a water-insoluble admixture of  $\text{Na}_3\text{AlF}_6$  cryolite salt in noticeable amounts from 7.7 to 15.5%, as well as an admixture of silicon nitride (up to 2.2%) and unreacted free silicon (up to 0.9%).

In this regard, in this work, the use of polytetrafluoroethylene  $\text{C}_2\text{F}_4$  in the azide SHS method as an initial carbidizing and activating reagent instead of carbon black and salt  $(\text{NH}_4)_2\text{SiF}_6$  was investigated, which promoted the formation of silicon carbide in large quantities, and in the form of nanofibers and nanoparticles [2]. In this case, the initial reaction equations for the synthesis of target AlN—SiC compositions with a molar phase ratio from 1:4 to 4:1 had the following form:



The results of thermodynamic calculations of these reactions are presented, according to which the adiabatic temperatures (2704–3216 K) are sufficient for the combustion regime, and the composition of the reaction products corresponds to the right parts of equations (1)–(5). The experimental study was carried out by burning the initial powder mixtures in bulk in a 4.5 L reactor in an atmosphere of gaseous nitrogen with a pressure of 4 MPa. The study showed that the synthesized compositions are agglomerates of powders from submicron particles ranging in size from 100 to 500 nm, the phase composition of which includes impurities of silicon nitride from 3 to 7%, cryolite salts from 4 to 15%, but the content of the SiC phase is large (from 11 to 50%) and much closer to the theoretical composition according to equations (1)–(5), in contrast to the results of [1].

Acknowledgments: The work was supported by the Russian Science Foundation under grant No. 23-29-00680.

## References

1. A.P. Amosov, Yu.V. Titova, G.S. Belova, D.A. Maidan, A.F. Minekhanova, *Powder Metallurgy and Functional Coatings*, **2022**, 4, 34.
2. V. V. Zakorzhevsky, V. E. Loryan, T. G. Akopdzhanyan, *Rus. J. Non-Ferr. Metals*, **2020**, 6, 675.

# Regularities of the combustion chemistry of PMMA in the oxidizer flow in microgravity

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At zero gravity, combustion is realized due to the heat and mass transfer in a stationary oxidizer or due to forced convection. Although the basic mechanisms of flame propagation are the same, the relative magnitudes and characteristics of heat and mass transfer, as well as the kinetics of chemical reactions in the flame, may be quite different. The influence of the forced convection rate on the chemical structure of a polymethyl methacrylate (PMMA) flame in an oxidizer flow ( $O_2+N_2$ ) under microgravity conditions was studied using numerical modeling. ANSYS Fluent software was used to solve a 2D problem of gas flow around a solid body with the full system of Navier–Stokes equations for a multicomponent mixture, taking into account thermal conductivity and thermal radiation and supplemented by the detailed kinetic mechanism. The chemical transformation in the flame was simulated using a kinetic mechanism comprising 45 reactions with the participation of 29 components [1]. The combustion of solid polymer includes preheating the polymer to the pyrolysis temperature, its pyrolysis and interaction of the pyrolysis products with oxygen. On the surface of the PMMA sphere, the pyrolysis reaction leading to the transition of the fuel from the condensed phase to the gas phase has been specified. The reaction rate is given in Arrhenius format as  $k=8.3 \times 10^{11} \times \exp(-E/RT)$ , where  $E=35$  kcal/mol [2]. Surface degradation is assumed to occur slowly; therefore, changes in the geometric dimensions during flame establishment are neglected.

The heat transfer and radiation in both the condensed and gas phases were considered in the modeling. On the PMMA surface, the pyrolysis reaction leading to the transformation of fuel from the condensed phase to the gas phase was specified. The forced convection velocity varied in the range from 3 to 100 cm/s. The thermal and chemical structure of the flame near the surface of PMMA sphere was analyzed at various velocities of the oxidizer flow. With an increase in the velocity from 3 to 10 cm/s, the maximum flame temperature increases from 1700K to 1793÷1799K. A further increase in the velocity was shown to result in a significant decrease in the maximum flame temperature to 1310K (at a flow speed 100 cm/s). At the same time the temperature gradient at the surface of the sphere increases that leads to an increase the surface temperature and, consequently, the rate of pyrolysis. Thus, a change in the flow velocity and, therefore, in the heat and mass transfer in the combustion zone leads to a change in the products composition near the surface and the chemical flame structure. Besides, with an increase in the speed of the oncoming flow of the oxidizer, the total heat release in the gas phase increases.

The maximum CO concentration increases as the forced convection rate increases. Analysis of the rates of fuel consumption reactions showed that at a low convection speed ( $v_{st}=3$  cm/s), the reaction with the H radical, which has the highest diffusion coefficient, plays a crucial role in MMA oxidation.

## References

1. T.A. Bolshova, I.E. Gerasimov, A.G. Shmakov, O.P. Korobeinichev, *Fire Saf. Jour.* **2023**, 138, 103807.
2. O.P. Korobeinichev, S.A. Trubachev, A.K. Joshi, A. Kumar, A.A. Paletsky, A.G. Tereshchenko, A.G. Shmakov, R.K. Glaznev, V. Raghavan, A.M. Mebel, *Proc. Combust. Inst.* **2021**, 38, 4867.



# Formation of complex organic molecules in prestellar cores: the role of non-diffusive grain chemistry

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Complex organic molecules (COMs) are detected at all stages of star formation, including prestellar cores. We present the results of astrochemical modeling of COMs in the prestellar core L1544. Our updated rate equations model includes, in particular, non-diffusive processes [1], new suggested chemical routes for acetaldehyde [2] and methane [3] ice formation and changing of H and H<sub>2</sub> desorption energies according to the part of grain surface covered by H<sub>2</sub> molecules [4]. The agreement with the observational data is very good (fig. 1).

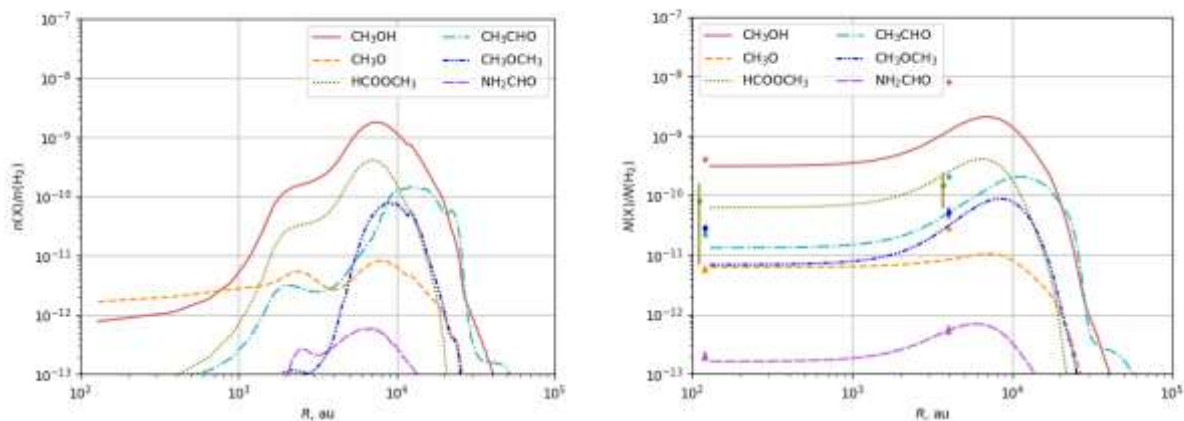


Figure 1. Radial profiles of modeled abundances (left) and abundances derived as column density ratios (right) of COMs obtained with our model. Dots indicate the observational abundances obtained by [5], arrows indicate observational upper limits, and vertical lines provide error bars.

Radical-radical reactions on grains surface between species such as CH<sub>3</sub>, CH<sub>3</sub>O and HCO efficiently proceed non-diffusively and play the key role in the formation of COMs in the ice. COMs are delivered to the gas phase via chemical desorption amplified by the loops of H-addition/abstraction surface reactions. Abundances of COMs in the ice are in the range 1%–2% (for methyl formate ice) or some tenths of percent (for such COMs as acetaldehyde and dimethyl ether) with respect to the abundance of water ice. The choice of parametrization of the efficiency of chemical desorption significantly affects the gas-phase COMs abundances. We also make the comparison of our updated non-diffusive model with the diffusive-only model and provide the constraints for the ratios of species' binding energies to their desorption energies.

The authors acknowledge the support of RSF via the Project 23-12-00315.

## References

1. M. Jin, R.T. Garrod, *ApJS* **2020**, 249, 26.
2. G. Fedoseev, D. Qasim, K.-J. Chuang et al., *ApJ* **2022**, 924, 110.
3. T. Lamberts, G. Fedoseev, M.C. van Hemert et al., *ApJ* **2022**, 928, 48.
4. R.T. Garrod, T. Pauly, *ApJ* **2011**, 735, 15
5. I. Jiménez-Serra, A.I. Vasyunin, P. Caselli et al., *ApJL* **2016**, 830, L6



# Ion chemistry in ammonia-hydrogen-oxygen flames

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Ammonia has recently been considered as a promising carbon-free fuel for internal combustion engines, gas turbines and other power plants. Ammonia has a low burning rate, so its reactivity can be greatly improved by co-firing with hydrogen. The use of ion-sensitive technologies opens up great opportunities for controlling the combustion of ammonia-hydrogen mixtures [1]. However, ionic chemistry in ammonia flames has been poorly studied, which is primarily due to the lack of experimental data on their ionic structure.

The goal of this work was to create a model for the kinetics of ion-molecular reactions in flames of  $\text{NH}_3/\text{H}_2/\text{O}_2/\text{Ar}$  mixtures. For this purpose, the cationic structure of flames of pre-mixed  $\text{NH}_3/\text{H}_2/\text{O}_2/\text{Ar}$  mixtures in the range of fuel excess coefficients  $\phi=0.8\div 1.2$  was studied using molecular beam mass spectrometry. The flames were stabilized on a flat burner at atmospheric pressure. Using a detailed chemical-kinetic model for the transformation of neutral components for the  $\text{NH}_3/\text{H}_2$  mixture flame, as well as data available in the literature on the kinetics of reactions involving the cations discovered in the experiment, a chemical-kinetic mechanism was developed, including 3 cations  $\text{NH}_4^+$ ,  $\text{NO}^+$  and  $\text{H}_3\text{O}^+$ , 4 anions and 34 reactions with their participation. Thermochemical data of cations were calculated using high-precision methods of quantum chemistry W2-F12.

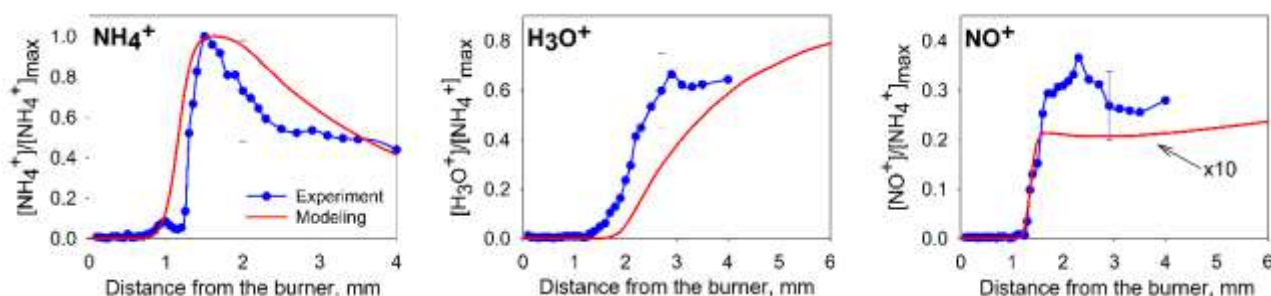


Fig. 1 Measured and calculated profiles of relative mole fraction of cations in stoichiometric flame.

Using the obtained mechanism, numerical calculations of the cationic structure of flames were carried out using Cantera 2.6 software [2]. Based on a comparison of experimental and simulation data, it was found that the proposed mechanism correctly describes the relative contents of  $\text{NH}_4^+$  and  $\text{H}_3\text{O}^+$ , but underestimates the  $\text{NO}^+$  content, which is shown on Fig.1 for stoichiometric conditions. The proposed model was analyzed and the main reaction pathways involving ions were established. The results obtained in this work will serve as the basis for further improvement of the model of ionic chemistry in ammonia flames.

This work was supported by Russian Science Foundation (project No. 23-23-00521)

## References

1. Hayhurst, A. N., & Taylor, S. G. (2002). The ions in fuel-rich hydrogen flames with added ammonia: measurements of the proton affinity of  $\text{NH}_3$  and the enthalpy of monohydration of  $\text{NH}_4^+$ . *Physical Chemistry Chemical Physics*, 4(4), 561-570.
2. Goodwin D. G., Moffat H. K., Speth R. L. Cantera: An object-oriented software toolkit for chemical kinetics, thermodynamics, and transport processes. – 2018.

# Quasi-periodic pulsations in active regions of the solar corona

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The aim of this work is the properties of acoustic wave dispersion in the solar corona and its role in the wave phenomena occurring in the corona. We believe that the dispersion and damping of acoustic waves can lead to the appearance of quasi-periodic pulsations in solar active regions such as coronal holes and loops [1]. The study is based on the previously proposed TCCCH-model of non-adiabatic acoustic waves in a high-temperature plasma, which takes into account the properties of the thermal conduction, radiative cooling and heating [2].

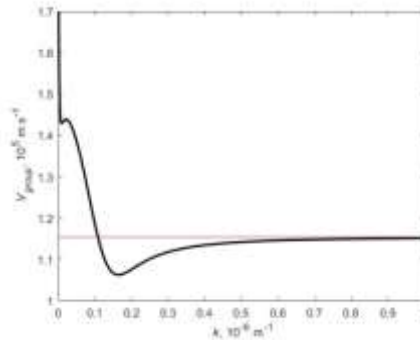


Figure 1. The group speed  $T = 1$  MK,  $n = 10^{15} \text{ m}^{-3}$

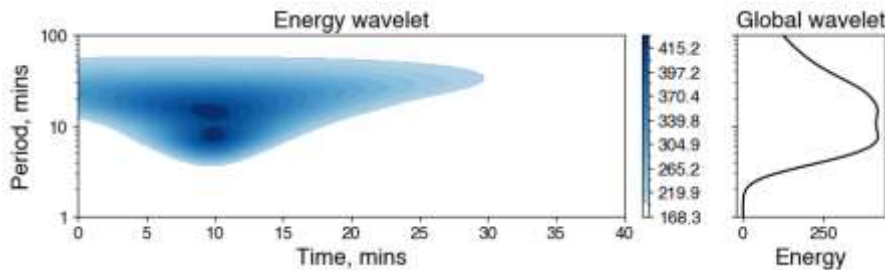


Figure 2. Wavelet-spectra of time signal at distance 67 Mm, with plasma parameters:  $T = 1$  MK,  $n = 0.33 \cdot 10^{15} \text{ m}^{-3}$

The effect of the thermal conduction leads to the formation of a local minimum of the group speed, which makes it possible for groups of waves with short and long period called (figure 1). It is shown that the frequency-dependent damping leads to the formation of two maxima in the spectrum (figure 2). This theoretical conclusion is confirmed by the results of the wavelet analysis (morlet) of model time signals. The periods and damping length can be used to estimate the plasma parameters and a length of the initial signal (Gauss shape) is  $d$ . For typical values of the physical parameters of the coronal plasma, it is possible to obtain periods close to the observed ones, for example, on figure 2 shown wavelet-spectra when it is two maxima with periods 14.3 and 8 mins at the same time, and  $d = 7.7$  Mm [3].

The work was carried out according to the state order of the Ministry of Education and Science of the Russian Federation (No. 075-03-2023-121/3 Development of new observational and theoretical approaches to space weather forecasting based on ground-based observations).

## References

1. S.B. Derteev, M.E. Sapraliev, N.K. Shividov, B.B. Mikhalyaev, *Physics* **2023**, 5, 215.
2. B.B. Mikhalyaev et al., *Solar Physics* **2023**, 298, 102.
3. S. Krishna Prasad, D. Banerjee, J. Singh, *Solar Physics* **2012**, 281, 67.

# Combustion of pellets from biomass and refused derived fuel

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Pelleted fuels are widely used to generate thermal energy in small boilers and household stoves. Most often, they are made from sawdust and other types of forestry waste. However, today the possibilities of expanding the component composition of pelletized fuels by involving low-grade components and various waste groups are being actively explored. In this work, the additional components in the production of fuel pellets are coal sludge, peat and a mixture of agricultural waste (rice husk and straw).

Fig.1 shows the ignition delay times of fuel pellets with the addition of coal slime (a), peat (b) and a mixture of rice husk and straw (c). Pellets without additives are characterized by minimal ignition delay times due to the highest content of volatiles in the sawdust composition. Among the considered additives, the minimum ignition delays were recorded for pellets with a mixture of agricultural waste due to the high content of volatiles, and, as a consequence, the high rate of formation of a vapor-gas environment at the stage of gas-phase ignition.

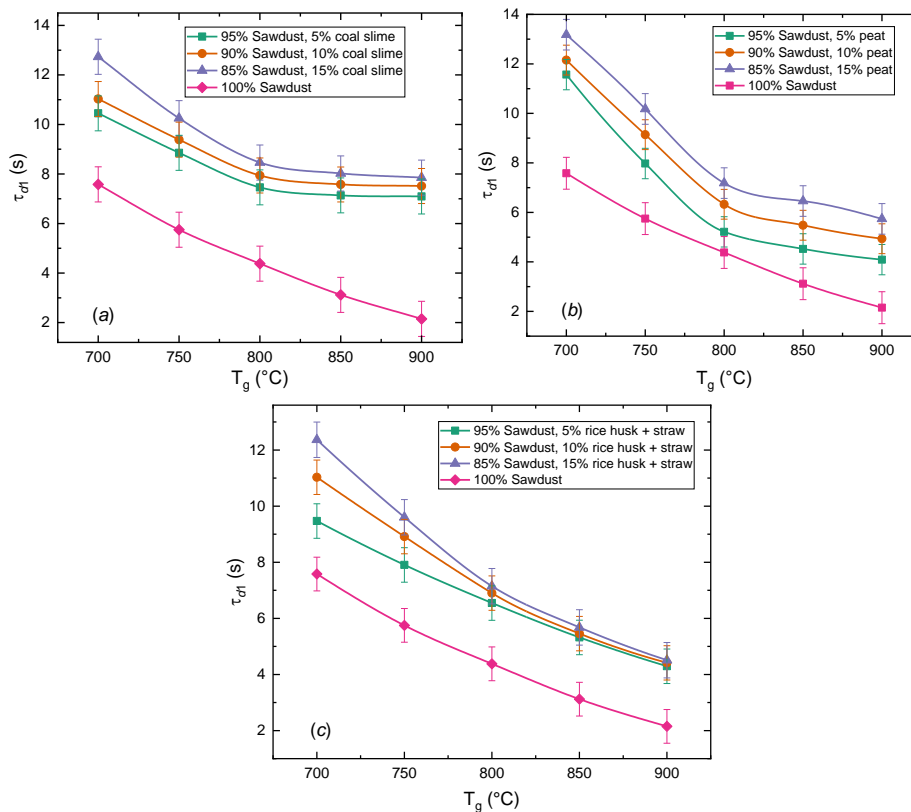


Fig.1. Ignition delay times of fuel pellets with addition of coal slime (a), peat (b) and rice husk + straw (c)

The greatest increase of ignition delay times with agricultural waste additives is observed in the temperature range  $700\text{ °C} \leq T_g \leq 800\text{ °C}$ . In this temperature range, an increase in the additive concentration from 5 wt% to 15 wt% led to an increase in the ignition delay time by up to 31%. In turn, at an oxidizing environment temperature of more than 800 °C, the difference in ignition delay times between pellets with different proportions of additives does not exceed 9%.

The study was supported by a grant from Russian Science Foundation No 23-79-10098.

# Study of the Initial Air-Fuel Mixture Temperature Effect on Ethane Flame Heat Release Rate Pulsation

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One of the problems of low-emission combustion chambers of gas turbine engines and power plants is the instability of their operation due to high-amplitude self-oscillations of gas pressure in the flame tube. High-amplitude pulsations of pressure and velocity occurred in the combustion chamber arising as a result of instability lead to fluctuations in engine thrust, flame blowout or flashback, as well as increased vibration load on the engine design components. These vibrations lead to increased heat transfer and thermal stresses of the flame tube, increased gas erosion of turbine blades, low- and high-cycle fatigue of design components, as well as a decrease in the accuracy of control systems. Flame heat release rate pulsations can be caused by changes in laminar flame speed, fuel composition, and changes in the environment. Experimental and numerical studies show that the initial air-fuel mixture temperature has a significant effect on the intensity of heat release rate pulsations in the flame front. An increase in the initial air-fuel mixture temperature at the combustion chamber inlet can lead to an increase in the amplitude of heat release pulsations, which can affect combustion efficiency and process stability. Therefore, studying the influence of the initial air-fuel mixture temperature on heat release rate pulsations in the flame front is of practical importance for optimizing the operation of burner devices, reducing pollutant emissions of harmful substances and increasing the efficiency of thermal processes.

The work carried out a computational study of the influence of the initial air-fuel mixture temperature at the model burner device on the heat release rate pulsations during ethane combustion. The combustion processes were simulated using the LES turbulence modeling approach with the Flamelet Generated Manifold combustion model. The pulsation amplitude of the speed of the air-fuel mixture at the inlet was 10%, the pulsation frequency varied in the range from 150 to 600 Hz.

As a result, the dependences of heat release pulsations on the frequency of the supplied mixture speed pulsations at initial temperatures of 300K, 400K and 500K were obtained. It is shown that when the initial temperature of the mixture changes, the peak values of heat release pulsations change their frequency and amplitude.

## Acknowledgment

The study was supported by the Russian Science Foundation, projects no. 23-79-01100, (<https://rscf.ru/project/23-79-01100/>).

# Firebrand Generation and Transport During Forest Fires: Experimental Approach

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In recent years, the number of forest fires has been increasing in the world and in Russia, which is associated with both natural factors and the growth of anthropogenic load. The combination of these factors leads to a decrease in the area of forest territories, reduces the renewability of forest resources, which in the long term leads to a decrease in the production of timber, sawn timber, paper and other derivative products on the scale of the Russian Federation. In addition, it should be noted that as a result of natural fires a significant amount of combustion products, soot, smoke is emitted into the atmosphere, and in the case of fires in contaminated (radioactively or chemically contaminated) territories, substances dangerous to life and health of the population are released into the atmosphere at significant heights for spreading.

The sources of forest fires can be both thunderstorms and anthropogenic influence. Often the spread of the fire front is accompanied by the firebrand transport, which are intermediate condensed products of combustion. Firebrand transport is directly related to turbulent processes occurring above the hearth, and provides jump-like spread of the front, the occurrence of spot fires, which leads to an increase in the fire area and complicates its extinguishing. Investigations of firebrands and smoldering particles can be divided into three important areas: particle generation, particle transport, and particle ignition [1-2]. One of the important characteristics of firebrands generated during natural fires is the range of transfer, as well as their flight paths. The use of an infrared camera in conjunction with this installation made it possible to determine the range of transfer of burning particles and their temperature.

This paper deals with an experimental study to evaluate the firebrand generation produced by the combustion of typical forest fuels (pine needles, twigs, leaves) and the effect on a model fuel bed. Experiments on the characterization of firebrands are performed using the only generator of firebrands in Russia and the large aerosol chamber (A.E. Zuev Institute of Atmospheric Optics). The volume of the chamber is 2000 m<sup>3</sup>. This chamber illuminates the influence of side and frontal wind, which is inevitably present in field conditions and affects the characteristics of firebrands.

This work was supported by the Russian Science Foundation (Grant No. 24-21-00069).

