

## MODELING OF SELF-IGNITION DELAYS OF METHANE–ALKANE–AIR MIXTURES

A. V. Arutyunov<sup>1,2</sup>, A. A. Belyaev<sup>1</sup>, A. V. Nikitin<sup>1</sup>, K. Ya. Troshin<sup>1</sup>, and V. S. Arutyunov<sup>1,3</sup>

<sup>1</sup>N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

<sup>2</sup>Faculty of Computational Mathematics and Cybernetics, Lomonosov Moscow State University, Leninskie Gory, Moscow 119991, GSP-1, Russian Federation

<sup>3</sup>Faculty of Fundamental Physics and Chemical Engineering, Lomonosov Moscow State University, Leninskie Gory, Moscow 119991, GSP-1, Russian Federation

**Abstract:** High content of methane homologues in associated petroleum gases (APG) with low resistance to detonation makes them unsuitable for use as fuel for power plants. To create effective technologies to reduce the concentration of methane homologues in APG, data on the detonation characteristics of these complex mixtures of hydrocarbon gases are needed. One of the most informative characteristics that determines the detonation resistance of gas mixtures is the delay of their self-ignition. The paper presents the results of computer simulation of self-ignition delays in stoichiometric binary and triple mixtures of methane with C<sub>2</sub>–C<sub>5</sub> alkanes and air. Satisfactory agreement of calculations with experimental data is obtained. Analytical expressions for estimating the self-ignition delay of the mixtures under consideration are proposed.

**Keywords:** methane; alkanes; combustion; self-ignition delay; computer modeling

**DOI:** 10.30826/CE19120302

## Acknowledgments

This work was performed within the framework of the Program of Fundamental Research of the Russian Academy of Sciences for 2013–2020 on the research issue of N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences No. 47.16. Theme number in Federal Agency for Scientific Organizations: 0082-2014-0004. State registration number of Center of Information Technologies Systems for Executive Power Authorities (CITIS): AAAA-A17-117040610283-3.

## References

1. Soloviyarov, A. A. 2015. Problemy ispol'zovaniya poputnogo neftyanogo gaza v Rossii [Problems of associated petroleum gas utilization in Russia]. *Oil and Gas Chemistry* 1:12–16.
2. Arutyunov, V. S., A. A. Kiryushin, V. M. Shmelev, and M. Yu. Sinev. 2010. Gazokhimicheskaya konversiya poputnogo gaza dlya maloy energetiki [Gas-chemical conversion of associated gas for small power units]. *Gazokhimiya* [Gas Chemistry] 1(11):16–20.
3. Nikitin, A. V., K. Ya. Troshin, A. A. Belyaev, A. V. Arutyunov, A. A. Kiryushin, and V. S. Arutyunov. 2018. Gazomotornoe toplivo iz poputnogo neftyanogo gaza. Selektivnyy oksikreking tyazhelykh komponentov PNG [Gas motor fuel from associated petroleum gas. Selective oxy-cracking of heavier components of APG]. *Oil and Gas Chemistry* 3:23–34.
4. Troshin, K. Ya., A. V. Nikitin, A. A. Belyaev, A. V. Arutyunov, A. A. Kiryushin, and V. S. Arutyunov. 2019. Experimental'noe opredelenie zaderzhki samovosplamneniya smesey metana s legkimi alkanami [Experimental determination of self-ignition delays of mixtures of methane with light alkanes]. *Combust. Expl. Shock Waves* 55(5):17–24. doi: 10.15372/FGV20190502.
5. Borisov, A. A., V. G. Knorre, E. L. Kudryashova, G. I. Skachkov, and K. Ya. Troshin. 1998. On temperature measurements in the induction period of ignition of homogeneous gas mixtures in a static admittance apparatus. *Chem. Phys. Rep.* 17(7):1323–1331.
6. Belyaev, A. A., A. V. Nikitin, P. D. Toktaliev, P. A. Vlasov, A. V. Ozerkiy, A. S. Dmitruk, A. V. Arutyunov, and V. S. Arutyunov. 2018. Analiz literaturnykh modeley okisleniya metana v oblasti umerennykh temperatur [Analysis of literature models of oxidation of methane at moderate temperatures]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 11(1):19–26.
7. Healy, D., D. M. Kalitan, C. J. Aul, E. L. Petersen, G. Bourque, and H. J. Curran. 2010. Oxidation of C<sub>1</sub>–C<sub>5</sub> alkane quaternary natural gas mixtures at high pressures. *Energ. Fuel.* 24(3):1521–1528.
8. Combustion Chemistry Center at NUI Galway: Database Mechanism of Natural Gas (including C<sub>5</sub>) Oxidation. Available at: <http://c3.nuigalway.ie/media/>

researchcentres/combustionchemistrycentre/files/mechanismdownloads/nc5\_49\_mech.dat (accessed August 29, 2019).

9. Nikitin, A. V. 2016. Kineticheskie zakonomernosti okisleniya legkikh alkanov i ikh smesey v srednetemperaturnoy

oblasti [Kinetics of light alkanes and their mixtures oxidation at medium temperatures]. Chernogolovka: IPCP RAS. PhD Diss. 127 p. Available at: [http://www.icp.ac.ru/media-store/EDUCATION/DIS-SOVET/Zatshita\\_disser/Disser\\_Nikitin.pdf](http://www.icp.ac.ru/media-store/EDUCATION/DIS-SOVET/Zatshita_disser/Disser_Nikitin.pdf) (accessed August 29, 2019).

*Received February 1, 2019*

## Contributors

**Arutyunov Artem V.** (b. 1994) — research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; PhD student, Faculty of Computational Mathematics and Cybernetics, Lomonosov Moscow State University, Leninskie Gory, GSP-1, Moscow 119991, Russian Federation; [aarutyunow@gmail.com](mailto:aarutyunow@gmail.com)

**Belyaev Andrey A.** (b. 1954) — Candidate of Science in physics and mathematics, leading research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; [belyaevIHF@yandex.ru](mailto:belyaevIHF@yandex.ru)

**Nikitin Aleksey V.** (b. 1988) — Candidate of Science in chemistry, senior research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; [ni\\_kit\\_in@rambler.ru](mailto:ni_kit_in@rambler.ru)

**Troshin Kirill Ya.** (b. 1949) — Doctor of Science in physics and mathematics, chief research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; senior teacher, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; [troshin@chph.ras.ru](mailto:troshin@chph.ras.ru)

**Arutyunov Vladimir S.** (b. 1946) — Doctor of Science in chemistry, professor, head of laboratory, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; head of laboratory, Institute of Problems of Chemical Physics, 1 Acad. N. N. Semenov Prosp., Chernogolovka 142432, Russian Federation; professor, Faculty of Fundamental Physics and Chemical Engineering, Lomonosov Moscow State University, Leninskie Gory, GSP-1, Moscow 119991, Russian Federation; [arutyunov@chph.ras.ru](mailto:arutyunov@chph.ras.ru)