

DETERMINATION OF THE AUTOIGNITION DELAY OF METHANE–ETHYLENE–AIR MIXTURES

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Abstract: The autoignition delays of stoichiometric methane–ethylene–air mixtures in the initial temperature range $T_0 = 800\text{--}1000\text{ K}$ and at a pressure $P_0 = 1\text{ atm}$ were determined experimentally by the method of autoignition in a static reactor and by kinetic modeling. It is experimentally established that as the concentration of ethylene in the mixture increases, the effective activation energy of the autoignition delay increases. On the basis of comparison with the delay of spontaneous ignition of methane–ethane–air mixtures, it is concluded that the detonation resistance of $\text{C}_2\text{--}\text{C}_3$ alkenes, including their mixtures with methane, does not exceed the detonation resistance of the corresponding alkanes.

Keywords: methane; ethylene; ethane; autoignition delay

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Figure Captions

Figure 1 Temperature dependence of the autoignition delay of stoichiometric methane–ethylene–air mixtures; $P_0 = 1\text{ atm}$. Concentration of ethylene in the mixture with methane: 1 – 0% (vol.); 2 – 5; 3 – 10; 4 – 20; 5 – 40; 6 – 60; 7 – 80; and 8 – 100% (vol.).

Figure 2 Dependence of the effective activation energy of the autoignition delay of stoichiometric methane–ethylene–air mixtures on the concentration of ethylene in the range of initial temperatures 800–1000 K at $P_0 = 1\text{ atm}$: 1 – experimental results; and 2 – results of kinetic modeling

Figure 3 Dependence of the autoignition delay of stoichiometric methane–ethylene–air mixtures on the concentration of ethylene at $P_0 = 1\text{ atm}$ and initial temperatures: 1 – 850 K; 2 – 900; 3 – 950; and 4 – 1000 K

Figure 4 Comparison of the dependence of the autoignition delay of stoichiometric methane–ethane–air (1) and methane–ethylene–air (2) mixtures on the concentration C of ethane or ethylene at $P_0 = 1\text{ atm}$ and $T_0 = 950\text{ K}$

Table Caption

Octane numbers of $\text{C}_2\text{--}\text{C}_5$ hydrocarbons of normal structure according to the motor (MON) and research (RON) method [11]

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References

- Arutyunov, A. V., K. Ya. Troshin, A. V. Nikitin, A. A. Belyaev, and V. S. Arutyunov. 2018. Computer modeling of self-ignition delays of methane–alkane mixtures. *J. Phys. Conf. Ser.* 1141:012153. doi: 10.1088/1742-6596/1141/1/012153.
- Troshin, K. Ya., A. V. Nikitin, A. A. Belyaev, A. V. Arutyunov, A. A. Kiryushin, and V. S. Arutyunov. 2019. Experimental determination of self-ignition delay of mixtures of methane with light alkanes. *Combust. Explos. Shock Waves* 55(5):526–533.
- Arutyunov, A. V., A. A. Belyaev, A. V. Nikitin, K. Ya. Troshin, and V. S. Arutyunov. 2019. Modelirovaniye zaderzhekh samovosplameneniya metanovozdushnykh smesey s dobavkami legkikh alkanov [Modeling of self-ignition delays of methane–alkane–air mixtures]. *Goren. Vzryv. (Mosk.) — Combustion and Explosion* 12(3):14–20. 2019. doi: 10.30826/CE19120302.
- Arutyunov, A. V., A. A. Belyaev, I. N. Inovenkov, and

- V. S. Arutyunov. 2019. Vliyanie vodoroda na normal'nyu skorost' goreniya metanovozdushnykh smesey pri povushennykh temperaturakh [The influence of hydrogen on the burning velocity of methane–air mixtures at elevated temperatures]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 12(4):4–10. doi: 10.30826/CE19120401.
5. Troshin, K. Ya., A. A. Belyaev, A. V. Arutyunov, A. A. Tsarenko, A. V. Nikitin, and V. S. Arutyunov. 2021 (in press). Vliyanie davleniya na samovosplamenenie metanovodorodnykh smesey [Influence of pressure on the self-ignition delay of methane–hydrogen mixtures]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 14(1).
6. Nikitin, A. V., K. Ya. Troshin, A. A. Belyaev, A. V. Arutyunov, A. A. Kirushin, and V. S. Arutyunov. 2018. Gazomotoroe toplivo iz poputnogo gaza. Selektyivnyy oksikreking tyazhelykh komponentov PNG [Gas motor fuel from associated petroleum gas. Selective oxycracking of heavier components of APG]. *Oil Gas Chemistry* 3:23–34. doi: 10.24411/2310-8266-2018-10301.
7. Arutyunov, V., K. Troshin, A. Nikitin, A. Belyaev, A. Arutyunov, A. Kiryushin, and L. Strekova. 2020. Selective oxycracking of associated petroleum gas into energy fuel in the light of new data on self-ignition delays of methane–alkane compositions. *Chem. Eng. J.* 381:122706. doi: 10.1016/j.cej.2019.122706.
8. Healy, D., D. M. Kalitan, C. J. Aul, E. L. Petersen, G. Bourque, and H. J. Curran. 2010. Oxidation of C₁–C₅ alkane quaternary natural gas mixtures at high pressures. *Energ. Fuel.* 24(3):1521–1528.
9. Combustion Chemistry Center at NUI Galway: Database Mechanism of Natural Gas (including C₅) Oxidation. Available at: http://c3.nuigalway.ie/media/researchcentres/combustionchemistrycentre/files/mechanismsdownloads/nc5_49_mech.dat (accessed November 14, 2020).
10. Kee, R. J., F. M. Rupley, E. Meeks, and J. A. Miller. 1996. CHEMKIN III. Livermore, CA: Sandia National Laboratories. Technical Report No. SAND96-8216.
11. Balaban, A. T., L. B. Kier, and N. Joshi. 1992. Structure-property analysis of octanenumbers for hydrocarbons (alkanes, cycloalkanes, alkenes). *MATCH Commun. Math. Co.* 28:13–27. Available at: http://match.pmf.kg.ac.rs/electronic_versions/Match28/match28_13-27.pdf (accessed April 2, 2020).
12. Wärtsilä Calculator. Available at: <https://www.wartsila.com/products/marine-oil-gas/gas-solutions/methane-number-calculator> (accessed April 2, 2020).

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