## References

1. Effect of small-scale wildfires on the air parameters near the burning centers / E.L. Loboda, D.P. Kasymov, M.V. Agafontsev, V.A. Tarakanova [et al] // Atmosphere. 2021. Vol. 12, № 1. Art. num. 75. URL: <https://www.mdpi.com/2073-4433/12/1/75>.
2. Experimental investigation of the effect of heat flux on the fire behavior of engineered wood samples / Kasymov D.P., Agafontsev M.V., Perminov V.V., Martynov P.S. [et al] // Fire. 2020. Vol. 3, № 4. P. 1–16. URL: <https://www.mdpi.com/2571-6255/3/4/61>.

# Neutralization of sulfur compounds by calcium-based additives in the filtration combustion processes

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Sulfur is a part of many solid fuels and combustible waste. The use of such fuels in modern conditions without capture and neutralizing acid gases ( $H_2S$ ,  $SO_2$ ) formed during combustion is unacceptable. The requirements for the purity of industrial emissions are constantly being tightened, therefore, new methods of sulfur capture are being actively developed and improved.

The aim of this work was to evaluate the effectiveness of using marble additives to neutralize sulfur during filtration combustion of the most common sulfur fuels and waste.

Two model compositions with additives of iron (II) sulfide and copper sulfate, sulfur dioxide and automobile tires were selected as objects of research.

The experiments were carried out in a laboratory quartz reactor with a diameter of 45 mm. In the course of the experiment, the temperature was recorded in five points of the reactor and samples of gaseous products were taken. Elemental analysis of solid and liquid combustion products was also performed.

Experiments have shown that during the filtration combustion of fuels containing sulfur, the addition of marble leads to a significant increase in the proportion of sulfur transferred to solid combustion products. Calcium carbonate absorbs the sulfur in the fuel in sulfide form most effectively: the addition of 50% marble allows 72% sulfur to be absorbed, and the addition of 90% marble – 85% sulfur. Similar additives of 50 and 85% marble to a model fuel containing copper sulfate can absorb only 15 and 31% sulfur, respectively.

For sulfurous coals the sulfur including is mainly in the form of sulfides, the addition of up to 50% marble to the charge allows, with a relatively small decrease in the heat of combustion of the product gas, to increase the proportion of absorbed sulfur by 3 times (up to 37%), and in some cases by 5 times (up to 60%).

At recycling of tires with organic sulfur, adding up to 50% marble to the charge allows to increase the proportion of absorbed sulfur by 2 times (up to 40%).

The obtained values of the degree of sulfur capture are not maximum, and can be increased by replacing marble with a more chemically active alkaline additive.

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.

This work funded by the Ministry of Science and Higher Education of Russian Federation, theme #FFSG-2024-0016.



# Experimental investigation of naphthalene growth via HACA mechanism

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Polycyclic aromatic hydrocarbons (PAH) and soot are the main pollutants, generated during incomplete combustion of hydrocarbon fuels, and pose a danger to human health and ecology as a whole. Although PAH are harmful to terrestrial beings, they attract a considerable interest in astrochemistry and astrobiology as potential precursors for biorelevant molecules, and therefore, the most primitive lifeforms [1]. One of the possible mechanisms of PAH formation is the mechanism of hydrogen abstraction – acetylene addition (HACA), which consists of consecutive H abstractions and additions of acetylene to the formed radical site [2].

In this work, we present a study of the naphthalene growth via the HACA mechanism by means of molecular beam mass spectrometry. During the experiment, the mixture of nitrosobenzene (precursor of phenyl) and acetylene was fed into a pyrolytic reactor via a piezoelectric pulse valve. In the reactor, the mixture is heated to a certain temperature and then expands into a vacuum chamber, forming a molecular beam. The molecular beam then undergoes soft single photon ionization by a 9<sup>th</sup> harmonic of an Nd:YAG laser (118 nm), and the ionized molecules are detected via a reflectron time-of-flight mass spectrometer (ReTOF). The experiments were conducted at combustion relevant conditions: pressures 100 – 600 Torr and temperatures 800 – 1200 K. Our results suggest that at lower temperatures and higher pressures naphthalene is predominantly generated via the Bittner-Howard route of the HACA mechanism, while at higher temperatures Frenklach's original pathway dominates.

This work was supported by the Ministry of Higher Education and Science of the Russian Federation under Grant No. 075-15-2021-597 "Origin and evolution of organic molecules in our Galaxy".

## References

1. Allamandola L. J. et al. Cosmic Distribution of Chemical Complexity //Ames Research Center. – 2009.
2. Frenklach M., Feigelson E. D. Formation of polycyclic aromatic hydrocarbons in circumstellar envelopes //The Astrophysical Journal. – 1989. – T. 341. – C. 372-384.



# Numerical Study of the Thermal Structure of Turbulent Diffusion Flame on the PMMA surface

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The numerical study of turbulent diffusion flame on the surface of solid combustible material has been carried out. The predictions were made using the open-source software Fire Dynamics Simulator (FDS) [1] employing LES technique for turbulent transfer modeling. Methylmethacrylate (product of PMMA pyrolysis) is assigned as the gaseous fuel component of gas-phase combustion reaction with corresponding values of molar weight and heat release.

A method is proposed to employ the coupled problem of flame propagation across the surface of a solid fuel. The entire computational domain is split into two sections: a relatively thin near-wall area (~5 mm) where laminar flow is present, and an external region that encompasses the flame plume where turbulence is prevalent. As a result, in the near-wall zone, the assumptions of laminar flow and two-dimensional formulation (if applicable) are accepted, enabling the use of a high-resolution numerical grid. This leads to a precise prediction of the temperature gradient and, consequently, the heat flux from the flame to the surface of the burning solid fuel [2].

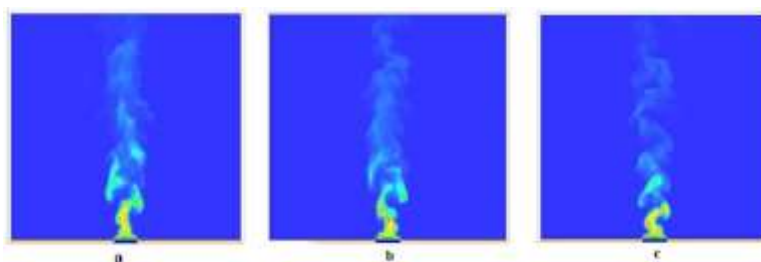


Fig.1 Horizontal turbulent flame structure at the time moments: a – 32.3 s, b – 32.7 s, c – 33 s

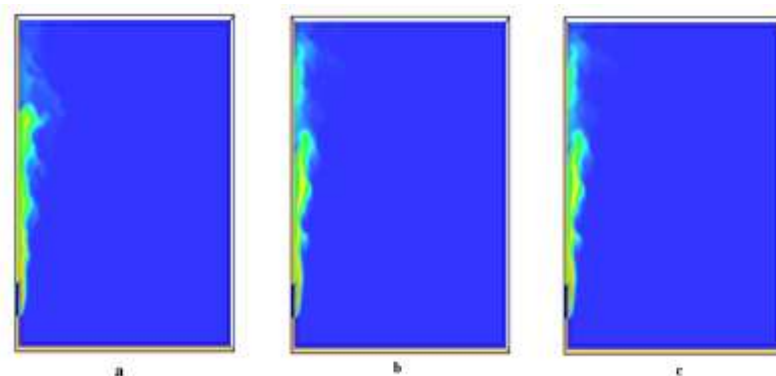


Fig.2 Vertical turbulent flame structure at the time moments: a – 19.2 s, b – 19.5 s, c – 19.8 s

This work was supported by the Russian Science Foundation (Project No. 22-79-10066).

## References

1. McGrattan K., Hostikka S., Floyd J., McDermott R., Vanella M. Fire Dynamics Simulator, Technical Reference Guide, Volume 1: Mathematical Model, NIST Special Publication 1018-1, Sixth Edition, November 2021. <http://dx.doi.org/10.6028/NIST.SP.1018>
2. Gabriela Morar, Alexander I. Karpov, Artem A. Shaklein Numerical Study of the Thermal Structure of Turbulent Diffusion Flame on the Horizontal Surface of PMMA, *Химическая физика и мезоскопия*, 2022, т.24, №4, с.463-472. <http://doi.org/10.15350/17270529.2022.4.37>

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

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The current work is the continuation of the paper [1]. The boundaries of critical phenomena such as onset of thermal-diffusive oscillations and blowing-off of the burner stabilized methane-air flames are found experimentally at different pressure in range from 1 to 4 bar. The critical mass flow rate where pulsations occur,  $M_{cr}$ , and corresponding frequency,  $f$ , are measured by analyzing the FFT of OH\* chemiluminescence signal. Also the mass flow rate at which flame blows-off,  $M_b$ , is determined. The obtained data allow us to find the methane-air flames' laminar velocity for different equivalence ratio at elevated pressure experimentally and compare it to numerical calculations. Experimental setup consist of the high-pressure chamber and the flat porous burner equipped with cooling and automatic ignition systems. Along the perimeter of the burner's porous media the nitrogen is supplied and a nitrogen atmosphere is created initially in chamber. Visual observation and detection the flame pulsations and blowing-off is made through the illuminators. The boundary of pulsations was found for  $\phi$  in range from 0.9 to 1.35 and boundary of blowing-off for  $\phi$  in range from 0.6 to 1.4 of methane-air flames for different pressure  $P = 1, 2, 4$  bar. Results are shown in Figure 1 with dashed and solid lines. For every pressure (black, blue, red is  $P = 1, 2, 4$  bar correspondingly) the flame between this lines is flat and stable.

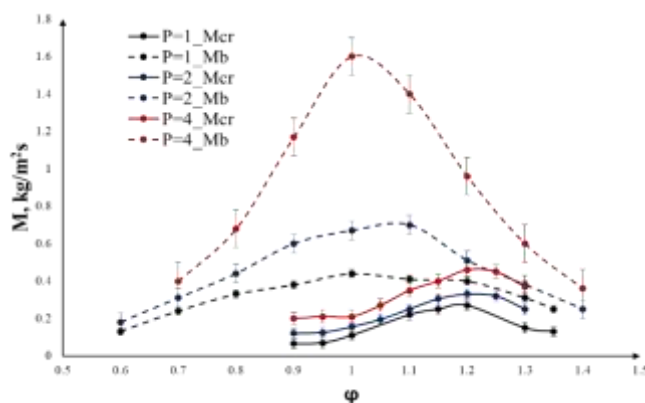


Fig.1. Experimentally measured boundaries of critical phenomena: the onset of pulsations (solid lines) and blowing-off (dashed lines) at different pressure.

Obtained data is very important for verification of detailed mechanisms. Mass flow rate of blowing-off allows find the flame laminar velocity experimentally. Critical mass flow rate and corresponding frequency allow compare different numerical models due to high accuracy of the experimental data.

## References

1. Moroshkina A. et al. Burner stabilized flames: Towards reliable experiments and modelling of transient combustion //Fuel. – 2023. – T. 332. – C. 125754.
2. Nechipurenko S. et al. Experimental observation of diffusive-thermal oscillations of burner stabilized methane-air flames //Combustion and Flame. – 2020. – T. 213. – C. 202-210.
3. Mislavskii V. et al. Diffusive-thermal pulsations of burner stabilized methane-air flames //Combustion and Flame. – 2021. – T. 234. – C. 111638.

# Inelastic cross sections for Ar\*-He complex

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Collision-induced transfer between the excited states of rare gas atoms (He, Ne, Ar, Kr, Xe) is a topic that has been the focus of many experimental and theoretical studies (there is considerable literature on this topic, so we list just a few representative papers here 1–4). This is a subject of direct relevance to processes occurring in electric discharge excited rare gases and rare gas mixtures (including the dynamics of He/Ne, Ar<sup>+</sup>, Kr<sup>+</sup>, Xe, and excimer lasers). From a theoretical point of view, the mechanistic details of energy transfer induced by collisions with ground state rare gas atoms is a problem that is amenable to investigation using high-level computational techniques. The collision-pair potential energy curves (PECs) and interaction between energy levels are a central part of energy transfer models, and they also determine the rate constants of nonradiative transitions between excited states. The objective of this work was to get elastic and inelastic cross sections for these states from PECs and curves of nondiagonal matrix elements.

The calculations of PECs, spin-orbit interactions and nonadiabatic coupling matrix elements reported here were carried out using the MOLPRO 2015 (5) electronic structure program for 49 spin-orbit states in total. Matrices with these elements were transformed to matrices for different values of total angular momentum projection on internuclear axis and represented as block diagonal matrix.

Diagonal matrix elements with new PECs are used for calculation of elastic scattering cross sections and wavefunctions. These wavefunctions are used for calculation of inelastic scattering cross sections with distorted wave Born approximation.

Calculated cross sections for inelastic processes can be used for calculation of rate constants of nonradiative transitions.

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

## References

1. J. Han, M. C. Heaven, *Optics Letters* **2014**, 39, 6541–6544
2. P. Mikheyev, A. Chernyshov, M. Svistun, N. Ufimtsev, O. Kartamysheva, M. Heaven, V. Azyazov, *Optics Express* **2019**, 27, 38759–38767.
3. A. A. Pershin, A. R. Ghildina, A. M. Mebel, V. N. Azyazov, P. A. Mikheyev, M. C. Heaven, *Journal of Chemical Physics* **2019**, 151
4. A. A. Pershin, P. A. Mikheyev, M. C. Heaven, A. M. Mebel, *Bulletin of the Lebedev Physics Institute* **2020**, 47, 300–302.
5. H.-J. Werner et al. MOLPRO, version 2015, a package of ab initio programs. **2015**  
<https://www.molpro.net/>.

# Propagation features of acoustic-gravity waves in a medium with thermal misbalance

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The heating and cooling processes have a significant effect on MHD waves propagating in the solar corona. Their influence is traditionally described in the framework of the approach proposed by Field [1]. This model considers a homogeneous medium in which, in the stationary state, heating and cooling, which depend on the temperature and density of the medium, compensate each other. When a perturbation appears in the medium, a misbalance of heating and cooling occurs, which changes the dispersion properties of the MHD wave and leads to the appearance of so-called thermal instabilities of various types (or, conversely, to the appearance of a steady state). However, this approach does not take into account the plasma structurization observed in real media.

In the current work, the effects of thermal imbalance and gravitational stratification of the medium are taken into account simultaneously. In the case when the influence of heat conduction can be considered weak or the temperature profile with height is close to linear, the condition of thermal equilibrium (zero equality of the heat release function) must be fulfilled in each spherical layer, and the condition of hydrostatic equilibrium must also be fulfilled. Simultaneous fulfillment of these conditions means that the profile of thermodynamic parameters with height is determined by the type of heat loss function, namely by the zeros of the heat-loss function.

In this work, we have obtained the relationship between the altitude profile of temperature, density, and pressure as a function of the parameters of the heating and cooling functions given as power functions of density and temperature. This relationship also opens up the possibility of determining the parameters of an unknown heating function from the known altitude profiles of thermodynamic parameters. In addition, a change in the acoustic cut-off frequency in the heat-releasing medium was found, which is associated with a change in the phase velocity of acoustic wave propagation in media with thermal misbalance.

The study was supported in part by the Ministry of Science and Higher Education of Russian Federation under State assignment to educational and research institutions under Project No. FSSS-2023-0009 and FFMR-2024-0017.

## References

1. G.B. Field, *ApJ* **1965**, 142, 531-567.

# Experimental study of low-temperature gasification of urotropine at different flux of filtering gas with obtaining combustible gaseous products

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The gasification of a solid porous hexamethylenetetramine (urotropine) during the filtration of high-temperature gas through it was experimentally studied. The aim of the work is to experimentally study the gasification of urotropine in a low-temperature gas generator at various values of the incoming gas flow.

Low-temperature gas generators are widely used in fire extinguishing systems, for spinning turbines, in airbags, etc. Depending on the application of the gas generator, various requirements are imposed on it, such as the absence of combustible products, high gas production with a minimum heat of combustion and maximum calorific value of gaseous products [1].

Experimental study was carried out to investigate the gasification of urotropine in a low-temperature solid fuel gas generator under varying inlet gas flows. The nitrogen was used as an inert filtering gas. The inlet gas flow was varied from 0.6 to 1.4 L/s with a step of 0.2 L/s. The initial temperature of inlet gas was equal to 910 K. The temperature at the reactor outlet was measured, and gas-sampling of products were collected. The time of fuel gasification was measured. It was shown that with an increase in the nitrogen flow, the time of urotropine gasification decreases. It has to do with an increase in the intensity of interfacial heat transfer with increasing nitrogen flow. Therefore, an increase in the inlet gas flow results to the decreases of gas generator operating time.

When the flux of incoming nitrogen was increased from 0.6 to 1.4 L/s, the average mass rate of urotropine gasification raised from 0.63 to 1.61 g/s. The fuel gasification rate showed an almost linear increase with a raise in the inlet nitrogen flow. This can be attributed to the higher intensity of interfacial heat exchange resulting from the increased nitrogen flow.

It has been shown that the ratio of mass flows of fuel gasification products and inlet gas does not depend on the value of inlet nitrogen flow. When varying the inlet gas flow from 0.6 to 1.4 L/s, the value of the mass flows ratio is constant and equals approximately 0.9 g/g. It is possible to calculate the calorific value of the gas outgoing from the gasifier by means of ratio of fuel gasification products flow and inlet gas one.

It has been shown that the gaseous products of urotropine gasification consist of nitrogen with small amount of hydrogen and hydrocarbons. The nitrogen in the gaseous products of urotropine gasification comes from the nitrogen cylinder. That is at this temperature (910 K) urotropine not only sublimated, but also decomposed to simpler gaseous products. The decomposition of urotropine molecules into simple substances at this temperature is very slow. The content of simple gaseous products does not exceed 4% vol.

This study was carried out as part of project no. 21-79-20008 of the Russian Science Foundation.

## References

M.V. Salganskaya, A.Yu. Zaichenko, D.N. Podlesniy, et al., *Acta Astronaut.* **2023**, 204, 682.

# Dynamics of sporadic combustion waves and single ball-like flame in straight channels

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In the last decade, there are a trend towards a transition to the ecofriendly technologies, more sparing to the environment. Examples of such promising technologies are the methods of lean hydrocarbon fuels burning and the transition to hydrogen power. Dilution of lean hydrocarbon fuels with hydrogen can increase flammability limits and efficiency, as well as reduce emissions. In this regard, the study of the combustion of lean gas mixtures with a low Lewis number is a relevant task.

The present study is devoted to a numerical study of the propagation dynamics of sporadic combustion waves of lean hydrocarbon fuels with low Lewis number consisting of a set of individual flame spots in straight channels within the framework of a three-dimensional reaction-diffusion model. As a result of numerical modeling, the dependences of the propagation velocity of a sporadic combustion wave, residual fuel concentration, and the number of flame spots on the channel size, mass flow rate, and radiative heat losses are obtained. Analysis of the numerical results shown the existence of a special transverse channel size, starting from which, as the channel size increases, the number of flame spots increases in proportion to the increase in the transverse channel size area. This critical diameter is proportional to the radiative heat loss intensity which is characterized by the mixture equivalence ratio. Thus, the presence of a universal size of flame spots is shown, which for its existence requires a certain area around it filled with a fresh mixture.

It was found that when a sporadic combustion wave propagates in a sufficiently narrow adiabatic channel, modes arise when, as a result of chaotic splitting of the reaction front into several combustion spots, only one of them "survives". In this case, the shape of the "surviving" combustion spot becomes almost spherical, in contrast to the cup-like flame in a sporadic combustion wave, i.e., it becomes similar to a drifting flame ball. In this case, the chemical reaction proceeds along the entire perimeter of the sphere, somewhat intensifying in the direction of the ball-like flame movement, since the fuel concentration in this region is higher. As a result of numerical modeling, it was found that when the mode of propagation of the combustion wave changes from sporadic to single ball-like flame, the combustion wave propagation velocity drops from close to adiabatic ( $\sim U_b$ ) to 0.1 - 0.2  $U_b$ , i.e. 5-10 times.

All this indicates that in this regime the dynamics of flame propagation is determined mainly by diffusion, similar to the way it is realized in flame balls. The study of the influence of radiation heat losses on the dynamics of the ball-like flame has shown that, unlike a sporadic combustion wave, a single drifting ball-like flame can exist in a wider range of changes in the radiation heat loss parameter, which is also predicted by theory. At the same time, the radius of the ball-like flame slightly decreases as the radiative heat loss increases.

Considering ball-like flame separately, by increasing the channel size, the asymptotic behavior of the fuel concentration distribution and its temperature along the symmetry axis is numerically investigated to determine whether this mode of combustion wave propagation is a classical representation of a flame ball.



# Crystallochemical approach to high-throughput screening of potential ionic electrides

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At present, about 200 structures of inorganic electrides are known, most of which were theoretically predicted but have not experimentally confirmed yet. This number amounts to only 0.1% of more than 200,000 crystalline compounds deposited in the Inorganic Crystal Structure database (ICSD). However, the real number of electrides can be much larger; the problem is that the electride properties are difficult for detecting both theoretically and experimentally. A number of criteria that indicate a crystal structure to be electride were proposed, but none of them is universal and sufficient. In particular, Dale and Johnson [1] highlighted eight important electride properties applicable for inorganic electrides. Most of these criteria are calculated by quantum-mechanics methods; hence, they are hard-to-obtain data that significantly depend on the initial calculation parameters. Thus the search for other criteria, which can be estimated by less resource-consuming methods, remains an actual task.

The excess electron can be considered as an anion or a pseudo atom in crystal structure. This means that we can apply crystallochemical methods, which are designed for the description of atoms, to the characterization of the interstitial electrons. We use for this purpose Voronoi polyhedra, which have exhibited their effectiveness for the representation of atoms in crystals of any chemical nature. An important geometrical property of atomic Voronoi polyhedron is that its vertices coincide with the points, which are most distant from the surrounding atoms, i.e. mimic the centers of structural cages. Like the  $\text{Cs}_7\text{O}\cdot 5e^-$  structure shown in the Figure 1, most of electrides have a positive charge imbalance, since they contain an excess number of metal atoms compared to the formally charge-balanced composition ( $\text{Cs}_2\text{O}$  for  $\text{Cs}_7\text{O}\cdot 5e^-$ ). Similar to the elementary substances, many metal-to-metal contacts exist in electrides. For this reason, we use atomic radii to determine the boundaries of the region not occupied by atoms and estimate the size of the localized electron domain with the modified Voronoi polyhedron (Figure 1).

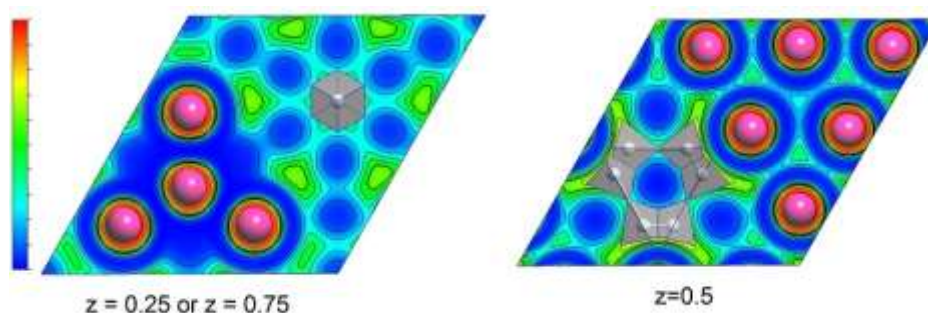


Figure 1. The electron localization function for the structure in sections at  $z=0.25$  (or  $0.75$ ) and  $0.5$ , on which the modified Voronoi polyhedra are superimposed, which are calculated using atomic radii.

## References

1. Dale S.G. and Johnson E.R. *J. Phys. Chem. A* **2018**, 122, 49, 9371.



# Numerical simulation of waveguide elements of an experimental microwave setup to determine the burning rate of energy condensed systems

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Condensed energetic materials (CEMs) are widely used as an energy source in modern propulsion systems of various applications. The CEM burning rate is one of the most vital parameters for the propulsion systems design. Its value is determined only experimentally, since combustion processes have not yet been fully studied. There are many experimental methods for determining the burning rate [1], but one of the most promising methods is microwave, because it has the highest measurement accuracy in time and space. At the same time, this method has a number of disadvantages, including necessity for the high accuracy of manufacturing structural elements of the experimental setup [2].

The voltage standing wave rate (VSWR) is one of the parameters by which the quality of a waveguide line is determined. For ideal systems it is equal to 1, for real devices it is in the range of 1.02-2. The occurrence of ghost reflections from local irregularities leads to an increase in VSWR, which negatively affects the accuracy of combustion rate measurements. Most commonly, ghost reflections occur at the wave-guides junctions, as well as in the transition region of the air-filled wave-guide to the CEM sample. Transition devices, such as dielectric antennas, are designed for removal of such disadvantages.

Dielectric permittivity is the main parameter of a dielectric material. The antenna itself is located in a tapered metal circular cross-section wave-guide and transmits an electromagnetic wave into the CEM sample with minimal ghost reflections. In this case, the dielectric permittivity of the antenna material and the sample under study should be close in value. For this reason, PLA plastic is used as the antenna material in this work. It also allows the possibility of antenna 3D printing [3].

This study includes the dielectric antenna outer surface profiling with further wave-guide section numerical modeling. Based on the simulations results, VSWR is determined in the frequency range 9-11 GHz, which are the operating frequencies of the electromagnetic wave generator. Additionally, the VSWR experimental determination for the experimental setup wave-guide section is carried out.

As a result of the current research, an antenna profile was obtained that ensures electromagnetic waves high-quality transmission in the wave-guide section with minimal ghost reflections. This technique made it possible to obtain high accuracy in determining the CEM burning rate. Dependence diagrams of VSWR in a given frequency range were obtained during numerical simulation, as well as for the experimental setup. The burning rate curves are shown with and without the use of a profiled antenna.

## References

1. V. Zarko, A. Kiskin, A. Cheremisin, Contemporary methods to measure regression rate of energetic materials: A review, *Prog. in Ener. and Comb. Sci.* **2022**, vol. 91, p. 16.
2. L.D. Strand, A.L. Schultz, G.K. Reedy, Microwave doppler shift technique for determining solid propellant transient regression rates, *J. Spacecraft*, **1974**, vol. 11, no. 2, pp. 75-83.
3. E. Huber, M. Mirzaee, J. Bjorgaard, M. Hoyack, S. Noghianian, I. Chang, Dielectric property measurement of PLA, *IEEE*, **2016**, pp. 88-92.

# Experimental study of flame spread over flame retardant glass fiber-reinforced epoxy resin in opposed oxidizer flow

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The high flammability of glass fiber-reinforced epoxy resin (GFRER) is a factor, that limits its propagation in industry. Traditional flammability and thermal stability tests can provide assessment of materials flammability in the most cases. The flame spread experiments under different ambient conditions are necessary to understand the mechanism of flammability reduction in details to develop new more effective materials and flame retardants.

This work is focused on flame spread over GFRER in opposed oxidizer flow. GFRERs with 35% and 50% binder content (BC) and addition of DDM-DOPO and graphene were prepared. It was noticed that the samples with lower limiting oxygen index (LOI) had higher downward flame spread rate (ROS) in opposed O<sub>2</sub>/N<sub>2</sub> mixture flow, but that was observed only near a flammability limit of the samples (LOC). At higher oxygen concentrations, there was no strict dependence between LOI values and flame propagation rate. Approximately the same gap between LOC and LOI values for GFRER samples was observed due to difference of the flame zone in LOI test and downward flame spreading experiments. In the downward flame spread in opposed oxidizing flow, DDM-DOPO and DDM-DOPO + graphene flame retardants slightly reduced ROS for GFRER with BC~35%. Moreover, the effect of flame retardants regarding the reduction in measured ROS for GFRER1 samples (with ~ 35%BC) at O<sub>2</sub> concentrations greater than 47.5 vol.% practically disappeared. For the samples with BC~52%, DDM-DOPO reduced ROS on ~15% for all tested O<sub>2</sub> concentrations. It was concluded, that the mixture of 5 wt.% graphene + 5 wt.% DDM-DOPO was more effective additive than only 5 wt.% DDM-DOPO additive for GFRER samples with different BC. The results of numerical simulation of flame propagation over the surface of GFRER have shown that the model is able to predict ROS and temperature for samples with binder content of ~33 ± 3%, while as the amount of binder increases, the role of the thermophysical properties of volatile pyrolysis products increases, which leads to underprediction of the model.

In conclusion, dependency between ROS, LOI and UL94 results were found. The obtained data may be used for improving numerical models, for designing effective reinforced non-combustible composites applied in the aircraft industry and for justifying standard flammability tests.

The study was financially supported by the Russian Science Foundation, grant no. 20-19-00295

# Experimental investigation of combustion limits of hydrogen/ methane/carbon monoxide/air/water vapor mixtures

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One way to high-volume hydrogen producing is vapor-oxygen methane conversion on the nuclear power station with the high temperature gas-cooled reactor [1]. The flowchart comprise group of reactors with the combustible and explosive mixtures, so-called conversion gas (congas), including hydrogen, methane, carbon monoxide, carbon dioxide with water vapor in quantity. In case of emergency depressurization congas can ignite with the certain probability, which limited by flammability limits of congas-air mixture.

It's necessary to develop numerical methodic validated on experimental data for calculation of flammability limits of several flammable gas mixture with diluent (water vapor and carbon dioxide). Large data set for individual flammable gases are contained in Coward and Jones paper [2]. Data for mixtures of two and more flammable gases with diluent are scarce. For example, flammability limits for interest gas mixtures (hydrogen, methane, carbon monoxide) in some ratio are presented in papers [3, 4, 5]. For validation of numerical methodic data in more wide range of gas mixture changes with water vapor is necessary.

In paper the flammability limits of methane-air-water vapor, methane-hydrogen-air-water-vapor ( $H_2:CH_4 = 2:1$  and  $1:2$ ) and hydrogen-carbon monoxide-air-water vapor ( $H_2:CO = 4:1$ ) mixtures are determined. Data for methane-air-water vapor are in a good agreement with the available data. Increasing of hydrogen content in mixture with methane expand flammability limits. Near the low flammability limit flame propagate by way of small floating flame kernel.

## References

1. Fateev S.A., Petrunin V.V., Kodochigov G.N., Marov I.V., Alexeev S.V., Ipatov P.L., Petrov A.Yu., Ponamarev-Stepnoy N.N., Shutikov A.V., Development of Atomic-Hydrogen Energy Technologies in the Rosatom State Corporation, Atomic energy. 2023, 133, 5-6, pp. 251–258
2. H.F. Coward, G.W. Jones, Limits of flammability of gases and vapors, US Bureau of Mines Bulletin 503, 1952.
3. Van den Schoor F, Verplaetsen F., The upper flammability limit of methane/hydrogen/air mixtures at elevated pressures and temperatures. Int J Hydrogen Energy. 2007, 32, pp. 2548–2552
4. I.Wierzba, Q.Wang. The flammability limits of  $H_2-CO-CH_4$  mixtures in air at elevated temperatures, Int J Hydrogen Energy. 2006, 31, pp. 485 – 489
5. I. Wierzba, V. Kilchyk. Flammability limits of hydrogen-carbon monoxide mixtures at moderately elevated temperatures. Int J Hydrogen Energy. 2001, 26, pp. 639–643

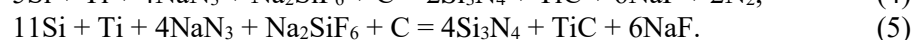
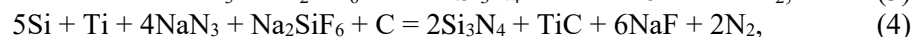
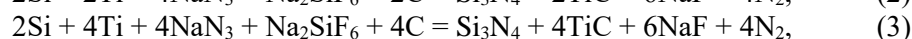
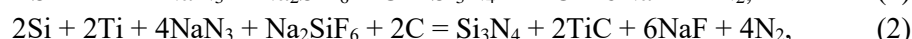
# Application of combustion of Ti-Si-Na<sub>3</sub>-Na<sub>2</sub>SiF<sub>6</sub>-C powder mixture for the synthesis of highly dispersed Si<sub>3</sub>N<sub>4</sub>-TiC ceramic composition

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Silicon nitride ceramics are capable of operating under high temperature and stress conditions due to their thermal conductivity, low coefficient of thermal expansion, and high resistance to thermal shock. However, the strength of Si<sub>3</sub>N<sub>4</sub> ceramics tended to decrease due to the formation of microcracks around large grains. Many efforts have been made to improve the mechanical properties of Si<sub>3</sub>N<sub>4</sub> by controlling the microstructure or creating various types of composites. Significant improvements in strength, toughness and damage resistance have been obtained in numerous ceramics such as AlN-SiC, Si<sub>3</sub>N<sub>4</sub>-SiC and Si<sub>3</sub>N<sub>4</sub>-TiC [1,2]. Titanium carbide (TiC) particles, characterized by a high elastic modulus, hardness and electrical conductivity, are introduced as a dispersion-strengthening phase into monolithic Si<sub>3</sub>N<sub>4</sub> ceramics to improve not only the strength, but also the fracture toughness and electrical conductivity of composite ceramics.

A Si<sub>3</sub>N<sub>4</sub>-TiC nanocomposite with high mechanical properties was obtained by hot pressing by adding 10 wt.% nanosized Si<sub>3</sub>N<sub>4</sub> particles and 15 wt.% TiC to a submicro-sized Si<sub>3</sub>N<sub>4</sub> matrix [3]. Layered composites have the highest strength, fracture toughness and wear resistance. Thus, a Si<sub>3</sub>N<sub>4</sub>-TiC ceramic nanocomposite for cutting tools using a Si<sub>3</sub>N<sub>4</sub> micromatrix with Si<sub>3</sub>N<sub>4</sub> and TiC nanoparticles showed better wear resistance than a sialon tool. Meanwhile, the wear of Si<sub>3</sub>N<sub>4</sub>-TiC composite ceramic cutting tool is mainly dominated by abrasion and adhesion, while the wear of sialon ceramic cutting tool is dominated by abrasion, adhesion, thermal cracking and peeling [4]. This paper explores the application of azide SHS, in which sodium azide powder and a halide salt (Na<sub>2</sub>SiF<sub>6</sub>) are used as a nitriding reagent. The compositions of the initial mixtures of powders for the synthesis of single-phase Si<sub>3</sub>N<sub>4</sub> and TiC are known, based on the analysis of which the following chemical reaction equations were used to synthesize the Si<sub>3</sub>N<sub>4</sub>-TiC composition with a molar phase ratio from 1:4 to 4:1:



Thus, despite the positive results of theoretical thermodynamic analysis, the considered experimental application of the azide SHS method did not allow us to synthesize the target composition of Si<sub>3</sub>N<sub>4</sub>-TiC powders in pure form, without the side titanium nitride phase (TiN) in the composition. But for the first time, the possibility of using combustion for the synthesis of compositions of highly dispersed nano-sized and submicron ceramic powders Si<sub>3</sub>N<sub>4</sub>-TiC and Si<sub>3</sub>N<sub>4</sub>-TiC-TiN with a particle size of less than 500 nm with a relatively low content of free silicon impurity (less than 1.5%) has been experimentally demonstrated, which is noticeable achievement.

Acknowledgments: The work was supported by the Russian Science Foundation under grant No. 23-29-00680.

## References

1. Amosov A.P., Belova G.S., Titova Y.V., Maidan D.A. *Synthesis of highly dispersed powder ceramic composition Si<sub>3</sub>N<sub>4</sub>-SiC by combustion of components in the Si-C-Na<sub>3</sub>-NH<sub>4</sub>F system*, Russian Journal of Inorganic Chemistry, T. 67, № 2, **2022**, 123-130.
2. Chunyan Tian, Ning Liu, Maohu Lu, *Thermal shock and thermal fatigue behavior of Si<sub>3</sub>N<sub>4</sub>-TiC nano-composites*, International Journal of Refractory Metals & Hard Materials 26, **2008**, 478-484.
3. Chaochao Ye, Xinyan Yue, Hongqiang Ru, Haibo Long, Xiao Gong, *Effect of addition of micron-sized TiC particles on mechanical properties of Si<sub>3</sub>N<sub>4</sub> matrix composites*. Journal of Alloys and Compounds, 709, **2017**, 165-171.
4. Xing Youqiang, Deng Jianxin, Feng Xiuting, Yu Sheng. *Effect of laser surface texturing on Si<sub>3</sub>N<sub>4</sub>/TiC ceramic sliding against steel under dry friction*. Materials and Design, 52, **2013**, 234-245.

# The Influence of Flame Retardants on the Combustion of Glass Fiber-Reinforced Epoxy Resin

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Glass fiber-reinforced polymers (GFRP) have good mechanical properties, making them a promising material for construction and aviation. In order to improve the epoxy resin based GFRP fire resistance, the samples with addition of DDM-DOPO (9,10-dihydro-9-hydroxy-10-phosphaphenanthrene-10-oxide-4,4'-diaminodiphenylmethane), CBz (phosphorus-containing cardanol-based benzoxazine) and graphene were prepared. Traditional flammability and thermal stability tests along with the experimental investigation and numerical modeling of flame spread over GFRPs were carried out. Graphene and DDM-DOPO exhibited comparable effectiveness in reducing the flame spread rate (ROS) at the same loading. 6wt% of DDM-DOPO addition in GFRP led to increasing limiting oxygen index (LOI) from 22.4 to 26.5 and self-extinguishing in UL94 test. The coupled numerical model of flame spread over the polymers has satisfactorily predicted DDM-DOPO gas-phase effect on decrease of ROS for glass fiber-reinforced epoxy resin. Also, the numerical model based on the decrease of combustible fuel and increase of noncombustible volatile pyrolysis products has predicted effect of graphene on decrease of ROS with a good precision. GFRP with the addition of phosphorus-containing CBz has shown a significant improvement in fire resistance (LOI=28.1) and achieved self-extinguishing in the UL94 test. Moreover, addition of CBz has not deteriorated mechanical properties of the samples. One more advantage of CBz, that it is fully bio-based, that makes it environmentally friendly for industrial use. GFRPs based on phosphorus-containing methacrylate ester binders were synthesized to prepare glass fiber reinforced samples. The samples had high LOI values (>31%), which were achieved due to chemically bound phosphorus in the molecules of the initial oligomers. The fire resistance test results according to FAR-25 (clause 867 (a)) showed that the samples (dimensions 140x150 mm) retained their integrity for 5 minutes under direct flame exposure with a temperature of 1100 °C. Furthermore, glass fiber reinforced polyimide resins have also been tested in flammability tests, demonstrating very high LOI values over 80 and low smoke production. As a result of this research, new fire-resistant GFRPs based on epoxy resin, phosphorus-containing methacrylate ester, and polyimide binder have been developed. These materials can meet modern requirements for safety, manufacturability, and economic efficiency, and can be used as structural materials in construction and aviation.

The study was financially supported by the Russian Science Foundation, grant no. 20-19-00295.



# Ignition, combustion, and emission performance of composite fuels from fossil and biomass derived components

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With the development of the transport and energy sectors, the consumption of liquid hydrocarbon fuels is growing [1]. Traditional liquid fuels include kerosene, alcohols, diesel fuels, gasoline and fuel oil, all of which have high calorific value and performance characteristics that allow them to be used in boilers and engines. The main disadvantages of these fuels are their high cost and the large amount of hazardous pollutants emitted during combustion [2]. Therefore, one of the promising research areas is the development of composite fuels based on liquid hydrocarbon fuels. One of the promising and carbon-neutral components is raw materials of biological origin, for example, vegetable oils and products of their thermochemical processing [3–5]. The present paper is aimed at studying the ignition and combustion characteristics, as well as determining the concentration of the main components of flue gases when burning mixtures based on diesel and biofuels.

The basis of the fuel blends was diesel fuel, and the additional components were vegetable oils and their by-products (fatty acid methyl esters). The proportion of the additive varied from 5 to 15%. The fuel mixtures were burned as droplets, the oxidizer (air) temperature varied in the range of 500–700 °C.

Oil additives had a fairly limited effect on the ignition inertia of composite fuels; the greatest effect was recorded at low temperatures in the combustion chamber; with increasing temperature, the ignition delay times practically did not vary. However, in the presence of an additive, the burning time increases depending on the mass fraction of the additive. The completeness of fuel burnout is determined by the ratio of CO<sub>2</sub> to CO. The highest ratio was observed when burning distilled tall oil. Similar results were recorded when using mixtures based on diesel fuel and this additive. A pattern was observed associated with an increase in the completeness of burnout of mixed fuel with a share of distilled tall oil of 5% as the temperature in the combustion chamber increased. In turn, the CO<sub>2</sub>/CO ratio when burning mixed fuel with a 10% share of distilled tall oil remained virtually unchanged compared to pure diesel. For fuel with a share of distilled tall oil of 15%, a slight decrease in this indicator was recorded.

Calculation of the dimensionless efficiency indicator, which also considers the cost of the fuel, its ash content and calorific value, showed that the most effective additives among raw oils are tall oil (15% share). Among the oil esters, the most promising is the methyl ester of fatty acids of used cooking oil with a share of 5%.

The study was supported by a grant from the Ministry of Science and Higher Education of Russia, Agreement No. 075-15-2024-543 dated April 24, 2024.

## References

1. S.V. Yazan, A.R. Altarazi, J. Yu. Abu Talib, *Energy*. **2022**, 238, 121910.
2. F. Perera, *Int. J. Environ. Res. Public Health*. **2017**, 15, 16.
3. M. Yahya, A. Dutta, E. Bouri, C. Wadström, G.S. Uddin, *Renew Energy*. **2022**, 197, 594.
4. M. Kiehadroulinezhad, A. Merabet, C. Ghenai, A.G. Abo-Khalil, *Heliyon*. **2023**, 9, e13407.
5. J.B. Krstić, A.B. Nježić, M.D. Kostić, B.D. Marić, *Process Saf. Environ. Prot.* **2022**, 168, 463.

# Combustion of non-uniformly hydrogen-air mixtures in partially obstructed closed volume

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Hydrogen-air mixture is combustible and explosive even with a low volumetric hydrogen content [1]. Research shows that evolution of a real emergency scenario with hydrogen combustion will most probably occur in non-uniform hydrogen-air mixtures with vertical gradients of hydrogen [2]. In that case, local regions of the mixtures with a stoichiometric ratio can form, the combustion of which often takes place in the regime of fast deflagration or detonation.

A quantitative description of thermobaric loads of probable emergency scenarios for large-scale facilities is carried out using numerical methods, the accuracy of which must be assessed based on the results of experimental data.

In this work, experiments on the combustion of a non-uniformly hydrogen-air mixture are carried out in a horizontally oriented channel of square cross-section  $0.6 \times 0.6$  m and length 12 m. In previous work [3], it was shown that in a channel with obstacles (blockage ratio  $BR = 0.6$ ) and at a stoichiometric ratio in the upper part of the facility, the flame propagated in the quasi-detonation regime. Probably, the transition to detonation did not occur because the presence of obstacles along the entire length of the channel contribute to "choking" the flame. To test this assumption, an experimental study of combustion in a closed volume with obstacles installed only in the first half of the channel was carried out.

Purpose of the work is determine the effect of partially obstruction on the transition from deflagration to detonation, as well as to obtain experimental data to verify numerical methods.

In work the speed of propagation of the flame front along the channel, the overpressure of the combustion wave and the maximum overpressure was determined. It was revealed that the transition to detonation took place in an unobstructed part of the channel.

## References

1. B.E. Gelfand, Thermogasdynamics of combustion and explosion of hydrogen. Saint Petersburg. Institute of Chemical Physics im. N. N. Semenov RAS, NPO Special Materials, **2009**, 119;
2. K.G. Vollmer, F. Ettner, T. Sattelmayer, e.a., *Comb. Sci. Tech.* **2012**, 184, 10-11;
3. S. A. Yakovlev, E. V. Bezhodov, V. V. Stakhanov, e.a. *Atomic Energy* **2023**, 134, 5-6.



# Dynamics of slow magnetoacoustic and entropy modes in flaring coronal loops

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Magnetoacoustic(MA) waves are observed in various regions of the solar corona in the form of intensity variations. The number of observed oscillations and waves makes it possible to use MA waves as a diagnostic tool for coronal plasma and its structures, such as coronal loops.

For practical needs of plasma diagnostics, it is sufficient to use a single-fluid system of MHD equations that describes the fundamental regularities of the macroscopic behavior of a quasi-neutral plasma in terms of its density, velocity, pressure, and magnetic field. Based on the system used, taking into account the thin flux tube approximation and/or an infinitely strong magnetic field approximation, the evolutionary wave equation and the dispersion equation, which is its partial solution, are obtained. The partial solution for magnetoacoustic waves allows us to obtain correct information on the wave parameters, in particular, phase velocities and wave increments. However, the solar corona plasma contains not only magnetoacoustic waves but also entropic waves. The observed perturbation is their superposition, for which the dispersion equation approach is not correct; an exact solution is needed. Thus, the main disadvantage of this method is the loss of important information about the observed phenomena and structures, since there is no exact solution to the evolution of an arbitrary initial perturbation, without which this problem can be solved only numerically.

In our work, we try to contribute to the problem of obtaining accurate analytical models. Within the framework of previous studies, a linear differential equation for slow MA waves in coronal loops has already been derived in the framework of the infinitely strong field approximation, taking into account non-adiabatic processes with given boundary conditions. In addition, the case of a weak influence of heating and cooling processes, as well as a strong influence of thermal conduction, was considered. The exact solution considering this formulation of the problem was obtained using the method of separation of variables (Fourier method) and Duhamel's principle or formula. The obtained solutions were applied to describe the possible dynamics of slow magnetoacoustic and entropy modes in flaring coronal loops.

This work was partially supported under the state assignment of the Ministry of Science and Higher Education of the Russian Federation (projects FSSS-2023-0009, FMR-2024-0017).

# POSTER TALKS

# Further Development of Multi-component Diesel Surrogate Model on Naphthanes for High Temperature Combustion

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Diesel fuel is widely used in transportation sections worldwide, such as in road- and railway, as well as in aviation. Despite its importance, the number of existing theoretical studies focused on its combustion characterization, particularly on kinetic surrogate modeling, remained limited. Together with the recently published diesel surrogate model in [1], three surrogate formulas were introduced which contain: n-dodecane, iso-octane, toluene and cyclohexane, with various mole fractions. As found in previous research, the high-temperature reactions of cyclohexane, as a simple naphthene molecule available, play important roles in determination of the high-temperature combustion behavior of the surrogate blends. Specifically important were the cascading dehydrogenation reactions of cyclohexane in prediction of ignition delay time data, and formation of the smaller poly aromatic hydrocarbons, such as benzene and naphthalene. Since in reality we have more complex naphthanes in different diesel mixtures, it is necessary to have the corresponding sub-model further developed. To this aim, the introduced surrogate formulas will be extended for high temperature ranges, and the corresponding kinetic model will be further extended, using the latest published propyl-cyclohexane sub-model (Fig 1). The simulation results will be compared with the high temperature ignition delay time, and laminar flame speed data; Further comparison with the previous results will be provided as well. Since the recently published model [1] was very consistent with ignition delay time data, the initial goal is to regenerate similar results. Clear changes may occur in the case of the simulation of laminar flame speed data, due to the new changes in surrogate model. At the end, the effective pathway toward formation of poly aromatic species will be investigated.

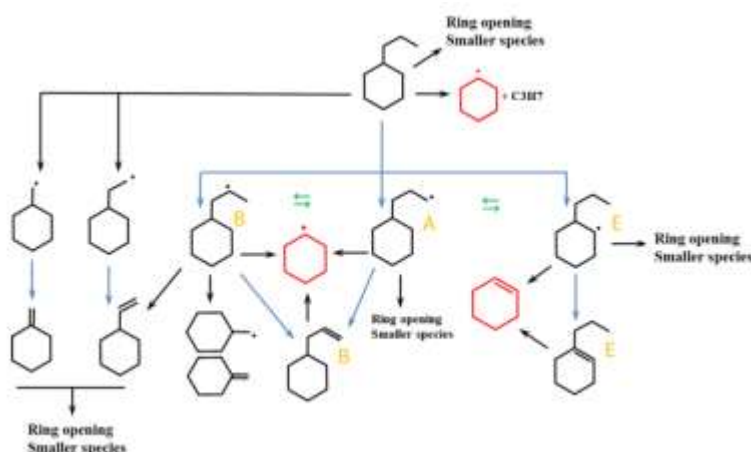


Fig 1. Principal scheme of the high temperature oxidation of propyl-cyclohexane [2].

## References

1. Abbasi, M., Slavinskaya, N., "Development of a 4-Component Surrogate Model for Combustion of Gasoil, including investigation of PAH Formation," in *10th INTERNATIONAL SEMINAR ON FLAME STRUCTURE*, Novosibirsk, Russian Federation, 2023.
2. Abbasi, M., Slavinskaya, N., Riedel, U., "Kinetic Modeling of Cyclohexane and n-Propylcyclohexane Oxidation with the PAH Precursor Formation.," in *Proc. 56th AIAA Aerospace Sciences Meeting*, Kissimmee, USA, 2018.

# Features of laser ignition of coal particles by laser radiation (review)

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Pulsed laser radiation in combination with time-resolving electron-optical equipment is a good tool for studying the primary processes of coal ignition and pyrolysis.

The radiation of the first harmonic of the YAG:  $Nd^{3+}$  laser in the free generation mode ( $\tau_1 = 120 \mu\text{s}$ ), as well as the first and second harmonics ( $\lambda = 1064 \text{ nm}$  and  $532 \text{ nm}$ ) in the Q-switching mode ( $\tau_1 = 12 \text{ ns}$ ,  $\tau_2 = 9 \text{ ns}$ ) influenced on tableted samples  $\rho = 1 \text{ g/cm}^2$  of coal microparticles ( $0.5 \div 63 \mu\text{m}$ ) in the metamorphism range from brown to anthracite. Absorption of radiation occurs in the surface layer  $d \sim 1 \mu\text{m}$ . Volumetric heating of microparticles is achieved in a time of  $\sim (0.5 - 2) \text{ ms}$ .

Free generation mode. When the critical value of the radiation energy density is reached.  $H_{cr}^1 \sim (0.3 \div 0.5) \text{ J/cm}^2$  on the surface of coal microparticles, reaction-active microprotrusions with a diameter  $d \geq 1 \mu\text{m}$  are ignited. The duration of combustion coincides with the duration of the radiation pulses. When  $H$  increases to  $H_{cr}^2$  values in a time interval of  $\sim 10 \text{ ms}$ , thermochemical reactions are initiated in the volume of coal microparticles, and volatile compounds are released and ignited in the gas phase. When the energy density reaches the value  $H_{cr}^3$  in the time interval of  $50 \div 100 \text{ ms}$ , the aromatic part of the coal macromolecules is ignited.

Q-switching mode. When the critical energy density  $H_{cr} \sim 0.2 \text{ J/cm}^2$  is reached in the laser radiation field, microprotrusions on the surface of coal particles are heated, electrons are emitted, an electron avalanche is formed and optical breakdown is accompanied by a continuous spectrum of luminescence, as well as a line spectrum of luminescence of laser-induced plasma, including excited atoms and ions of  $\text{C}^+$ ,  $\text{C}_2^+$ ,  $\text{H}$ ,  $\text{O}$ ,  $\text{Ca}^+$ ,  $\text{Al}$ ,  $\text{Fe}$ ,  $\text{Fe}^+$ ,  $\text{Mg}^+$  and  $\text{C}_2$ ,  $\text{CN}$ ,  $\text{OH}$ , formed from the evaporated substance in the surface breakdown channels. Plasma lifetime  $\sim 1 \mu\text{s}$ . When the energy density reaches the value  $H_{cr}^2$  in the time interval of  $200 \div 500 \mu\text{s}$  after exposure to the laser pulse, thermochemical reactions are initiated in the volume of coal particles and their combustion occurs. Models of the processes described above are discussed.

When the critical value of energy density  $H_{cr} \sim 0.2 \text{ J/cm}^2$  is reached in the laser radiation field, microprotrusions on the surface of carbon particles are heated, electrons are emitted, an electron avalanche is formed, and optical breakdown is accompanied by a continuous luminescence spectrum, as well as a line spectrum of C atoms and ions,  $\text{C}^+$ ,  $\text{C}_2^+$ ,  $\text{H}$ ,  $\text{O}$ ,  $\text{Ca}^+$ ,  $\text{Al}$ ,  $\text{Fe}$ ,  $\text{Fe}^+$ ,  $\text{Mg}^+$  and  $\text{C}_2$ ,  $\text{CN}$ ,  $\text{OH}$  molecules formed from the evaporated substance in the surface breakdown channels. Plasma lifetime  $\sim 1 \mu\text{s}$ . When the energy density reaches the value  $H_{cr}^2$  in the time interval of  $200 \div 500 \mu\text{s}$ , thermochemical reactions are initiated in the volume of coal particles and their combustion occurs. Models of the processes described above are discussed.

The work was carried out within the framework of the state assignment FRC CCC SB RAS (project No. 1022041700063-6).

# The efficiency of combustor perforated plate

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Modern combustion chambers operate at conditions, which are associated with the high temperatures and pressures, so the issue of cooling the walls is relevant. There are different types of cooling systems: film, convective, convective-film, transpiration and perforation, which is the most promising, as it allows for more efficient use of the cooling resource.

To analyze the influence of various geometric parameters on the efficiency of perforation cooling, a sector of the annular combustion chamber with six rows of holes with a diameter of 0.85 mm and a pitch of 8 mm was taken as the initial data. The wall thickness is 1.6 mm, the cold air temperature at the inlet is 957K, the hot air temperature is 1800K, which corresponds to the temperature conditions of modern combustion chambers.

During the work, various geometric parameters of the holes were investigated, which are technologically feasible and can be implemented into the design of the combustion chamber. The following parameters were changed:

- 1) Angles of inclination of holes;
- 2) Rotation angles of holes;
- 3) Recesses on the hot surface;
- 4) Types of hole geometry;
- 5) The order of the holes (linear and staggered).

The associated calculation was carried out in the Ansys Fluent program. The wall material was chosen EI868 (XH60BT). When specifying the material, the values of thermal conductivity and heat capacity were taken into account depending on temperature.

The efficiency parameter was taken to be the value  $\eta$ , which is defined as the ratio of the difference in the temperature of the hot air at the inlet and the adiabatic temperature of the wall to the difference between the temperatures of the hot and cold air. A comparison is made of the dependence of cooling efficiency along the length of the wall on geometric parameters. Recommendations are given for the selection of holes for the most effective cooling of the flame tube walls of modern combustion chambers.

# Synthesis of the simplest alcohols and nitrogen-substituted PAHs in the interstellar medium

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Complex organic molecules (COM) are molecules containing six or more atoms of hydrogen, carbon, nitrogen or oxygen - they make up about a third of all molecules found in the interstellar medium [1]. Establishing the ways of their formation is critically important for explaining the fundamental processes governing the poorly understood chemistry of the interstellar medium and for determining organic molecules capable of forming in space conditions. Modern astrochemical models believe that COMs are formed in cold molecular clouds on dust particles - silicate or carbon nanoparticles covered with a thin layer of ice consisting of water, methanol, carbon monoxide, carbon dioxide, ammonia, formaldehyde and methane [2] - as a result of exposure to cosmic radiation at temperatures reaching up to 10 K. During the gravitational collapse of a molecular cloud, molecules from the dust particles can sublime into the gas phase, since the temperature of the dust particles increases due to the non-isothermal phase of the collapse, and then due to heating from the hot core [1]. These molecules then enter the protoplanetary disk, planets and other bodies in star systems. A recent analysis of the organics in comet 67P has found many organic substances, much more diverse and complex than expected based on currently accepted chemical models [3], therefore, there is still no fundamental understanding of the level of molecular complexity of COM that can be achieved in deep space.

The purpose of the work is to study the radical substitution reaction involving components of space ice, leading to the formation of the simplest alcohols, and about revealing the mechanisms of the chemical conversion of acetonitrile radicals into diazines (pyrimidine and pyridazine) in the gas-phase and ice-phase reactions. Geometry optimization of all possible stationary and transient states was carried out at the long-range corrected hybrid density functional  $\omega$ B97X-D level of theory with Dunning's correlation-consistent cc-pVTZ basis set in Gaussian 09. The ice-phase conditions were created by applying the SCRf (PCM, solvent water) approach in Gaussian that allows calculations to be performed in the presence of a solvent by placing the solute in a cavity within the solvent reaction field. The energy refinement was carried out according to the extrapolation scheme to the complete basis set E(CBS), the phenomenological velocity constants depending on temperature were calculated in the Abstraction subroutine of the MESS package.

## References

1. E. Herbst, The synthesis of large interstellar molecules // *International Reviews in Physical Chemistry*. — 2017. — Vol. 36. — P. 29.
2. A. C. A. Boogert, P. A. Gerakines, D. C. B. Whittet, Observations of the Icy Universe // *Annual Review of Astronomy and Astrophysics*. — 2015. — Vol. 53. — P. 541.
3. Altwegg K., Balsiger H., Berthelier J. J. et al. Organics in comet 67P – a first comparative analysis of mass spectra from ROSINA-DFMS, COSAC and Ptolemy // *Monthly Notices of the Royal Astronomical Society*. — 2017. — Vol. 469. — P. 130.



# Reactions in cryogenic methane films initiated by ultraviolet vacuum radiation

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The study examined cryogenic reactions in methane ice initiated by ultraviolet vacuum radiation. Studying reactions initiated by cosmic radiation in methane-containing cosmic ices is of significant scientific interest, because methane is abundant in the Solar System and interstellar medium [1, 2]. Ice films with a thickness of at least 100 nm on a substrate were obtained by deposition of methane from the gas phase onto a copper surface at a temperature of 5 K. Irradiation was carried out using the ninth harmonic of a Nd:YAG laser with a wavelength of 118 nm, which was obtained by nonlinear frequency conversion of the third harmonic on Xe atoms. The reaction products were detected using a quadrupole mass spectrometer.

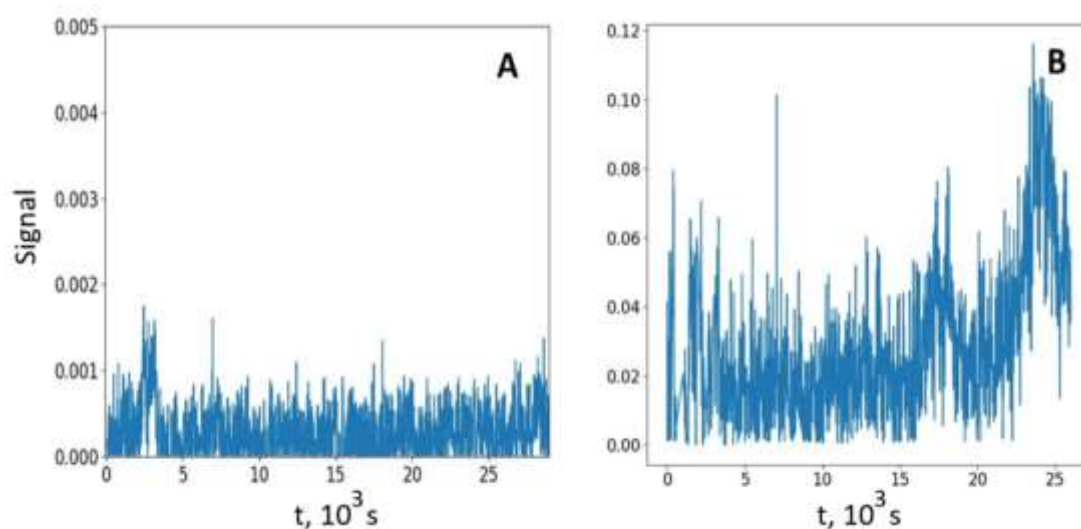


Figure 1. Temperature-programmed desorption (TPD) dependencies of the mass channel  $M/z = 29$  for unirradiated (A) and irradiated (B) methane ice samples

As a result, a peak at  $M/z = 29$  amu corresponding to the  $C_2H_5^+$  fragment was found in the mass spectra of the reaction products. Figure 1 shows the temperature-programmed desorption (TPD) dependencies of the mass channel  $M/z = 29$  for unirradiated and irradiated methane ice samples. This peak appeared at intermediate and late times and was associated with the fragmentation of propane and butane molecules. Furthermore, for a more comprehensive study of chemical processes, it is planned to subject the icy film to prolonged exposure to ultraviolet radiation or to use particles with greater penetration depth, such as electrons with energies on the order of several keV.

## References

1. S. Protopapa, W. Grundy, S. Tegler, and J. Bergonio. Absorption coefficients of the methane–nitrogen binary ice system: Implications for Pluto. *Icarus*. **2015**, 253, pp. 179-188.
2. S. Tegler et al. Methane and nitrogen abundances on Pluto and Eris. *The Astrophysical Journal*. **2010**, 725, 1, p. 1296.

# Testing of monolithic chromato-desorption systems with organic solvents under extreme conditions

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At the present stage of development of analytical chemistry several important tasks are being solved, one of which is the improvement of existing methods and means of preparation of gas and liquid mixtures of known composition, as well as the creation of fundamentally new methods of obtaining standard samples.

Today, one of the understudied dynamic methods of production of the mixtures is the creation of a flow of organic solvents with a certain content of the target component released from the monolithic polymer matrix.

The purpose of this work is to study the possibility of obtaining constant concentrations of organically-soluble analytes in organic media during the operation of monolithic chromato-desorption systems (MHDS) under extreme conditions.

Monolithic chromato-desorption systems were manufactured using a modified two-component epoxy resin as a matrix material. *N*-octane was used as a solvent. As analytes, several saturated fatty acids – tetradecanoic acid, pentadecanoic acid, hexadecanoic acid, and octadecanoic acid – were chosen. The analytes under study have high solubility in nonpolar organic solvents.

The manufactured experimental samples were studied in dynamic mode of extraction using a specially designed extraction system at temperatures of 50, 80 and 120°C and an eluent flow rate of 3 cm<sup>3</sup>/min, using *n*-octane as the eluent.

According to the results of chromatographic analysis of octane solutions of organically-soluble analytes, it can be concluded that to obtain quasi-stationary concentrations in the dynamic extraction mode it is necessary to ensure the passage of 500-600 cm<sup>3</sup> of extractant through the samples under study at a flow rate of 3 cm<sup>3</sup>/min. The error of maintaining constant concentrations does not exceed 10%.

A comparative evaluation of the degree of extraction of organically-soluble analytes from MHDS at different temperatures in the dynamic mode of extraction was carried out. It was found that the increase in extraction temperature leads to an increase in the content of the studied organically-soluble analytes in *n*-octane.

As a result of the experiment, it was concluded that the use of fabricated MHDS allows to obtain solutions of *n*-octane with known analyte content in dynamic extraction mode at 50, 80 and 120°C.

The results obtained can be used to create solutions with known content of organically-soluble analyte by dynamic method.

# Measurements of the oxygen dissociation rate constant with verification of modern models of hydrocarbon combustion

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The dissociation rate of molecular oxygen ( $O_2$ ) is one of the most important kinetic parameters in the study of combustion and high-temperature air flows. It was shown that in modern models of hydrocarbon combustion there is still no consensus on the value of the rate of dissociation of molecular oxygen. It was also shown that the accuracy of knowing the rate of this reaction requires special attention, as one of the components of the "core" of any comprehensive combustion models. Therefore, to resolve existing contradictions, new, more accurate measurements of the dissociation rate of molecular oxygen at temperatures close to conventional combustion were carried out. The presented rate constant of the  $O_2$  dissociation reaction with a very low uncertainty will undoubtedly contribute to the development of more reliable modern combustion models.

The data available in the literature on measurements of the rate coefficient of molecular oxygen dissociation were considered and structured. Modern models of hydrocarbons combustion were analyzed considering values of the  $O_2$  dissociation rate constant. Precision measurements of the rate of  $O_2$  dissociation behind shock waves at temperatures of  $2500\text{--}5000 \pm 50$  K and pressures of 1.2–2.5 bar were carried out using atomic resonance absorption spectrometry on O atom (O-ARAS). The ARAS measurements of the absolute concentration of oxygen atoms were calibrated in the conditions of complete dissociation of  $N_2O$  and  $O_2$ , considering the temperature splitting of the calibration curves. Using kinetic modeling, a detailed analysis of experimental uncertainties was carried out with an assessment of the influence of impurities of various origin at the dissociation of  $O_2$ . An updated expression for the rate constant of the reaction  $O_2 + Ar = 2O + Ar$  was obtained in the form  $k_{\text{diss}} (\pm 15\%) = 1.30 \cdot 10^{14} \cdot \exp(-108.95 \text{ [kcal/mol]} / RT) \text{ cm}^3 \text{ mol}^{-1} \text{ s}^{-1}$ . A significant influence of the  $O_2$  dissociation rate constant on the predictive ability of modern models of hydrocarbons (on the example of biofuels) combustion at high temperatures was shown. Recommendations were formulated on the use of the corresponding oxygen dissociation rate constant in the development and/or refinement of combustion kinetic models.

This study was funded by RSF project № 23-1900407.

# Astropolarimetry: reduced form of statistical equilibrium equations

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In a typical astrophysical spectropolarimetry study, it is assumed that the gas surrounding an exoplanet is irradiated by the nearest star, causing polarization of the atoms in the gas. Then the polarized gas emits or scatters polarized light, which is observed from Earth (transit spectroscopy). The interaction between polarized atoms and polarized radiation is described by statistical equilibrium equations (SEE), which are usually given in a rather complicated form [1](=DL). In this work we reformulated them in a new form, which is shorter and its physical meaning is easily verifiable, but it is equivalent to initial DL's expressions. The SEEs for the density-matrix elements  $\rho_{mm'} = \langle m | \rho | m' \rangle$  describe polarization of gas species by radiation:

$$\frac{d}{dt} \rho_{mm'} = -i2\pi\nu_{mm'} \rho_{mm'} + \sum_{nn'} \rho_{nn'} T_A(m, m', n, n') + \sum_{pp'} \rho_{pp'} [T_E(m, m', p, p') + \dots \text{ where } m, m', m'', n,$$

$n', \dots$  are eigenvectors of atomic Hamiltonian. In our case  $|m\rangle = |\tau, j, m\rangle$  and  $|m'\rangle = |\tau, j, m'\rangle, \dots$  etc.

Usually there are seven terms here, only three are shown. Let us consider only the second term, that describes absorption of light via transition  $\tau_l j_l m_l \rightarrow \tau, j, m$ . Using the algebra of irreducible spherical tensor operators (ITOs) DL rewrote the SEEs in the ITO-form like

$$\frac{d}{dt} \rho_Q^K(\tau j) = -i2\pi\nu_L g_{\tau j} Q \rho_Q^K(\tau j) + T_A + \dots \text{ where } T_A \equiv \sum_{\tau_l j_l K_l Q_l} \rho_{Q_l}^{K_l}(\tau_l j_l) \sum_{K_r Q_r} 3(2j_l + 1) \times$$

$$\times (-1)^{K_l + Q_l} \sqrt{(2K + 1)(2K_l + 1)(2K_r + 1)} \begin{pmatrix} K & K_l & K_r \\ -Q & Q_l & -Q_r \end{pmatrix} \begin{pmatrix} j & j_l & k \\ j' & j'_l & k'_l \\ K & K_l & K_r \end{pmatrix} B(\tau_l j_l \rightarrow \tau j) J_{Q_r}^{K_r}(\nu_{\tau_l j_l \rightarrow \tau j})$$

here Einstein coefficient is  $B(\tau_l j_l \rightarrow \tau j) = C_A |\langle \tau j || d || \tau_l j_l \rangle|^2 / (2j_l + 1)$ , the polarization tensor

is  $J_{q'q}(\nu) \equiv \iint I_{q'q}(\nu, \Omega) d\Omega / 4\pi$ , where  $I_{q'q}(\nu, \Omega) = \sum_{\alpha, \beta = \pm 1} \mathbf{b}_{\beta, \alpha}(\nu, \Omega) D_{\alpha q}^1(\Omega) D_{\beta q'}^1(\Omega)$ , here

$I_{\beta, \alpha}(\nu, \Omega)$  is the photon flux tensor, and  $C_A \equiv 32\pi^4 / 3h^2 c$ . In this work, an extension of the ITO vector algebra has been proposed, which involves coupling two ITOs into a third one

, where one of the terms is a complex conjugate and therefore is not an ITO.

This approach has been applied to rewrite the SEEs. Thus, the rate coefficient  $T_A$  in our form is

$$T_A = \frac{3C_A}{\sqrt{2K + 1}} \sum_{\tau_l j_l K_l K_r} (\rho^{(K_l)}(\tau_l j_l) \otimes J^{(K_r)*})_Q^{(K)} \langle \tau (j \otimes j^*)^{(K)} || (d^{(k)} \otimes d'^{(k')*})^{(K_r)} || \tau_l (j_l \otimes j_l^*)^{(K_l)} \rangle. \quad \text{It}$$

has two terms, the reduced matrix element of the dipole moments and the vector product of the tensors  $\rho^{(K_l)}(\tau_l j_l)$  and  $J^{(K_r)*}$ : in all our equations polarimetry and geometry are clearly separated.

## References

1. (DL) E.L. Degl'innocenti, M.Landolfi *Polarization in Spectral Lines*, Springer, 2004

# Preparation of $Ti_3SiC_2$ and $Ti_3AlC_2$ MAX phases from $TiSi_2$ -C and $TiAl$ -C by SHS in river sand shield

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Currently, MAX phases remain a hot topic for research due to their unique properties and possible areas of application [1]. The main problems in obtaining the MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$  by the SHS method are associated with the phase heterogeneity of the synthesis product and the presence of impurity phases of titanium carbide TiC and titanium silicides  $TiSi_2$ ,  $Ti_3Si_5$  (in the case of  $Ti_3AlC_2$  - titanium intermetallic compounds  $TiAl$ ,  $Ti_3Al$ ,  $TiAl_3$ ). This problem arises for many reasons, including the fact that during SHS in combustion mode, due to high reaction temperatures, part of the low-melting powder element of the charge evaporates, thereby violating the stoichiometry and reducing the amount of MAX phase in the resulting product. For the synthesis of MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$  in the initial charge, many authors use not elemental powders, but their compounds to increase the number of MAX phases in the product [2, 3].

The work carried out a study of the effect of replacing low-melting charge powders: silicon and aluminum with their chemical compounds - titanium disilicide ( $TiSi_2$ ) and titanium intermetallic compound ( $TiAl$ ). The samples were obtained by the SHS method in air in a protective shell of sand. As a result of the studies, it was established that replacing titanium and silicon powders with titanium silicide powder  $TiSi_2$  in the initial charge during the synthesis of the porous frame of the MAX-phase  $Ti_3SiC_2$  by the SHS method leads to the appearance of a silicon carbide phase SiC and an increase in the titanium carbide phase TiC relative to the MAX phase  $Ti_3SiC_2$  in the resulting product. When replacing silicon by 50 wt% of the mass, the amount of silicon carbide phase reached 46 wt% of the total mass of the resulting SHS frame. At the same time, the amount of titanium carbide decreased to 12 wt% compared to the stoichiometric composition. The amount of the  $Ti_3SiC_2$  MAX phase in the composition of the porous frame obtained by the SHS method in air with an increase in the amount of replacement of silicon with titanium disilicide  $TiSi_2$  decreases from 66 wt% to 20 wt% of the total mass. Replacing titanium and aluminum powders with titanium aluminide  $TiAl$  powder in the initial charge leads to an increase in the amount of titanium carbide phase TiC and titanium aluminide  $TiAl$  relative to the MAX phase  $Ti_3AlC_2$  in the resulting SHS composite. The maximum amount of MAX phase in the resulting composites does not exceed 35 wt%. For comparison, when using elemental powders in the initial charge after SHS, the amount of the MAX phase  $Ti_3AlC_2$  fluctuates around 52 wt%.

Acknowledgments: The research was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation within the framework of the state task (theme no. AAAA12-2110800012-0).

## References

1. Gonzalez-Julian J, *J Am Ceram Soc.* **2020**, 1–32, 44.
2. Hwang SS, Lee SC, Han J, Lee D, Park S, *J Eur Ceram Soc.* **2012**, 32(12), 3493–500.
3. Tang Hai, Feng Yi, Huang Xiaochen, Dou Yakun, Ding Dongdong, Xia Meng, Tian Pei, Qian Gang, Zhang Xuebin, *Rare Metal Materials and Engineering*, **2017**, 46(8), 2108-2113.

# Synthesis of porous MAX phases $Ti_3SiC_2$ and $Ti_3AlC_2$ by combustion in air and river sand

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MAX phases occupy an intermediate position in properties between ceramics and metals and are attractive for use in energy, mechanical engineering and other industries due to their unique properties [1]. Porous MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$  can be used as filters, bone bioimplants, in catalysis and electrochemistry. A new method for producing cermets is also known, in which a hot porous workpiece from the MAX phase immediately after combustion synthesis (CS) in air serves as a base (skeleton) for spontaneous filling with molten metal [2].

Porous skeletons of the MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$  were obtained using the CS method under the simplest conditions of reactorless combustion in air or in a backfill of river sand. The total porosity (open and closed) is 60% by volume, of which the proportion of open pores is more than 40%. The average pore size ranges from 10 to 350  $\mu m$ . Quantitative XRD of the resulting porous skeletons showed that the content of the MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$  is about 60 wt.%. In addition to the MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$ , a titanium carbide phase TiC of about 40-50 wt.% and a titanium silicide phase  $TiSi_2$  (or titanium aluminide TiAl in the synthesis of  $Ti_3AlC_2$ ) were formed in an amount of 2 – 5 wt.%. It was found that the fractional composition (particle size) of the initial titanium and carbon powders, as well as the form of the powdered carbon (graphite or soot) significantly influence the macrostructure of the porous CS skeletons of the MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$ . It has been experimentally proven that the CS skeleton, obtained using coarse titanium powder of the TPP-7 grade and graphite powder of the S-2 grade, better preserved the cylindrical shape of the original pressed charge billet and has a uniform fine-porous macrostructure without macrodefects (cavities, cracks, delaminations), and also has the highest, compared to other brands of titanium and carbon powders used, uniaxial compressive strength of 104 MPa. The influence of the composition of the gas atmosphere and vacuum on the formation of surface films formed during the production of porous skeletons of MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$  by the synthesis in combustion mode was studied. During the CS of the MAX phases  $Ti_3SiC_2$  and  $Ti_3AlC_2$  in air, oxide-nitride films about 100  $\mu m$  thick were formed on the surface of the samples, and about 20  $\mu m$  thick by the synthesis in the river sand backfill.

Acknowledgments: The research was carried out with the financial support of the Ministry of Science and Higher Education of the Russian Federation within the framework of the state task (theme no. AAAAA12-2110800012-0).

## References

1. M.W. Barsoum, *MAX phases: Properties of machinable ternary carbides and nitrides*, Weinheim: Wiley-VCH, **2013**.
2. A.P. Amosov, E.I. Latukhin, E.R. Umerov, D.M. Davydov, *Izvestiya Vuzov. Poroshkovaya Metallurgiya i Funktsional'nye Pokrytiya (Powder Metallurgy and Functional Coatings)*, **2022**, 3, 24.



# Chemical structure of laminar hydrogen flames with the addition of tetraethoxysilane

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Flame synthesis is a scalable technology for the continuous production of inorganic oxide-based functional materials used for energy storage, catalysis, sensing, medical applications, and many other applications. A range of flame fusion technologies are used across the industry to produce tons of nanomaterials. At the same time, the development of these technologies proceeds mainly through empirical trial and error, since the complexity of the physicochemical processes of transformation and growth of particles in a flame does not allow establishing a clear connection between the synthesis parameters and the final properties of the resulting particles. One of the problems here is the lack of reliable knowledge about the detailed mechanisms of pyrolysis and oxidation of precursors [1].

This work aims to study the kinetics of tetraethoxysilane (TEOS) oxidation in a hydrogen flame. TEOS was chosen as the main object, since it is considered as a SiO<sub>2</sub> nanoparticle precursor. Laminar premixed flames of H<sub>2</sub>/O<sub>2</sub>/Ar mixtures of different stoichiometry with a small TEOS additive were investigated. The flames were stabilized over a flat flame burner at atmospheric pressure and examined with the molecular-beam mass-spectrometric setup. The reactants, stable and intermediate products of TEOS decomposition including radicals were detected.

To get insights to the TEOS oxidation kinetics the mechanism of tetramethoxysilane (TMOS) oxidation from the work of Zhang et al. [2] was adopted. The key reactions of TEOS consumption were assessed and implemented to the Zhang mechanism. The rate of production and sensitivity analyses were performed to elucidate the key reaction pathways.

## References

1. C. Schulz, T. Dreier, M. Fikri, H. Wiggers, *Proc. Combust. Inst.* **2019**, 37, 83–108.
2. Y. Zhang, J. Xia, Q. Fang, B. Mei, W. Li, T. Li and Y. Li, *Combust. Flame.* **2022**, 242, 112169.

# Radical substitution reactions between light alkanes and their radicals

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Alkanes, or paraffins, with the general chemical formula of  $C_nH_{2n+2}$ , have the simplest structure among organic molecules, which range in complexity from the smallest hydrocarbon, methane, to macromolecules such as polyethylene. Alkanes are the major constituents of natural gas and crude oil and thus the direct conversion of abundant and low-cost hydrocarbon feedstocks into value-added products has the potential to be a revolutionary technology in the chemical industry. Selectively converting propane to propene, for instance, is a process with tremendous applicability due to the huge demand of propene for the production of polypropene and commodity chemicals, such as acrylic acid, acrylonitrile, and cumene [1]. Also of practical interest are processes of alkanes molecular weight growth, in which light and abundant molecules such as methane or ethane form heavier saturated hydrocarbons used in industry, for example, butane, which is used in the synthesis of maleic anhydride and acetic acid [2].

In this work, we consider radical substitution reactions between alkanes and alkynes, resulting in the formation of a heavier alkane and atomic hydrogen. These processes could lead to an increase in the molecular weight of saturated hydrocarbons and the branching of their structures. In present work, we focused on reactions between methane, ethane and propane and their radicals.

Optimized geometries and vibrational frequencies for reagents, products and transition states of considered reactions were obtained on wB97-XD/cc-pVTZ level of theory. The intrinsic reaction coordinate method was used to more accurately study potential energy surfaces. Electronic energies were refined using the CCSD(T)/cc-pVTZ method.

As a result of the work, potential energy surfaces of radical substitution reactions occurring between light saturated hydrocarbons containing up to 3 carbon atoms and their radicals were obtained. It has been shown that the considered reactions could lead to alkanes molecular weight growth.

## References

1. Tang X., Jia X., Huang Z. Challenges and opportunities for alkane functionalisation using molecular catalysts // *Chemical Science*. – 2018. – T. 9. – №. 2. – C. 288-299.
2. Baerns M., Buyevskaya O. Simple chemical processes based on low molecular-mass alkanes as chemical feedstocks // *Catalysis Today*. – 1998. – T. 45. – №. 1-4. – C. 13-22.

# Calculation method for lean flame blowout limit of CH<sub>4</sub>/H<sub>2</sub>/air combustion considering laminar flame speed values

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In recent years both in Russia and abroad, much attention has been paid to the issue of using hydrogen-containing fuel-air mixtures (FAM) utilized, in particular, in industrial gas turbine power plants, to reduce the content of CO<sub>2</sub> and CO in the combustion products. The use of hydrogen in fuels comes with a number of advantages. It is known that the hydrogen addition to the fuel-air mixture increases the stability limits of the engine by the lean blowout limit, and, as it is known, combustion of lean mixtures leads to a decrease in the nitrogen oxides emission.

In this study, the validation of the method for determination of the stability limits of a model combustion chamber by lean blowout limit was carried out at different hydrogen content in a premixed methane-hydrogen combustion. Self-reported experimental data were used to validate the model.

The specific feature of the applied mathematical model of turbulent combustion is the consideration of the laminar flame speed dependence on the temperature, pressure and fuel-air mixture composition. As a result, the values of laminar flame speed SL calculated in Fluent and Chemkin software products were obtained. The discrepancy between the SL values obtained by Ansys Fluent and the values obtained by the verified Chemkin methodology disagree to a smaller extent at hydrogen additions of 10-20%. However, as the hydrogen content in the fuel increases, the discrepancy between the laminar flame speed values calculated in Fluent increases significantly, which can have a significant effect in lean flame blowout simulation. Thus, the use of SL values obtained by the verified computational methodology from Ansys Chemkin improves the predictive ability of the lean flame blowout calculation method, which can be used in the preliminary design of combustion chambers operating on methane-hydrogen mixtures.

## Acknowledgment

The study was supported by the Russian Science Foundation, projects no. 22-79-10205, (<https://rscf.ru/project/22-79-10205/>).

# Rate constants for the interaction of para-pyridyl with O<sub>2</sub>: Theoretical study

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Despite the development of green energy and research on the use of environmentally friendly fuels, many industrial enterprises currently use coal as fuel. Although coal combustion studies have been conducted for many years, their predictive ability is often insufficient in modern conditions, as requirements for reducing harmful emissions become more stringent every year.

Theoretical, in particular quantum chemical, methods make it possible to reduce the cost of expensive experiments, as well as obtain results for processes that are difficult to carry out experimentally.

As a model system to describe the combustion of coal, one can use a pyridine molecule, which, on the one hand, has an aromatic structure, and on the other hand contains a nitrogen atom. Nitrogen in coals is predominantly contained in heterocyclic structures in rings of the six-membered pyridine and five-membered pyrrole type. When modeling the combustion of fuel-bound nitrogen, it is generally assumed that heterocyclic nitrogen is rapidly released as tar and as volatile compounds HCN and NH<sub>3</sub>. Pyridine and pyrrole are expected to be at least as reactive as HCN with respect to oxygen, so more realistic models of the oxidation of coal nitrogen functionality should include studies of the oxidation mechanisms of the pyridine and pyrrole ring structures.

The oxidation of pyridine most likely occurs due to the interaction with molecular oxygen of pyridine radicals. For pyridine, the formation of three radicals is possible: ortho-, meta- and para-pyridyls, depending on the position of the radical in the ring of the molecule.

This work is devoted to the theoretical study of reaction pathways between para-pyridyl and molecular oxygen. The geometries of reactants, products, intermediates, and transition states of the reactions of ortho- and meta-pyridyl radicals with O<sub>2</sub> were optimized at the level of density functional theory using the  $\omega$ B97XD functional with the 6-311G\*\* basis set. The vibrational frequencies were calculated at the same level of theory to characterize stationary points as local minima or transition states, to obtain zero-point energy (ZPE) corrections, and for use in partition function calculations. Additionally, the optimized  $\omega$ B97XD geometries were used to refine single-point energies using the combined ab initio G3 (MP2, CC) method. The potential energy surface of the interaction of para-pyridyl with molecular oxygen was constructed. Research reaction can proceed along 2 paths, the shortest of which is leading to the formation of 1 $\lambda$ 2-pyrrole, while the formation of other products (HCO + HCN, 1 $\lambda$ 2-pyrrole and 1 $\lambda$ 3,4-oxazine) proceeds through a significantly larger number of barriers.

# **Development of a method for determining the flashback limits when using methane-hydrogen fuel in the combustion chambers of gas turbine engines**

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To design new low-emission combustion chambers that stably operate on methane-hydrogen fuels, it is necessary to reliably determine the boundaries of stable operation of combustion chambers, in particular, the conditions for the occurrence of flashback into the burner device. The solution to this problem is possible using computational gas dynamics methods. However, at present, mathematical models of methane-hydrogen fuel combustion have been verified only in a narrow range of parameters under study. Also, there are insufficient experimental results of studies of the combustion of methane-hydrogen-air mixtures under various conditions in relation to complex technical devices, which does not allow qualitative verification of mathematical models.

The paper proposes a method for determining the boundaries of flashback when using methane-hydrogen fuel, the use of which reduces the error in predicting flashback from 40-50% to 5% in burner devices of combustion chambers of gas turbine engines and power plants. A kinetic mechanism for the oxidation of methane-hydrogen fuel has also been developed, which makes it possible to simulate the laminar flame speed with higher accuracy in relation to the operating process parameters of the combustion chambers of aviation gas turbine engines and power plants, characterized by an additional set of elementary reactions and refined rate constants. New dependencies have been proposed that make it possible to simulate the laminar flame speed of a methane-hydrogen flame in relation to the operating process parameters of the combustion chambers of aviation gas turbine engines and power plants, differing by taking into account a wider range of temperatures, pressures, mixture composition and the type of fuel used. The paper presents the results of validation of the proposed method for determining the boundaries of flashback in a model combustion chamber, which is a prototype of the low-emission combustion chambers used with preliminary mixture preparation, as well as the combustion chamber of the GTE-65.

## **Acknowledgment**

The study was supported by the Russian Science Foundation, projects no. 22-79-10205, (<https://rscf.ru/project/22-79-10205/>).

# Mathematical and physical modeling of crown forest fires initiation and spread

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Forest fires are extremely complex and destructive natural phenomena which depend on availability of fuel, meteorological conditions and an initial ignition. The overall purpose of forest fires research is a better understanding of the phenomena so that firefighting techniques can be improved, controlled burnings can be undertaken with more confidence, and lives and property might be preserved. It is presented mathematical model of forest fire which is based on an analysis of known experimental data and using concept and methods from reactive media mechanics [1]. In this paper the theoretical investigation of the problems of crown forest fire initiation and spread in windy condition were carried out. It takes in to account the mutual interaction of the forest fires and atmosphere flows. It is assumed that the forest during a forest fire can be modeled as 1) a multi-phase, multistoried, spatially heterogeneous medium; 2) in the fire zone the forest is a porous-dispersed, two-temperature, single-velocity, reactive medium; 3) the forest canopy is supposed to be non-deformed medium (trunks, large branches, small twigs and needles), which affects only the magnitude of the force of resistance in the equation of conservation of momentum in the gas phase, i.e., the medium is assumed to be quasi-solid (almost non-deformable during wind gusts); 4) let there be a so-called “ventilated” forest massif, in which the volume of fractions of condensed forest fuel phases, consisting of dry organic matter, water in liquid state, solid pyrolysis products, and ash, can be neglected compared to the volume fraction of gas phase (components of air and gaseous pyrolysis products); 5) the flow has a developed turbulent nature and molecular transfer is neglected; 6) gaseous phase density doesn't depend on the pressure because of the low velocities of the flow in comparison with the velocity of the sound. The study is based on numerical solution of Reynolds equations for chemical components and equations of energy conservation for gaseous and condensed phases. The forest during a forest fire is modeled as a two-temperature multiphase non-deformable porous reactive medium. A discrete analog for the system of equations was obtained by means of the control volume method [2]. The model proposed in the article gives a detailed picture of changes in temperature fields and concentrations of components over time, and also determines the influence of various conditions on the spread of a crown forest fire with a non-uniform distribution of reserves of forest combustible materials and their moisture content. The results of calculation of the rate of crown forest fire spread obtained agree with the laws of physics and experimental data for the cases when the forest fire spread through the crowns of forest under the influence of wind. The results of calculation give an opportunity to evaluate critical condition of the crown forest fire initiation and spread, which allows applying the given model for preventing fires.

This work was supported by the Russian Science Foundation (Grant No. 24-21-00069).

## References

1. A.M. Grishin, *Mathematical Modeling Forest Fire and New Methods Fighting Them*, Tomsk: Publishing House of Tomsk University (Russia), 1997.
2. S.V. Patankar S.V., *Numerical Heat Transfer and Fluid Flow*. New York, Hemisphere Publishing Corporation, 1981.



# Investigation of the soot growth process in a flame by the 2D-LII method

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Knowledge about the mechanisms of formation and properties of polycyclic aromatic hydrocarbons (PAHs) and ultrafine ( $\leq 5$  nm) carbon nanoparticles or precursors of soot particles with sizes smaller than ordinary soot (10-50 nm) contained in the exhaust of internal combustion and jet engines is necessary for reducing harmful emissions during combustion processes. Taking into account the absorption and emission of radiation by such particles allows to determine their contribution to the thermal balance of the atmosphere, which affects climate change. Monitoring the number of such compounds per unit volume of air allows to assess the danger to human health due to their carcinogenic properties. Also, 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 ultrafine carbon nanoparticles which are practically transparent to visible radiation.

One of the useful methods in this field is the well-known and widely used laser-induced incandescence (LII) method. Two-dimensional laser-induced incandescence (2D-LII) and time-resolved laser-induced incandescence (TiRe-LII) methods are the promising laser-optical methods for studying the soot precursors formed below the soot formation flame region. In this study the results of 2D-LII and TiRe-LII methods implementation for the investigation of the early stages of the soot particles formation and growth during the hydrocarbons combustion are presented.

The laminar flat premixed flame was stabilized with a kinetic McKenna type burner, which allows to form a flame with horizontally uniform parameters. To verify this fact, vertical and radial temperature measurements were carried out using ultrathin type B thermocouples. The combustion of ethylene – air ( $\varphi = 2.1$ ,  $C/O = 0.7$ ) and acetylene – air ( $\varphi = 1.8$ ,  $C/O = 0.72$ ) mixtures was investigated.

Using a composition of cylindrical lenses the beam of a nanosecond Nd:YAG laser at the first harmonic (1064 nm) was deployed in a vertical laser plane along the height of the burner to heat the entire central section of the flame and obtain a height- and width-distributed incandescence signals from laser-heated carbon particles on the nanosecond ICCD camera K018UV. The camera shot was synchronized with the laser pulse using a pulse/delay generator. The laser beam size was 0.7 mm x 15 mm, energy density was maintained at  $\sim 0.15 - 0.2$  J/cm<sup>2</sup>. Laser beam profiles were obtained using BEAMAGE-4M beam profiler. A comprehensive camera setup was carried out to register the emission of ultrafine soot particles and their precursors in the flame in the visible spectrum. Using narrowband filters, diagnostics was configured in the wavelength ranges corresponding to the most intense radiation of ultrafine carbon nanoparticles in accordance with the Swan bands.

As a result of the conducted research, vertical and radial temperature profiles of the studied flames were obtained. Spatially and time resolved flame particles incandescence signals were carried out using 2D-LII and TiRe-LII methods. The profiles of the volume fraction of the studied particles were calculated from the obtained ICCD images of the flame using a LII mathematical model. The calculations of the sizes of the studied particles based on the attenuation of the incandescence signals were started.

This study was funded by RSF, project No. 23-19-00407.

# **The dynamics of sulfur compounds release investigation at combustion and its absorption by the calcium-based additives**

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Currently, coal is still one of the main types of fuel. The significant disadvantages of coal as a fuel is the sulfur presence, mainly in the form of sulfides: pyrite ( $\text{FeS}_2$ ), as well as chalcopyrite ( $\text{CuFeS}_2$ ) and marcasite (iron polysulfide,  $\text{FeS}_2$ ). When such coals are burning, hydrogen sulfide, sulfur dioxide and carbon dioxide are formed, and harm the environment when they entering in the gas phase. Taking into account the volume of coal processed annually, it is necessary to take measures to reduce emissions of sulfur-containing gases.

The aim of the work is to determine the ability of marble in direct contact with sulfurous brown coal to absorb sulfur compounds released as coal burns out, as well as the residual sulfur content in the continuation of coal combustion, and the dynamics of the release of sulfur compounds into the gas phase in processes of combustion are studied.

Eight cuvettes were simultaneously loaded into the furnace, at the bottom of which particles of Tula coal were filled in, on top of which a layer of marble particles was poured (in a mass ratio of 1:1). The particle mass of both coal and marble was the same, and was 10.0 g. The average particle size of coal and marble was 5 mm.

The studied samples were heated from room temperature to 1200°C. During heating, when the temperature reached 500°C, the first cuvette was removed, and then, after heating the furnace, the next cuvette was removed for every 100°C. After cooling, the particles of calcined marble and unburned coal were separated from each other and given for analysis.

When particles of sulfurous brown coal and marble particles filled on top of it burn in a cuvette, as the coal burns, the proportion of sulfur contained in it decreases almost linearly, and the proportion of sulfur absorbed by marble and its output into gaseous products increases.

The chemical composition of marble are also have changes with heating and combustion of coal. At temperatures of 500 – 800°C, the decomposition of  $\text{CaCO}_3$  practically does not occur, sulfur is mainly absorbed as  $\text{CaS}$ . Active decomposition of  $\text{CaCO}_3$  begins at temperatures of 800 – 1000°C, and is almost completely completed at 1000 – 1200°C. After burning of loading in layers coal and marble particles in the furnace, the marble was mainly converted into  $\text{CaO}$  (and some sufficient amount of  $\text{CaCO}_3$ ) and  $\text{CaS}$ .

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.

This work funded by the Ministry of Science and Higher Education of Russian Federation, theme #FFSG-2024-0016.

# Thermal decomposition of sulfur brown coal at different heating rates

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Despite the fact that coal is one of the "dirtiest" fuels, its use in energy and other industries is gradually increasing [1]. In this regard, it becomes very relevant to search for methods of using coal with minimal damage to the environment.

The purpose of the work is to study the sulfur content in solid products under various modes of heat treatment of sulfurous brown coals. The object of the study was the sulfurous brown coal of the Moscow basin, characterized by a predominance of sulfide sulfur in the form of pyrite ( $\text{FeS}_2$ ), chalcopyrite ( $\text{CuFeS}_2$ ) and marcasite (polysulfide of iron,  $\text{FeS}_2$ ).

The experiments were carried out in a muffle electric furnace. Coal particles weighing 25.0 g were suspended in the furnace, the particle size was 1.5, 2.5 and 5.0 mm. Rapid heating was carried out in the temperature range from 500 to 1200°C with a holding time at a given temperature for 15 seconds. With gradual heating, the samples were simultaneously placed inside the furnace and heated from room temperature to 1200°C. When the required temperature is achieved, one of the samples was removed from the furnace, cooled and weighed, then given for elemental analysis.

Experiments are shown that at rapid heating of coal, dehydration and carbonation processes mainly occur. The sulfur contained in the coal remains almost completely in the solid residue.

At the gradual heating from 300 to 900°C, pyrolysis processes are mainly carried out, and intensive release of volatiles are occurred. At a temperature of 900°C, carbonation is almost completely completed. In the temperature range from 900 to 1200°C, the oxidation of the coke residue occurs at a constant rate. The sulfur content in the solid residue is determined by the temperature and intensity of oxidation of the organic mass of coal. The best temperature conditions for the thermal processing of this coal is the range of 1000-1200°C, this regime makes possible to burn the carbon contained in the coal, but does not lead to complete combustion of the sulfur-containing compounds contained in the one.

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.

This work funded by the Ministry of Science and Higher Education of Russian Federation, theme #FFSG-2024-0016.

## References

1. Russia's Energy strategy for the period up to 2035 / <https://minenergo.gov.ru/node/18038>, 09.06.2020.

# Gas-phase Formation of Phenanthrene and Dibenzofulvene via the Reaction of Fluorenyl and Methyl Radicals

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It is known that Polycyclic Aromatic Hydrocarbons (PAH) are products of fossil fuels combustion processes, which, in turn, leads to the formation of soot. Methyl (CH<sub>3</sub>) plays an important role in the formation of cyclic aromatic compounds by interacting with monocyclic and polycyclic hydrocarbon radicals, including fluorenyl (C<sub>13</sub>H<sub>9</sub>). Early studies of the reaction of methyl with carbocyclic compound cyclopentadienyl (C<sub>5</sub>H<sub>5</sub>) [1,2] showed that the resulting compound would be benzene (C<sub>6</sub>H<sub>6</sub>) or fulvene (C<sub>6</sub>H<sub>6</sub>), confirming the significant role of methyl in the development of five-membered rings.

The current study examines the formation of tricyclic polycyclic aromatic hydrocarbons (PAHs) in the reaction between methyl and fluorene. The initial addition of radicals results in the formation of various complexes, with relative energies of -71.3 kcal/mol and -40.4 kcal/mol, for compounds connected at C-1 (i1) and C-3 (i1\_1), respectively. After the separation of atomic hydrogen, isomerization of the subsequent complexes leads to various three-ring isomers, such as C<sub>14</sub>H<sub>10</sub>, through an intermediate pathway (i1). This pathway produces basic products such as dibenzofulvene (at 53.9 kcal/mol), phenanthrene (at 39.5 kcal/mol), and 1-methylidenfluorene (at 76.4 kcal/mol). After calculating kinetics for this pathway, dibenzofulvene was found to be the most advantageous product, under all conditions considered. The less favorable pathway for the i3 complex results in products such as anthracene at 45.0 kcal/mol, benzoazulene at 74.3 kcal/mol, and 3-methylidenfluorene at 72.5 kcal/mol. These products are least profitable and have low branching coefficients, indicating their possible formation only under high temperatures and pressures.

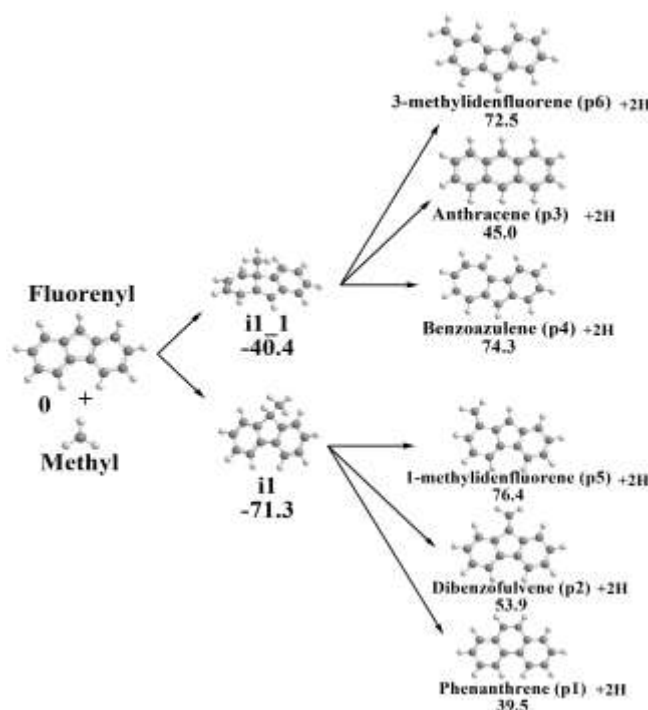


Fig. 1. Schematic diagram of the reaction between methyl and fluorenyl radicals

## References

1. S. Sharma, W.H. Green. *J. Phys. Chem. A*. **2009**, 113, 8871.
2. V.S. Krasnoukhov, D.P. Porfiriev, I.P. Zavershinskiy, V.N. Azyazov, A.M. Mebel. *J. Phys. Chem. A*. **2017**, 121(48), 9191.

# The methylidyne radical with the benzonitrile reaction potential energies and molecular parameters

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The reaction of the methylidyne (CH) radical with benzonitrile (C<sub>6</sub>H<sub>5</sub>CN) molecule was studied at a collision energy of 5.0 kJ/mol with ab initio calculations of the potential energy surface (PES). At low temperatures in deep space, a large amount of nitriles are present in the atmosphere of Saturn's moon Titan [1, 2], as well as in interstellar molecular clouds. Reactions of nitriles with the methine radical CH are of interest, as potential initial step in the study of biological molecules. In particular, in the course of the reaction with cyanide molecules, a nitrogenous base, structural blocks in DNA chains, can be formed. In addition, the formation of linear and cyclic radicals is possible with the release of the corresponding products: atoms, molecular particles, ethylene, etc.

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

Those results were utilized in Rice–Ramsperger–Kassel–Marcus calculations of the product branching ratios at the zero pressure limit – common approach in modelling of the cold molecular clouds chemistry. Mechanism identified emphasizes importance of the CH+C<sub>6</sub>H<sub>5</sub>CN reaction as an important supplier of the initial bricks for building heterocyclic hydrocarbons in extreme environments.

## References

1. R.I. Kaiser, A.M. Mebel, V.V. Kislov, et al., *Astrophysical journal.*, **2009**, 701, 2
2. X.Gu, Y.S. Kim, R.I. Kaiser, A.M. Mebel, et al., *Proceedings of the National Academy of Sciences of the United States of America*, **2009**, 106, 38
3. D. Xu, D. Li, *Astrophysical journal.*, **2016**, 833, 90.
4. Adler, T.B., *The Journal of Chemical Physics*, **2007**, 127, 22.
5. Knizia, G., *The Journal of Chemical Physics*, **2009**, 130, 5.
6. Chai, J.-D., *Physical Chemistry Chemical Physics.*, **2008**, 10.
7. J.-D. Chai, M. Head-Gordon, *Physics Chemical Journal.*, **2008**, 128.
8. Marcus, R.A., *Philosophical Transactions of the Royal Society of London. Series A: Physical and Engineering Sciences.* – **1990**, 332.
9. P. J. Robinson, K. A. Holbrook, «Unimolecular Reactions», Wiley: New York, **1972**.



# Energy-saturated materials based on silicon and halogen-containing polymers

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The purpose of this study was to study the combustion process of highly dispersed silicon powder in a mixture with various fluorine-chlorine-containing polymers (fluoroplastics F-4, F-40, F-42, F-3, F-32) depending on the ratio of the components. Thermodynamic calculations were carried out using the TERMPS program and experimental studies of compacted samples were carried out when the fuel content varied from 10 to 90% wt. with determination of burning time and energy illumination in the wavelength range of 0.5-20 microns.

Industrial silicon powder of the Kr-1 brand, with an average particle size of 16-19 microns, was used as fuel. The preparation of the compositions was carried out according to the methodology accepted in the pyrotechnic industry. The samples were molded using the method of blind pressing on a PSU-50A hydraulic press in accordance with GOST 310-60 at a pressure of 100 MPa in a press tool with a diameter of 16.2 mm without a shell. The samples were tested in a vertical combustion chamber without air blowing.

Based on the results of thermodynamic calculations, it was established that the highest combustion temperatures are achieved with a silicon content of 20-25% wt. for systems with F-3, F-32, F-4 and 5-10% wt. silicon content for systems with F-40, F-42 in the case of using the mixture's own oxidizing elements. With the additional participation of an oxidizing agent, the combustion temperature increases over the entire range of changes in fuel concentration, with a sharp rise observed in the silicon content range of 10-30% wt. It should be noted that the highest combustion temperature is achieved for the silicon system with F-4. Among the condensed combustion products are carbon, silicon carbide and unburned silicon, which are formed by the interaction of reagents without the participation of the environment; silicon dioxide formed with the additional participation of the environment. The amount of a particular product depends on the silicon content in the pyrotechnic composition. Also among the combustion products there are substances in a gaseous state, fluorides and chlorides of silicon, oxides of carbon, and hydrogen in the case when atmospheric oxygen takes part in the chemical interaction.

As a result of experimental studies, an extreme dependence of combustion parameters with maximum values of linear combustion rate (1.8-3.0 mm/s) and energy illumination (180-380 W/m<sup>2</sup>) was established at a fuel content of about 50 wt. percent. Concentration limits of flammability are 30-80% by weight fuel content. Within these limits, stable combustion is maintained, while the compaction coefficient becomes smaller with increasing silicon content. The highest values of irradiance are achieved for silicon systems with F-4 and F-40 and amount to 360-380 W/m<sup>2</sup>. The nature of the resulting solid combustion products depends on the ratio of the components. Up to a fuel content of 50% wt. during combustion, sooty combustion products are intensively formed. Microscopic analysis of these products showed that they are thread-like formations. Further, when the silicon content increases to more than 50% wt. the amount of soot combustion products is reduced. A solid combustion product is formed in the form of regular rings.

It should be noted that pyrotechnic compositions based on silicon and fluoropolymers burn in the spin mode, in which a small luminous spot appears on the surface of a cylindrical sample, moving in a spiral along the outer part of the sample.



# Measuring gas temperature in Ar-He plasma using diode laser absorption spectroscopy

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An optically pumped rare gas laser (OPRGL) is a new laser system that converts the radiation from laser diodes into high-power radiation with a quality close to the diffraction limit. In order to determine the limiting characteristics and optimal operating modes of the OPRGL, it is necessary to create a mathematical model of the active medium. The construction of such a model is complicated by the lack of data on the rate constants of processes involving metastable atoms of heavy rare gases. The operating pressure of the OPRGL is of the order of atmosphere, leading to elevated gas temperatures in the plasma. In view of this, it is necessary to know the temperature dependence of these constants in order to construct an OPRGL model. Therefore, the measurement of the rate constants must be accompanied by the measurement of the gas temperature in the plasma, which is the goal of our work.

In the experiment, the production of metastable argon atoms  $1s_5$  was carried out in a pulse-periodic discharge ignited between a pair of titanium electrodes located inside the discharge chamber.

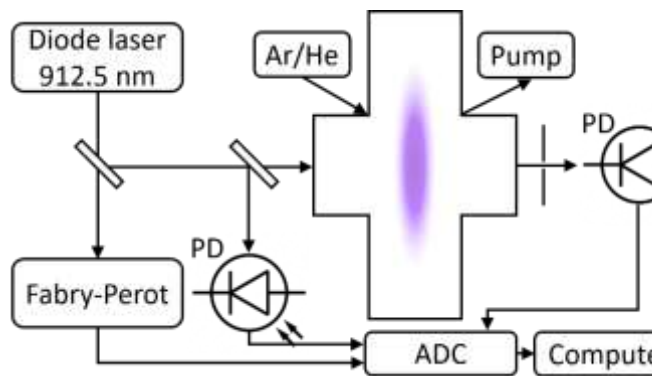


Figure 1 – Experiment scheme

Radiation from a tunable diode laser with a wavelength of about 912.3 nm was introduced into the interelectrode space. In front of the camera, the beam was split and entered the reference channel and the Fabry-Perot interferometer. In the signal channel, the power of the laser beam passing through the plasma was measured as a function of time. The time scale was converted to a

frequency scale using a Fabry-Perot interferometer.

Approximation of the experimental absorption line by the Voigt profile using the Levenberg-Marquardt algorithm allowed the determination of the full width at half maximum (FWHM). The Voigt contour is a convolution of the Gaussian and Lorentz functions, and the dependence of the FWHM of the Voigt profile on temperature and pressure is determined by the expressions:

$$\begin{aligned} \text{FWHM} &= 0.5346 * \text{WL} + \sqrt{0.2166 * \text{WL}^2 + \text{WG}^2}, \\ \text{WL} &= 2 * 3.22 * p * \xi * (T/300)^{-0.7} * 0.001 + \text{WL}_{\text{las}}, \\ \text{WG} &= \text{WG}_{300} \sqrt{T/300}, \end{aligned}$$

where  $p$  is the pressure in Torr,  $\xi$  is the collisional broadening coefficient,  $\text{WL}_{\text{las}}$  is the laser spectral linewidth,  $\text{WG}_{300}$  is the Gaussian broadening at 300 K. A comparison of the experimental FWHM and that calculated using the formula made it possible to determine the gas temperature in the plasma.

The report will present the results of temperature measurements at various experimental parameters.

# Theoretical study of 1-acenaphthyl oxidation with molecular oxygen

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A pressing issue is the formation of soot and polycyclic aromatic hydrocarbons (PAHs) during incomplete combustion of hydrocarbon fuels, since they are chemical compounds harmful to humans and the environment [1,2]. Reducing unwanted emissions is possible by switching to cleaner and more efficient fuel combustion systems. Designing such equipment requires the use of more advanced kinetic models of PAH oxidation, since large PAH molecules are used as model molecules in studies of chemical interactions on soot [3–6].

Previous theoretical [7] and experimental works [8] have determined that acenaphthylene occupies an important place in the mechanism of PAH and soot growth according to HACA. Further studies [9, 10] have shown that, due to the peculiarities of the edge structure, the rate constants of addition to the five-membered ring of acenaphthylene are the highest. The latter circumstance has created interest in studying the mechanism of oxidation of 1-acenaphthyl by molecular oxygen.

Molecular parameters and relative energies were obtained using the composite calculation scheme G3(MP2,CC)//B3LYP/6-311G(d,p), providing chemical accuracy. The connectivity of the stationary states through the corresponding transition states was confirmed by IRC calculations. The values of the rate constants and relative yields of the reaction products were calculated for different conditions within the RRKM-ME theory with kinetic accuracy.

Potential energy surface (PES) analysis revealed that the most energetically favorable reaction channels are those leading to O atom abstraction and CO abstraction. The reaction kinetics and relative yields were studied for the 0.01-100 atm pressure range and 500–2500 K temperature range. Competitive behavior of the reaction products was found at low pressure. At high temperatures and low pressures, the O abstraction channel dominates, while at low temperatures and pressures, the CO abstraction channel dominates. The relative yields of the products are equal at a temperature of  $\approx 77$  K.

This work was supported by the Ministry of Higher Education and Science of the Russian Federation under Grant No. 075-15-2021-597 "Origin and evolution of organic molecules in our Galaxy".

## References

1. H. N. Sharma et al., *Energy & Fuels* **2012**, 26, 9.
2. A. Raj, G. R. da Silva, S. H. Chung, *Combustion and flame* **2012**, 159, 11.
3. K. Sendt, B. S. Haynes, *Combustion and flame* **2005**, 143, 4.
4. M. S. Celnik et al. *Proceedings of the Combustion Institute* **2009**, 32, 1.
5. M. Frenklach et al. *Symposium (International) on Combustion* **1985**, 20, 1.
6. M. Frenklach *Physical chemistry chemical Physics* **2002**, 4, 11.
7. V. V. Kislov, A. I. Sadovnikov, A. M. Mebel *The Journal of Physical Chemistry A* **2013**, 117, 23.
8. D. S. N. Parker et al. *Angewandte Chemie International Edition* **2015**, 54, 18.
9. P. Liu et al. *Combustion and Flame* **2019**, 199.
10. P. Liu, Z. Li, W. L. Roberts *Combustion and Flame* **2021**, 230.

# **Solid-phase extraction of synthetic dyes from wastewater and their analysis by HPLC**

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The analysis of synthetic dyes in wastewater is an urgent task of modern analytical chemistry, since an increased content of dyes in wastewater can have a negative impact on the environment. To monitor the content of dyes in various objects, reverse-phase high-performance liquid chromatography (RP HPLC) is often used, which allows one to reliably determine the content of substances of interest.

The purpose of this work was to create and evaluate the metrological characteristics of a method for analyzing synthetic dyes in wastewater from enterprises with a high content of inorganic salts. The chromatographic system used in this work consisted of a high-pressure pump manufactured by Knauer, separation was carried out on a Kromasil 100-5-C18(w) reverse-phase column (4.6 × 250 mm) in gradient elution mode. Acetonitrile and ammonium acetate solution were used as the mobile phase. Detection of synthetic dyes was carried out using an Azura diode array detector.

The paper presents the results of concentrating 10 synthetic dyes on commercially available solid-phase extraction cartridges, which are suitable for working with aqueous solutions with a high content of inorganic salts. For each substance, the degree of concentration from distilled and model wastewater was calculated, which varies from 2 to 98%. The highest degree of concentration of the analyzed cartridges when operating in conditions close to real wastewater was shown by the “Diapak P” cartridge, with a pH of the concentrated solution equal to 4. Based on the results of this work, a method for the simultaneous determination of 10 synthetic food colors (SFC) (E102, E104, E110, E122, E124, E129, E131, E133, E142, E151) in aqueous and organic solutions.

The results of the work may be useful in the field of analytical monitoring of the content of synthetic dyes in wastewater from enterprises. The intermediate precision limit of the technique did not exceed 5%, and the expanded measurement uncertainty was less than 10%.

# Ignition of coal microparticles by continuous laser radiation of various wavelengths

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Bituminous coals are one of the main energy sources for thermal power engineering. In this regard, improving coal combustion methods with the highest efficiency and the least damage to the environment is an urgent task.

For practical application research using relatively inexpensive continuous-wave semiconductor lasers is of the greatest interest. In this work, we studied the ignition of widely used coal grades B (brown or lignite), DG (long-flame gas or high volatile C bituminous coal), G (gas or high volatile B bituminous coal), Zh (fat or high volatile A bituminous coal), K (coke or medium volatile bituminous coal) and A (anthracite) using radiation from continuous-wave semiconductor lasers with lengths waves  $\lambda_1 = 450$  nm and  $\lambda_2 = 808$  nm with adjustable radiation power up to 10 W and 20 W, respectively.

Coal particles with a granulometric distribution of  $0.5 \div 63$   $\mu\text{m}$  were used. A considerable number of particles is contained in the range of  $10 \div 40$   $\mu\text{m}$ , the maximum distribution is at 20  $\mu\text{m}$ . The experiments used samples of bulk density with  $\rho = 0.4$   $\text{g}/\text{cm}^3$ , which were placed in a copper holder with a diameter of 5 mm and a depth of 2 mm.

A study of the kinetic characteristics of coal microparticles ignition was carried out during exposure to laser radiation lasting 1 second at wavelengths  $\lambda_1 = 450$  nm and  $\lambda_2 = 808$  nm. The ignition delay times  $t_z$  were measured depending on the radiation power density  $W_p$  and the critical values of the ignition energy density of pulverized coal fuel samples were determined.

The process of laser ignition of microparticles of pulverized coal fuel has statistical nature. This is manifested both in the statistics of the sample ignition delay time  $t_z$  at a fixed radiation power, and in the probabilistic nature of the critical density of the laser radiation power  $W_{cr}$  required for sample ignition. For a fixed wavelength of laser radiation the energy consumption  $E_{cr}$  for ignition increases with the rise of coalification degree in the studied grades of coal. The energy consumption for igniting of each type of coal is less when using radiation with  $\lambda_1 = 450$  nm than radiation with  $\lambda_2 = 808$  nm. Interpretations of the results are given according to concepts obtained using pulsed laser ignition of coals.

The research was carried out through a grant from the Russian Science Foundation No. 22-13-20041, <https://rscf.ru/project/22-13-20041/> and through a grant from the Kemerovo Region - Kuzbass (agreement with No. 2 dated 03/22/2022).

# **Numerical and experimental study of NO<sub>x</sub> formation during hydrogen combustion in a model combustion chamber with a cluster microflame burner device**

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At present, atmospheric pollution by nitrogen oxides NO<sub>x</sub>, which are formed in the combustion chambers of gas turbine engines and power plants, is a serious environmental problem. In addition, reducing greenhouse gas emissions (or carbon footprint) to combat global climate change has become a relevant issue in recent years. And while ultra-lean premixed combustion technologies are used to address the issue of reducing nitrogen oxide emissions, fuels with lower carbon content must be used to reduce the carbon footprint. An alternative fuel that does not contain C atoms is hydrogen. The use of hydrogen as a fuel in traditional combustion chambers with burner devices providing combustion in a swirling flow is impossible due to the high probability of flame flashback upstream, as well as the occurrence of gas auto oscillations in the combustion chamber. This is due to the fact that the combustion process of hydrogen is different from that of methane due to the large difference in physical and chemical properties (calorific value, rate of chemical reactions, etc.).

Research shows that with a high hydrogen content in the fuel, a transition to a fundamentally different design of the burner device is necessary (BD). An example of such a device is the so-called cluster microflame burner. The cluster microflame BD concept is based on the integration of two key technologies: low NO<sub>x</sub> combustion and flame flashback-resistant combustion. Low NO<sub>x</sub> emissions are ensured by intensive mixing of fuel and air using a coaxial jet system. Each coaxial jet consists of a central fuel jet surrounded by an annular air stream. Immediately after the coaxial jet exits the perforated plate orifice, a high level of turbulence is generated in the jet due to abrupt expansion and interaction with adjacent jets. In this way, rapid mixing of fuel and air is ensured, which creates conditions for organizing a combustion process with low NO<sub>x</sub> content by reducing the volume of high-temperature zones.

The aim of this work is to conduct experimental studies of hydrogen combustion in a model combustion chamber with a cluster microflame BD developed at Samara University to estimate the level of nitrogen oxides emission, as well as to develop a methodology for numerical modelling of hydrogen combustion and validation of the developed mathematical model.

## **Acknowledgment**

The study was supported by the Russian Science Foundation, projects no. 22-79-10205, (<https://rscf.ru/project/22-79-10205/>).

# Gas-phase synthesis of phenylacetylene in the reaction of 1,3-butadiene with the butadiynyl radical

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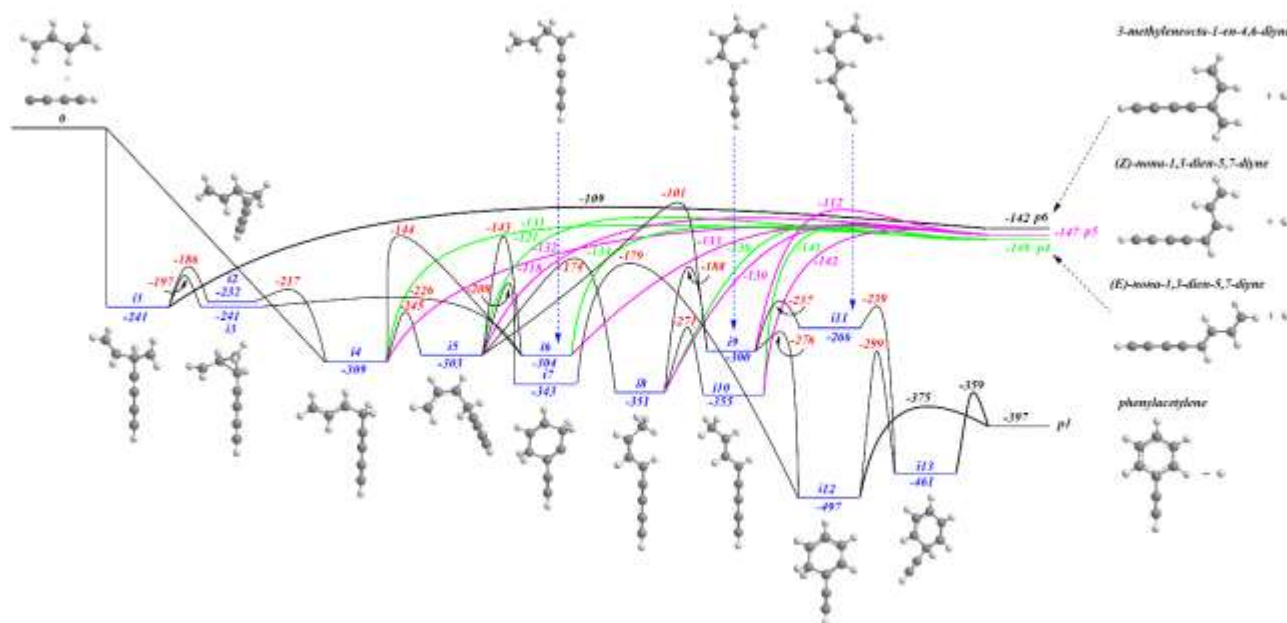
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Up to 20% of the interstellar carbon store is considered to be concentrated in polycyclic aromatic hydrocarbons (PAHs) – molecules containing multiple fused aromatic rings – along with their protonated, ionised, (de)hydrogenated, alkylated, and nitrogen-substituted derivatives [1].

The formation of alkylated PAHs is even less understood. Alkylated aromatics such as methylphenanthrene (C<sub>15</sub>H<sub>12</sub>), methyltriphenylene (C<sub>19</sub>H<sub>14</sub>), methyl-, dimethyl-, and trimethylnaphtalene (C<sub>11</sub>H<sub>10</sub>, C<sub>12</sub>H<sub>12</sub>, C<sub>13</sub>H<sub>14</sub>) were detected in carbonaceous chondrites such as Murchison, Allende, Aguas, Zarcas, Mukundpura, and Kolang. A recent study [2] has shown the formation of isomers of the simplest dimethyl-substituted benzene – xylenes.



This study is devoted to the investigation of the formation of an even more exotic type of cyclic aromatic hydrocarbons, alkynylated cyclic aromatic hydrocarbons [3]. These include, for example, phenylacetylene. It was found that during the reaction of the 1,3-butadiene molecule with the butadienyl radical, phenylacetylene is formed with a fairly large branching ratio. Fig. 1 shows the main diagram of the potential energy surface (PES) of the reaction of 1,3-butadiene and butadienyl radical, obtained on the basis of the analysis of the RRKM calculations.

## References

1. I.A. Medvedkov, A.A. Nikolayev, C. He, Z. Yang, A.M. Mebel, R.I. Kaiser, *Molecular Physics*. **2023**, 122(7-8), e2234509.
2. I.A. Medvedkov, A.A. Nikolayev, C. He, Z. Yang, A.M. Mebel, R.I. Kaiser, *Angew. Chem. Int. Ed.* **2024**, 63(5), e202315147.
3. G.R. Kiel, H.M. Bergman, T.D. Tilley, *Chemical science*. **2020**, 11(11), 3028.



# Ignition of microparticles of coals of different ash content by laser pulses

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Coal fuel is widely used in thermal power engineering. The development of methods for igniting fuel using laser radiation will eliminate the use of fuel oil for these purposes, that gives an economic and environmental effect. An adequate description of the laser action mechanism on coal particles does not currently exist. Therefore, it is necessary to obtain more experimental materials, including the study of various brands of coals and their ignition processes in the time interval of  $10^{-8}$ - $10^{-3}$  s.

The effect of ash content on the coals laser ignition characteristics is of interest. High ash content has an adverse effect on the calorific value [1] and also causes structural elements erosion of coal furnaces and environmental pollution [2].

In this work we conducted studies of laser ignition of brown (or lignite) coal microparticles using samples with bulk density  $\rho = 0.5 \text{ g/cm}^3$  before demineralization (original) with an ash content of 10.1% and after demineralization with an ash content of 0.5%. The kinetic and energy characteristics of ignition at various stages when exposed to pulsed laser radiation ( $\lambda = 1064 \text{ nm}$ ,  $120 \mu\text{s}$ ) were determined.

The energy characteristics of the ignition of brown coal microparticles with different ash contents under the influence of a continuous laser with a radiation wavelength of  $\lambda = 808 \text{ nm}$  were measured. A comparison of the results of the ash content influence was made when exposed to pulsed and continuous laser radiation on microparticles of brown coal. Thermogravimetric measurements of the studied samples were carried out.

In a demineralized sample exposed to laser pulses of different energy densities  $H$ , the same ignition stages are observed as in the original sample but the energy characteristics change. At the stage of release and ignition of volatile substances  $\tau = 1 \div 5 \text{ ms}$ , the critical ignition energy density  $H = 1.9 \text{ J/cm}^2$  for the original sample and  $H = 2.8 \text{ J/cm}^2$  for the demineralized one. At the stage of ignition of the nonvolatile residue  $\tau = 10 \div 50 \text{ ms}$ , the critical energy density is  $H = 2.3 \text{ J/cm}^2$  for the original sample and  $H = 5.4 \text{ J/cm}^2$  for the demineralized one. When samples are exposed to continuous laser radiation, the same patterns are observed as during pulsed irradiation. The absorbed radiation energy density required to ignite the initial sample is  $E = 31.5 \text{ J/cm}^3$ , for the demineralized sample  $E = 51.4 \text{ J/cm}^3$ . The results of measuring the energy characteristics of laser ignition, thermogravimetric measurements during heating at a rate of  $10 \text{ }^\circ\text{C/min}$  of initial and demineralized samples, as well as measuring the amount of burnt masses of samples under laser irradiation with the same doses allow us to draw a conclusion about the catalytic effect of the mineral part of coal particles on the burnout rate.

The research was carried out through a grant from the Russian Science Foundation No. 22-13-20041, <https://rscf.ru/project/22-13-20041/> and through a grant from the Kemerovo Region - Kuzbass (agreement with No. 2 dated 03/22/2022).

## References

1. Filippenko Yu.N., Rudavina E.V., Chernyavskiy N.V., *Modern sci.: Researches, Ideas, Results, Technologies*. **2010**, 1(3), 44-47.
2. Alekhovich A.N. // *Energetik*. 2008, 3, 8-12.

# The effect of N<sub>2</sub> presence on the interstellar ice analogs infrared spectra

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Surfaces of interstellar dust grains are the place, where plenty of the chemical reactions occurs in cold and dark interstellar clouds. Molecules freeze out on this surfaces or form on them from separate atoms or radicals. Observing the chemical composition of interstellar ices that consist of those molecules is very helpful in the determination of evolutionary paths for different types of clouds. Additionally, interstellar complex organic molecules can be formed efficiently in interstellar ices. Owing to space telescopes, IR spectra of dust and its ice mantles can be received and interpreted in accordance with laboratory experiments [1].

The observed bulk of interstellar ice consists of H<sub>2</sub>O, CO, CO<sub>2</sub>, CH<sub>3</sub>OH, NH<sub>3</sub>, CH<sub>4</sub> [1]. The presence of the molecules, which cannot be observed in infrared light and radio quiet at the same time, such as N<sub>2</sub>, H<sub>2</sub>, O<sub>2</sub> is also predicted [1, 2, 3].

N<sub>2</sub> in the gas phase is an infrared and radio inactive molecule. Despite this fact, there are still both direct and indirect ways, which allow to observe N<sub>2</sub> on the surface of dust grains. The most important is affecting an absorption feature of another molecules [4]. Also, N<sub>2</sub> can be found by its own infrared absorption features in condensed phase [5] due to small dipole induced by neighbouring molecules. It is supposed that upper limit of icy N<sub>2</sub> abundance relative to H<sub>2</sub>O ice is 70 % along lines of sight toward background stars and 30 % for embedded sources [5].

In our study, we present the first systematic research of N<sub>2</sub> in astronomically relevant environments. It consists of binary ice mixtures with such compounds as H<sub>2</sub>O, CO<sub>2</sub>, CO, CH<sub>4</sub>, CH<sub>3</sub>OH with N<sub>2</sub> abundance 5, 10, 20 and 40 % relative to the main component. Binary mixtures were made to verify the reproducibility of our experimental data with those received by Ehrenfreund and others for CO and CO<sub>2</sub> [4]. For the first time the effect of N<sub>2</sub> presence on the H<sub>2</sub>O infrared spectrum, CO<sub>2</sub> bending mode are demonstrated and discussed. In addition, the effect of N<sub>2</sub> presence in seventh compound ice mixture is revealed. The composition of ice mixture is taken from fitting of James Webb Space Telescope infrared spectrum of Chamaeleon I performed by Dartois [6].

This research work is funded by the Russian Ministry of Science and Higher Education via the State Assignment Contract FEUZ-2020-0038 and the Russian Science Foundation via RNF 23-12-00315 agreement.

## References

1. A.C.A. Boogert, P.A. Gerakines, and D.C.B. Whittet, *Annu. Rev. Astron. Astrophys.*, **2015**, 53.
2. A.G.G.M. Tielens, *Rev. Mod. Phys.*, **2013**, 85, 3.
3. E.F. van Dishoeck, *Faraday Discuss.*, **2014**, 168.
4. P. Ehrenfreund, A.C.A. Boogert, P.A. Gerakines, A.G.G.M. Tielens, E.F. van Dishoeck, *Astron. Astrophys.*, **1997**, 328.
5. J. Elsila, L.J. Allamandola, S.A. Sandford, *Astrophys. J.*, **1997**, 479
6. Dartois E., Noble J.A., Caselli P. et al.. *Nat. Astron.* **2024**, 8.

# Study of clumps in atomic zones of photodissociation regions

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Photodissociation region (PDR) observations such as Orion Bar [1] or S187 [2] show that prolonged clumps can be formed in them. thermal PDR parameters can be described with the usage of generalised heat-loss function:

$$\mathfrak{S}(\rho, T) = \Lambda(\rho, T) - \Gamma(\rho, T), \quad (1)$$

where  $\Lambda(\rho, T)$  is the heating rate,  $\Gamma(\rho, T)$  is the cooling rate.

Heating and cooling misbalance may lead to the instabilities. One of these instability types is isentropic one [3]. This type of instability leads to amplitude growth of initial pressure disturbance which has occurred in the medium before. On the late evolution steps, the disturbance can assume the shape of shockwave pulse, which parameters are described only by (1) [4].

In this work, we have researched an evolution of initial disturbance which spreads in the isentropically unstable medium with the parameters of Orion Bar PDR. The view of function (1) and numeric parameters are taken from [5, 6]. Numerical modelling in the Athena MHD programming package [7] shows that regardless of the initial disturbance amplitude, the shockwave pulse reaches the amplitude predicted by analytical method [4, 8]. At the same time, the growth time of the pulse is influenced by the initial conditions: for initial low-density amplitudes (Fig. 1a), the growth time is about 40 thousand years, and for high-density amplitudes (Fig. 1b) it is 8 thousand years.

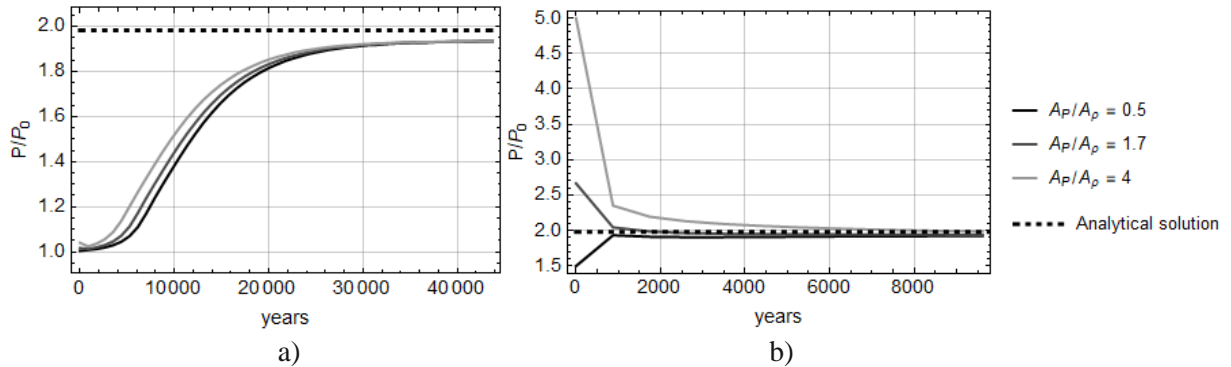


Fig. 1. Dependency of shockwave pressure amplitude on time with different values initial magnitude ratio  $A_p/A_p$ : a) with initial disturbance amplitude  $A_p = 0.1$ ; b) with initial disturbance amplitude  $A_p = 1$ .

The study was supported in part by the Ministry of Science and Higher Education of Russian Federation under State assignment to educational and research institutions under Project No. FSSS-2023-0009 and FFMR-2024-0017.

## References

1. E. Habart, R. Le Gal, C. Alvarez et al. *Astron. Astrophys.* **2023**, 673, A149.
2. P. Zemlyanukha, I.I. Zinchenko, E. Dombek et al. *Mon. Not. R. Astron. Soc.* **2022**, 515, 2445.
3. G.B. Field *Astrophys. J.* 1965, 142, 531.
4. N. Molevich, D. Riashchikov. *Phys. Fluids.* **2021**, 33, 076110.
5. K.V. Krasnobaev, R.R. Tagirova. *Mon. Not. R. Astron. Soc.* **2017**, 469, 1403.
6. C. Joblin, E. Bron, C. Pinto et al. *Astron. Astro-phys.* **2018**, 615, A129.
7. J.M. Stone, T.A. Gardiner. P. Teuben et al. *Astrophys. J. Suppl. Ser.* **2008**, 178, 137.
8. D.S. Riashchikov, I.A. Pomelnikov, N.E. Molevich. *Bull. Lebedev Phys. Inst.* **2022**, 49, 3

# Activation energy of lean methane-hydrogen-air mixtures

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In the modern world, pollution is seen to be an enormous problem, and other fuels, for instance, hydrogen, are considered to reduce the CO<sub>2</sub> emissions usually associated with hydrocarbons. However, hydrogen is very explosive and has high temperatures of combustion in air. Moreover, over the world there is developed infrastructure only in relation to natural fuels such as gasoline, natural gas, methane, and others. So, the next more convenient step towards the use of hydrogen could be a methane-hydrogen mixture.

Even though modern computational power gives the opportunities to undertake calculation within reduced and detailed reaction kinetics, the one-step reaction models are still of great interest in cases of complex reacting flows and geometries. In several papers, the parameters of one-step reaction models are selected so as to better describe the dependence of laminar burning velocity or the heat release rate on the parameters of a combustion system [1-3]. Despite the one-step reaction model is convenient and widespread for modelling combustion processes, selection of reaction rate parameters is opened.

In this work, the overall activation energy of the combustion of lean hydrogen–methane–air mixtures (equivalence ratio  $\varphi = 0.7$ – $1.0$  and hydrogen fraction in methane  $\alpha = 0, 2, 4$ ) is experimentally determined using thin-filament pyrometry of flames stabilized on a flat porous burner under normal conditions ( $p = 1$  bar,  $T = 20$  °C) [4, 5].

The experimental setup includes the flat porous burner which position can be regulated vertically, the gas mixture supplying system, thin filament made of silicon carbide (SiC) to measure the gas temperature, and the thermal imager OPTRIS PI. The flow rate of the gas can be adjusted by el-Flow controllers. By measuring the gas temperature dependence on the height above the burner, it is possible to determine the maximum flame temperature, which is close to the temperature of adiabatic combustion. According to the Arrhenius theory, changing the mass flow of the gas  $M$  and measuring the maximum temperature  $T$  it is possible to find the activation energy  $E_a$  for certain methane-hydrogen concentration in the mixture as a slope of the line.

As a result, it was found that the activation energy ( $E_a=256$  kJ/mol) is universal for investigated methane-hydrogen mixtures. Additionally, pre-exponent dependency of equivalence ratio was estimated that allows to create one-step reaction model based on experimental data, which provide the match with laminar flame velocity, calculated using models with detailed mechanisms for lean fuel mixtures.

## References

1. C. Westbrook, F. Dryer, *Combust. Sci. Technol.* 1981, 27, 31.
2. T. Coffee; A. Kotlar; M. Miller, *Combust. Flame.* 1983, 54, 155.
3. T. Coffee, A. Kotlar, M. Miller, *Combust. Flame.* 1984, 58, 59.
4. A. Moroshkina, A. Ponomareva, V. Mislavskii, E. Sereshchenko, V. Gubernov, V. Bykov, S. Minaev, *Fire.* 2024, 7, 42.
5. A. Moroshkina, A. Ponomareva, V. Mislavskii, E. Sereshchenko, V. Gubernov, V. Bykov, S. Minaev, *Combustion Theory and Modelling.* 2023, 27, 1.

# Thermodynamic assessment of the composition of mixed solid fuel for the gas generator of a high-speed flying vehicle

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The goal of the present study is to develop a method for calculating an energetically optimal ratio of the solid propellant and fuel in the low-temperature gas generator. A method is proposed for calculating the optimal ratio of the volume fractions of the solid propellant and solid fuel in the gas generator of a high-velocity flying vehicle. The self-burning solid propellant and gasified fuel are consecutively arranged in the charge of the gas generator. The ratio of the volumes of the solid propellant and fuel in the gas generator is determined by their physical and chemical properties. An increase in the density and heat of combustion of the solid propellant and also in the fuel porosity leads to reduction of the volume fraction of the solid propellant in the gas generator. An increase in the fuel density, specific heat, specific heat of sublimation, and temperature of sublimation of the fuel leads to an increase in the volume fraction of the solid propellant in the gas generator.

In the case of using such fuels as the lattice-type copolymer polymethylmethacrylate, cross-linked polystyrene, or hexamethylene, the required volume fraction of all considered solid propellants does not exceed 10%. In the case of cross-linked polyethylene used as a fuel, the volume fraction of the solid propellant is 20–30%. The minimum heat of combustion of the solid fuel in the gas generator with a total volume of 1 m<sup>3</sup> is observed for the lattice-type copolymer polymethylmethacrylate (approximately 20 000 MJ/m<sup>3</sup>) in combinations with all solid propellant types considered in the study. The maximum heat of combustion is obtained for cross-linked polystyrene (approximately 30 000–31 000 MJ/m<sup>3</sup>) in combinations with all solid propellant types. Thus, these compositions are optimal from the viewpoint of the energy performance among all compositions considered in the study.

Reduction of the solid fuel porosity leads to a linear increase in the volume fraction of the solid propellant and the total heat of solid fuel combustion. However, the solid fuel porosity cannot be reduced to zero because some porous space is needed for filtration of hot gases of solid propellant combustion.

This study was carried out as part of project no. 21-79-20008 of the Russian Science Foundation.

## References

1. M.V. Salganskaya, A.Yu. Zaichenko, D.N. Podlesniy, et al., *Acta Astronaut.* **2023**, 204, 682.



## Characteristics of algae biomass-derived biochars

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Marine macroalgae have high potential among renewable energy sources due to their rapid growth, efficient carbon dioxide absorption, and ability to avoid competing with farmland for limited space. The global production of macroalgae has been growing steadily each year at a rate of 10%, and currently amounts to approximately 36.9 wet metric tons worldwide. Meanwhile, the total value of the global algae production market is estimated to be around 11.8 billion US dollars.

Different types of biofuels can be produced through the thermal processing of algae biomass, including biogas (a mixture of hydrogen, methane and carbon oxides), bio-oil, and biochar. A variety of technologies can be used for these purposes, including gasification, pyrolysis, hydrothermal liquefaction, and other methods [1]. Various thermochemical conversion techniques employing different heating rates, such as pyrolysis, torrefaction and hydrothermal carbonation, are utilized in the manufacturing of biochars derived from biomass feedstocks like algae. The biochar output can find application as an energy source, in agriculture, for wastewater remediation of heavy metals, as well as other uses. The objective of this study is to experimentally investigate the production of biochars from algae biomass at different pyrolysis temperatures. It also aims to analyze the elemental composition and characteristics of the biochars produced.

Biochars were produced through the pyrolysis of algae under inert atmospheric conditions at different temperatures in a laboratory quartz unit [2]. Thermogravimetric analysis was carried out to compare the yield of biochar and its ash content. As the temperature of algae pyrolysis increases, the elemental composition of the biochars produced gradually undergoes changes. The lower calorific values of algae's and biochars were determined based on their elemental compositions. The values were calculated using the Mendeleev formula. The obtained biochars showed a complex branched surface with high microporosity and a specific surface area of tens of  $\text{m}^2 \text{g}^{-1}$ .

Much of the available seaweed is not being fully utilized because it contains a high amount of moisture and decays quickly. However, algae could be employed if they are pretreated through processes like drying or pyrolysis, which produces biochar, to reduce their moisture content before decay sets in. These pretreatments would help overcome the challenges posed by algae's natural moisture levels and perishability in order to make better use of this abundant resource.

This work funded by the Ministry of Science and Higher Education of Russia, theme #FFSG-2024-0016 «Development of physical and chemical foundations of promising technologies and materials for energy-efficient use of traditional and alternative carbon-containing resources» and theme #FEFF-2022-0027 «Carbon balance of biomorpholithosystems of the coast and adjacent marine areas of the marginal seas of the Far East». This work was performed using the equipment of the Federal Research Center of Problems of Chemical Physics and Medicinal Chemistry RAS (<http://www.icp.ac.ru/en>).

### References

1. M. V. Tsvetkov, A. Yu. Zaichenko, D. N. Podlesniy et al., *E3S Web of Conferences*. **2024**, 474, 01012.
2. A. A. Belmesov, A. A. Glukhov, R. R. Kayumov et al., *Coatings*. **2023**, 13(12), 2075.



# Interaction of pyridine radicals with molecular oxygen: Theoretical study

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Around the world, coal-fired power plants continue to play an important role in electricity generation because coal is a less expensive, more abundant and reliable energy resource compared to oil and natural gas. At the same time, environmental issues force strict control over emissions of pollutants from coal combustion. These compounds include, in particular, nitrogen oxides (NO<sub>x</sub>), which are poisonous to humans. The main nitrogen functional groups in coals are predominantly in the form of heterocyclic aromatic structures, including pyridine and pyrrole rings. In this regard, the pyridine molecule can be considered as a model for studying the transformations of nitrogen during coal combustion. The purpose of this study is to describe the interaction of pyridine radicals with molecular oxygen.

The geometries of reactants, products, intermediates, and transition states of the reactions of ortho- and meta-pyridyl radicals with O<sub>2</sub> were optimized at the level of density functional theory using the ωB97XD functional with the 6-311G\*\* basis set. The vibrational frequencies were calculated at the same level of theory to characterize stationary points as local minima or transition states, to obtain zero-point energy (ZPE) corrections, and for use in partition function calculations. Additionally, the optimized ωB97XD geometries were used to refine single-point energies using the combined ab initio G3(MP2,CC) method.

As a result of the study, it was found that the reactions of ortho-, meta- and para-pyridyls with molecular oxygen have a similar mechanism and give products that are similar in structure. The main pathways of the reactions were studied in detail and potential energy surfaces of the interactions of ortho-, meta- and para-pyridyls with molecular oxygen were constructed.

# Impact of non-adiabatic heating and cooling on the gravitational stratification of the solar atmosphere

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The solar atmosphere is a natural laboratory for studying plasma physics. One of the features of this medium is the presence in it of heating and cooling processes that depend on the thermodynamic parameters of the plasma. The balance of these processes ensures the existence of the solar atmosphere itself. Moreover, this balance must be observed at different heights, at which the plasma density and temperature, as well as the magnitude of the magnetic field, are different. Thus, the height profiles of thermodynamic parameters should be determined, on the one hand, by the pressure gradient caused by solar gravity and, on the other hand, by the balance of heating and cooling, the powers of which depend, for example, on the plasma density and temperature. In the case of heating and cooling, given as power functions of temperature and density, analytic profiles of thermodynamic parameters from height were obtained and their dependence on the power indices was shown.

In [1], it was proposed to use observational data on the height profiles of temperature and density in the Sun's gravitational field to obtain information on the heating of the solar corona. Under the assumption that the heating and cooling powers of the medium are equal in the regions of the quiet Sun and long-lived coronal structures, it is shown that the height profiles of temperature and density are determined by the type of functional dependences of heating and cooling on the density and temperature of the medium.

In the current work, the known model of medium cooling calculated with the CHIANTI database [2] and the height profiles of temperature and number density obtained on the basis of measurements in [3] are used. The heating function was modeled as a power dependence on temperature and density and such power values were found at which the observed height profiles are realized and the medium is stable. In addition, the characteristic damping times of MHD waves associated with the effect of thermal imbalance were calculated for the considered regions.

The study was supported in part by the Ministry of Science and Higher Education of Russian Federation under State assignment to educational and research institutions under Project No. FSSS-2023-0009 and FFMR-2024-0017.

## References

1. D. S. Riashchikov, N. E. Molevich, D. I. Zavershinskii, *MNRAS* **2023**, 522, 572.
2. G. Del Zanna, K. P. Dere, P. R. Young, E. Landi, *ApJ* **2021**, 909, 38.
3. D. J. Pascoe, A. Smyrli, T. Van Doorselaere, *ApJ* **2019**, 884, 43.

# Singlet potential energy surface of C<sub>3</sub>H<sub>2</sub>+O<sub>2</sub> interaction

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The development of complex oxidation mechanisms of intermediate compounds formed during hydrocarbon fuel combustion is among the most important directions of quantum-chemical research. One such compound is propenylidene (C<sub>3</sub>H<sub>2</sub>) and its isomers. The reaction mechanisms of these compounds are largely determined by the composition of the air-fuel mixture [1], and a thorough understanding of the chemistry of individual isomers in the singlet and triplet states is becoming more and more demanded. This work is part of a comprehensive study and aims to form the potential energy surface of the C<sub>3</sub>H<sub>2</sub>+O<sub>2</sub> reaction in the singlet state, for future combination of singlet and triplet surfaces and reaction rate constants calculation.

Optimized molecular geometries were calculated for reactants, products, intermediates, and transition states using the wB97XD hybrid density functional theory method with the 6-311++G(d,p) basis function set. The corresponding potential energy surface is formed. A simplified surface showing only the main reaction pathways for the various isomers is presented in Figure 1. All calculations were performed in the Gaussian 09 program.

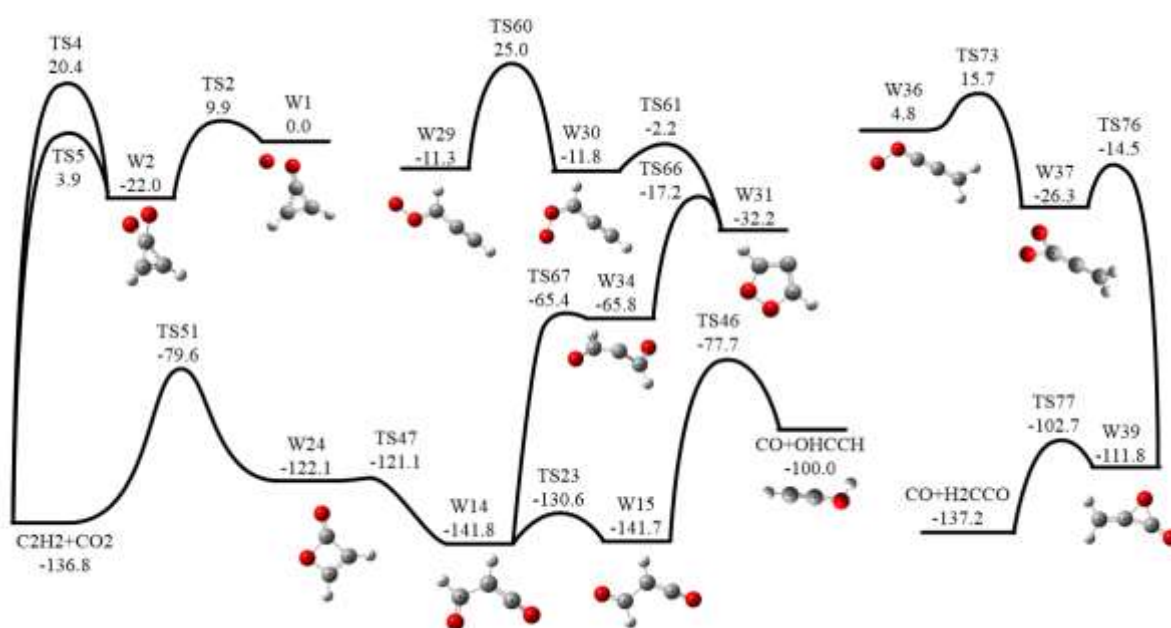


Fig.1 The main pathways on the obtained singlet potential energy surface, relative energies in kcal/mol.

## Acknowledgment

The study was supported by the Russian Science Foundation, projects no. 22-79-10205, (<https://rscf.ru/project/22-79-10205/>).

## References

1. T.L. Nguyen, A.M. Mebel, R.I. Kaiser A Theoretical Investigation of the Triplet Carbon Atom C(3P) + Vinyl Radical C<sub>2</sub>H<sub>3</sub>(2A') Reaction and Thermochemistry of C<sub>3</sub>H<sub>n</sub> (n = 1–4) Species, J. Phys. Chem. A 2001, 105, 13, 3284–3299. DOI:10.1021/jp003224c

# Methodology for plotting a distillation curve for multicomponent fuels with the addition of ethers

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The purpose of the study is to review and validate methods for calculating saturated vapor pressure for multicomponent fuels with the addition of ethers. The results of the work should improve the reliability of modeling the distillation curve of composite fuels consisting of both petroleum derivatives and biocomponents. The developed methodology will be applied in the following areas:

- Simulation of the evaporation process. The distillation curve shows at what temperatures and pressures the evaporation of various fuel fractions occurs and compares the obtained values with the fuel requirements.
- Creation of fuel models (surrogates). The resulting methodology will improve virtual fuel models (surrogates), which simulate the behavior of real fuel when studying the engine operating process.

The technique for constructing a distillation curve is described in [1]. The main factors determining the accuracy of the distillation curve calculation are the number of iterations and the reliability of the saturated vapor pressure of the mixture components. An increase in the number of iterations without a significant increase in calculation time is ensured by the use of specialized software [2]. To select the optimal method for calculating the saturated vapor pressure of components, an analysis of existing methods for both petroleum fuels and ethers was carried out. The results of calculations using various methods were compared with reference data and with the results of experimental determination of saturated vapor pressure. As a result of the study, the optimal method for calculating saturated vapor pressure was determined [3], which provides the most reliable construction of the distillation curve of multicomponent fuels with the addition of ethers.

This work was funded by a grant from the Russian Science Foundation (project No. 23-69-10006) <https://rscf.ru/project/23-69-10006/>.

## References

1. Morales, M. H., Tsapenkov, K. D., Zubrilin, I. A., Yakushkin, D. V., Semenikhin, A. S., Sazhin, S. S., & Matveev, S. G. (2023). Formulation of Surrogates of Hydrocarbon Fuels Using Selected Physico-Chemical Properties Related to Atomization, Heating, Evaporation and Combustion Behaviours. *Combustion Science and Technology*, 1–23.
2. Pat. 2023614390 Russian Federation. FM Configurator V1 [Text] / Zubrilin I.A., Ostapyuk Ya.A., Tsapenkov K.D., Hernandez Morales M., Kuznetsov A.Yu., Yakushkin D.V., Yastrebov V.V.; applicant and copyright holder Samara University; application 12/12/2022; publ. 03/01/2023.
3. V.V. Raznoschikov, I.A. Demskaya. Mathematical model for calculating the thermophysical properties of synthetic liquid fuel // *Electronic journal "Proceedings of MAI"*. Issue No. 50

# The influence of N<sub>2</sub> content on the yield of ozone in a dielectric barrier discharge under conditions of plasma-initiated combustion

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The dielectric barrier discharge (DBD) is a topic of interest in accelerating chemical processes in lean fuel-air mixtures and stabilizing combustion through plasma. Its technical simplicity and adaptability to different gas flow setups make it a valuable tool [1,2]. To enhance and validate kinetic models of DBD plasma assisted combustion, comprehensive experimental data on gas mixture composition in the discharge afterglow is essential. In this work, additional measurements of ozone number densities [O<sub>3</sub>] at the output of the DBD were carried out using the experimental setup described in [3].

Figure 1(a) illustrates the typical dependencies of ozone number densities [O<sub>3</sub>] at the output of DBD on electrical power for various N<sub>2</sub> content values at a constant total flow rate of O<sub>2</sub>/N<sub>2</sub> gas mixture of 9 L min<sup>-1</sup>. The O<sub>2</sub> content is calculated using the expression  $\eta = [\text{O}_2] / ([\text{O}_2] + [\text{N}_2])$ . The expected decrease in [O<sub>3</sub>] with decreasing  $\eta$  is observed, although the nature of this decrease is nonlinear. This nonlinearity is more evident in Figure 1(b), which displays the dependencies of [O<sub>3</sub>] on electric power from Figure 1(a) divided by  $\eta$ . It is apparent that the efficiency of converting molecular oxygen into ozone improves with the increase in N<sub>2</sub> content at a constant gas flow rate. This phenomenon cannot be attributed to more effective cooling of the mixture, as the thermal conductivity coefficients of O<sub>2</sub> and N<sub>2</sub> are nearly identical across a wide temperature range. Another intriguing observation is that the yield of [O<sub>3</sub>] with a 2% N<sub>2</sub> mixture is approximately 10% higher than that with 100% O<sub>2</sub>. A precise explanation of these findings necessitates a comparison of the experiment with a numerical model, which will also facilitate the verification and description of the "memory effect" from [3].

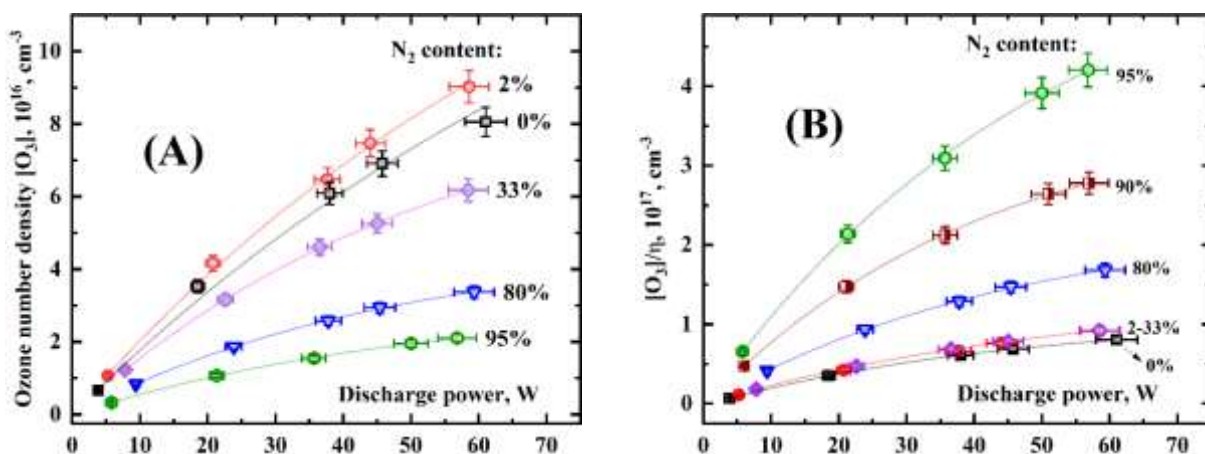


Figure 1. a) Power-dependences of [O<sub>3</sub>] at the output of DBD in O<sub>2</sub>/N<sub>2</sub> mixtures at a pressure 1 atm and a flow rate 9 L min<sup>-1</sup>; b) data from figure (a), divided by oxygen content  $\eta$

## References

1. Shah Z. A. et al. *International Journal of Hydrogen Energy*. **2023**, 51, 354-374.
2. Johnson P. N. et al. *Combustion and Flame*. **2023**, 255, 112927.
3. Torbin A. P. et al. *Plasma Sources Science and Technology*. **2022**, 31, 035017.



# Numerical simulation of the time-of-flight mass spectrometer of the cryogenic surface processes apparatus: influence of the inhomogeneity of the source region field

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As part of the work on launching a new experimental facility for the study of astrochemical processes under laboratory conditions, a time-of-flight (TOF) mass spectrometer [1] with an ion mirror [2] was built and tested for the identification of complex organic molecules. Preliminary simulations of the TOF mass spectrometer in the Simion [3] software package showed that the mass resolution  $M/\Delta M$  can reach  $\sim 1600$ , and the ion collection efficiency  $\varphi$  could be as high as 75% [4]. In the constructed mass spectrometer, the ion source contains mounting elements - bolts and nuts, protruding 3-5 mm beyond the extraction plate (Fig. 1, Right panel). These elements create a non-uniform electric field, which can penetrate into the centerline of the source and affect the trajectories and flight time of the ions, leading to "broadening" of the ion packet and affecting its focusing. This effect is amplified due to the potential difference between the extraction plate and the mounting elements. To evaluate the effect of the inhomogeneity of the electric field, the corresponding changes were introduced into the simulation (Fig. 1, Left panel). The calculations showed a decrease in  $M/\Delta M$  to 1000 and reduction of  $\varphi$  to 10%.

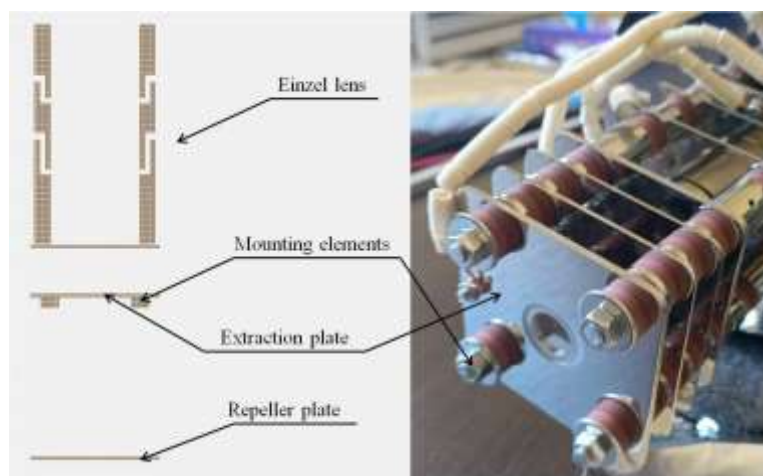


Fig. 1. Right panel: Computer simulation of the ion source of a TOF mass spectrometer with an ion mirror; Left panel: ion source photo.

The effect inhomogeneity of the electric field in the ion source region can be alleviated by equalizing the potentials on the mounting elements and the extraction plate. Simulations have shown that in this case,  $M/\Delta M$  improves to 1200, and the  $\varphi$  can reach 60%, sufficient for sensitive detection of complex organic molecules in our experiments.

## References

1. W.C. Wiley, I.H. McLaren, Review of Scientific Instruments.1955, 26, 1150–1157.
2. B.A. Mamyurin, *et al* J. of Exp. and Theor. Phys. 1973, 64, 82-89.
3. SIMION for the personal computer in reflection, <https://simion.com/info/>
4. D.S. Trufanov. I.O. Antonov, XXI Russian Optics, Laser Physics and Plasma Physics. Youth Conference, 2023, 2, 263-264.



# Experimental optimization of the time-of-flight mass spectrometer of the cryogenic surface processes: mass spectrum of butadiene

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The experimental optimization of the time-of-flight mass spectrometer of the "Cryogenic Surface Processes" setup (CSP) was carried out. During the optimization, the mass spectrum of butadiene ( $M/z = 54$ ) was obtained for the linear mode (Fig. 1). The time of flight was  $t = 29.1 \mu\text{s}$ , the peak width  $\Delta t = 0.7 \mu\text{s}$ , and the mass resolution  $M/\Delta M = t/2\Delta t \sim 22$ . The low value of mass resolution is explained by the penetration of external fields from the walls of the vacuum chamber into the ion source region. In future work, the mass resolution will be increased to the design value ( $>400$  in linear mode [1] and up to 2000 in mass-reflectron mode [2]) by reducing the distance between the electrodes in the ion source to prevent the penetration of external fields.

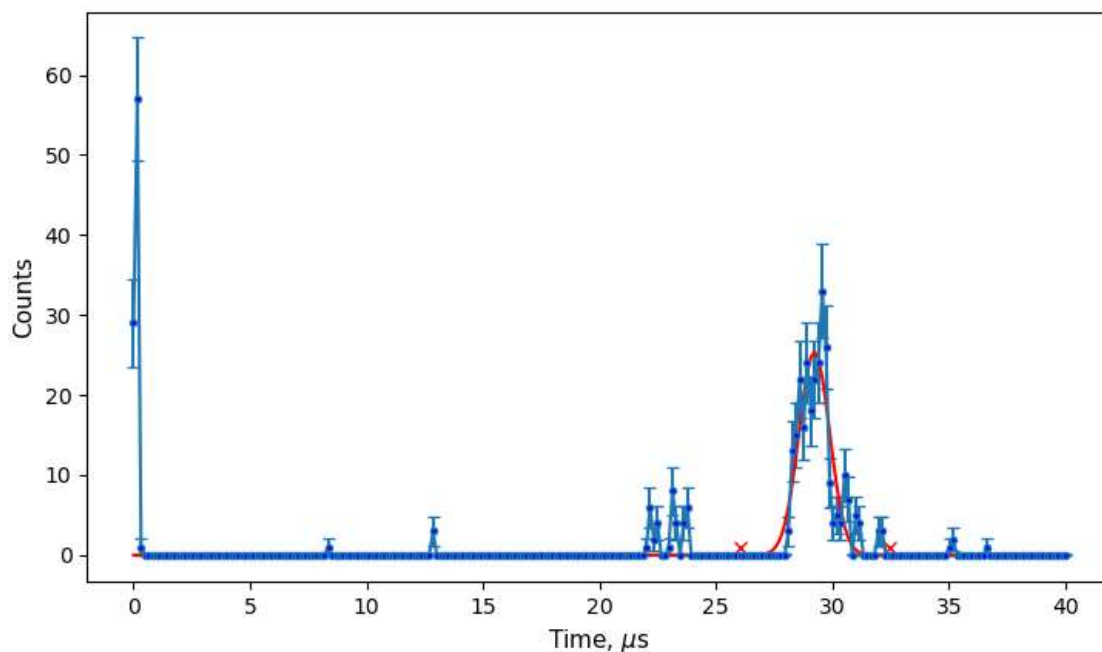


Figure 1. Mass spectrum of butadiene for the linear mode. A fitted Gaussian is shown by the red line

## References

1. W.C. Wiley, I.H. McLaren, Review of Scientific Instruments. 1955, 26, 1150–1157.
2. B. A. Mamyurin, V. I. Karataev, D. V. Shmikk, V. A. Zagulin Journal of Experimental and Theoretical Physics. 1973, 64, 82–89.

# Investigation of soot and PAHs formation during hydrocarbons pyrolysis with kinetic modeling and optical density measurements in UV-VIS range

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The process of soot formation during the combustion and pyrolysis of hydrocarbons is of interest to researchers due to emission of soot particles and their precursors, polycyclic aromatic hydrocarbons (PAHs). Soot contributes to global warming [1], and many PAHs are carcinogens [2]. Thus, the development of the soot and PAHs formation models is an important task that scientists face today. The greatest difficulties are associated with the kinetics of PAHs formation and the nucleation of “young” soot particles.

This work investigates the pyrolysis of hydrocarbons (CH<sub>4</sub>, C<sub>2</sub>H<sub>4</sub>, C<sub>2</sub>H<sub>2</sub> and C<sub>6</sub>H<sub>6</sub>) diluted in argon behind the reflected shock waves. Experiments were performed on the shock tube of standard construction using light extinction diagnostic in temperature range of 1630-2552 K and pressures 2.85-7.85 bar. The measurement wavelengths were 633, 405 and 313 nm. Extinction at a wavelength of 633 nm is a standard method for the soot yield diagnostic. As it can be seen from work [3] the maximum wavelength of absorption tends to decrease with decreasing of the molecular mass of PAH. Thus, the decrease of the extinction wavelength makes it possible to observe the absorption contribution not only from condensed particles, but also from the gas phase reacting mixture. Extinction caused by particles at wavelengths of 313 nm and 405 nm was estimated with the literature on soot optical properties data from [4,5] for separation from the absorption of gas phase.

This work resulted in the obtaining temperature dependencies of the optical density of reacting hydrocarbon mixtures at wavelengths of 633 nm, 405 nm and 313 nm. It was shown that the well-known “bell-shaped” temperature dependence at 633 nm, persists at 313 and 405 nm. The exception is the case of acetylene at a wavelength of 313 nm, where the optical density stays at the same value at high temperatures after reaching its maximum. The highest soot yield was observed in benzene and acetylene. It was shown that the left and right branches of the “bells” of optical density at 313 and 405 nm cannot be explained only by the absorption of condensed particles and the contribution of gas phase to the extinction was observed in experiments. Kinetic modeling of hydrocarbons pyrolysis studied in the experiment was carried out with the help of CRECK mechanism [6]. It was shown that the calculated soot yield was not in the agreement with the experimental data for benzene and acetylene. A possible reason is there is no polyynes path of soot formation in kinetic scheme.

This work was supported by RSF 23-19-00407.

## References

1. B. Moorthy et al. *Toxicol. Sci.* **2015**, 145.
2. T. C. Bond et al. *J. Geophys. Res. Atmos.* **2013**, 118.
3. F. J. Bauer et al. *Appl. Phys. B.* **2021**, 127, 115.
4. E. V. Gurentsov et al. *High Temp.* **2022**, 60.
5. F. Migliorini et al. *Phys. Chem. Chem. Phys.* **2021**, 23.
6. W. Sun et al. *Proc. Combust. Inst.* **2021**, 38.

# Influence of aluminum powder additives on the acoustic conductivity of the burning surface of solid propellant

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During the operation of a solid propellant (SP) rocket engine, with its selected geometric parameters and given fuel characteristics, the development of high-frequency pressure fluctuations is possible, due to close values of the natural frequencies of the combustion chamber and the combustion process. High-frequency instability of the combustion chamber contributes to the emergence and development of vibration or resonant combustion, leading to an uncontrolled increase in pressure and, ultimately, to the destruction of the combustion chamber [1]. In this regard, there is a need to conduct experimental studies in order to determine the characteristics of the acoustic conductivity of the fuel at the specified frequencies and subsequent assessment of the performance of the combustion chamber design.

The main source of amplification of acoustic vibrations is the burning surface of SP. The process of amplification of small disturbances of gas phase parameters, which are always present in the form of turbulent noise, is associated with the response of the combustion surface in the form of an additional portion of combustion products and energy. At a certain ratio between the frequency of disturbances and the frequency corresponding to the relaxation time of the combustion wave, the initial small pressure disturbance is amplified, which leads to the emergence of a vibrational combustion mode.

Currently, interest in research into high-frequency instability has increased significantly [2-4], which is associated with the development of promising fuel compositions containing new components (active combustible binders, metal nanopowders, combustion catalysts, etc.). The burning rate of such compositions is significantly higher than that of traditional SP compositions.

This paper presents the methodology and results of studying the acoustic conductivity of the combustion zone of SP samples using a two-end combustion chamber (T-chamber). Model mixed SP containing aluminum powders of industrial grades ASD-4, ASD-6 and ASD-8 were selected as experimental samples.

The experimental results on the influence of the dispersion of aluminum powders on the development of acoustic vibrations in the resonator of the T-chamber can be explained by the difference in the average sizes and concentrations of particles of condensed combustion products of mixed SP (aluminum oxide  $\text{Al}_2\text{O}_3$ ) formed during the combustion of aluminum powders of different dispersion in the composition of mixed SP, which dampen the resulting acoustic vibrations.

This work was supported by the Ministry of Education and Science of the Russian Federation within the framework of state contract No. FSWM-2020-0036.

## References

1. B.V. Rauschenbach, Moscow: Fizmatgiz. **1961**. 500 p.
2. W. Su, N. Wang, J. Li, Y. Zhao, M. Yan, *J. of Sound and Vibration*. **2013**, 333(8), 2226-2240.
3. A.A. Kuroyedov, D.M. Borisov, P.A. Semenov, *Elec. J. Trudy MAI*. **2018**, 98, 4.
4. V.A. Arkhipov, S.A. Volkov, L.N. Revyagin, *Russ. J. Phys. Chem. B*. **2012**, 6(3), 384-389.

*Научное издание*

International Conference on Physics and Chemistry  
of Combustion and Processes in Extreme Environments  
(Samara, Russia, 2-6 July 2024)

**Proceeding of the conference**

**/ Edited by V.N. Azyazov & A.M. Mayorova/**

Подписано в печать 18.06.2024

Формат 60 х84/8. Бумага ксероксная. Печать оперативная.

Объем – 13,75 усл. печ. л. Тираж 100 экз. Заказ № 126

Отпечатано в типографии издательства «Инсома-Пресс»  
443080, г. Самара, ул. Санфировой, 95, литер 4, офис 416,  
тел. 8 927-005-93-31, E-mail: [insoma@bk.ru](mailto:insoma@bk.ru)

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