

MODELING OF FLAMELESS COMBUSTION OF LARGE DROPLETS OF NORMAL AND IZOMERIZED HYDROCARBONS IN MICROGRAVITY CONDITIONS

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Abstract: Comparative calculations of combustion of large (2.8 mm) droplets of four liquid octanes — *n*-octane, 2-methylheptane, 2,2-dimethylhexane, and 2,2,4-trimethyl pentane — are performed for microgravity conditions. The temperature histories obtained for droplet combustion were shown to be qualitatively similar to those obtained for self-ignition of homogeneous fuel–air mixtures: the oxidation and combustion rates of fuel droplets also decrease with the degree of branching in the molecule structure in the line from *n*-octane to reference iso-octane (2,2,4-trimethylpentane). This theoretical conclusion corresponds well with the results of space experiment “Zarevo” with droplets of pure *n*-dodecane and iso-dodecane as well as with droplets of *n*-dodecane/iso-dodecane solutions of different composition.

Keywords: alkanes; iso-octanes; detailed kinetic mechanism; multistage self-ignition; radiation quenching of droplet flame; flameless combustion of droplet

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References

1. Dietrich, D. L. 2010. MCDA/FLEX. *AIAA Aerospace Sciences Meeting*. Orlando, FL. doi: 10.2514/6.2010-1110.
2. Farouk, T., and F. L. Dryer. 2011. Microgravity droplet combustion: Effect of tethering fiber on burning rate and flame structure. *Combust. Theor. Model.* 15(4):487–515. doi: 10.1080/13647830.2010.547601.
3. Nayagam, V., D. L. Dietrich, P. V. Ferkul, et al. 2012. Can cool flames support quasi-steady alkane droplet burning? *Combust. Flame* 159(13):3583.
4. Frolov, S. M., V. Ya. Basevich, and S. N. Medvedev. 2016. Modeling of low-temperature oxidation and combustion of droplets. *Dokl. Phys. Chem.* 470(2):150–153.
5. Basevich, V. Ya., A. A. Belyaev, S. N. Medvedev, V. S. Posvyanskii, F. S. Frolov, and S. M. Frolov. 2010. Simulation of the autoignition and combustion of *n*-heptane droplets using a detailed kinetic mechanism. *Russ. J. Phys. Chem. B* 4(6):995–1004.
6. Basevich, V. Ya., A. A. Belyaev, V. S. Posvyanskii, and S. M. Frolov. 2010. Mechanism of the oxidation and combustion of normal paraffin hydrocarbons: Transition from C₁–C₆ to C₇H₁₆. *Russ. J. Phys. Chem. B* 4(6):895–994.
7. Basevich, V. Ya., S. N. Medvedev, S. M. Frolov, F. S. Frolov, B. Basara, and P. Priesching. 2016. Makrokineticheskaya model' dlya rascheta emissii sazhi v dizele [Macrokinetic model for calculation of soot emissions in diesel engine]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 9(3):36–46.
8. Frolov, S. M., V. Ya. Basevich, S. M. Medvedev, and F. S. Frolov. 2018 (in press). Nizkotemperaturnoe besplamennoe gorenie krupnoy kapli n-dodekana v usloviyakh mikrogravitatsii [Low-temperature flameless combustion of a large drop of *n*-dodecane under microgravity conditions]. *Russ. J. Phys. Chem. B* 37(5).
9. Frolov, S. M., V. Ya. Basevich, S. N. Medvedev, and F. S. Frolov. 2017. Besplamennoe gorenie krupnoy kapli n-dodekana v usloviyakh mikrogravitatsii [Flameless burning of large *n*-dodecane drops in microgravity conditions]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 10(3):36–42.
10. Basevich, V. Ya., A. A. Belyaev, S. M. Medvedev, S. M. Frolov, and F. S. Frolov. 2018 (in press). Detal'nyy kineticheskiy mekhanizm okisleniya i gorenija oktanov [Detailed kinetic mechanism of oxidation and burning of octanes]. *Russ. J. Phys. Chem. B* 37(6).
11. Basevich, V. Ya., A. A. Belyaev, S. N. Medvedev,

- V. S. Posvyanskii, F. S. Frolov, and S. M. Frolov. 2016. A detailed kinetic mechanism of multistage oxidation and combustion of isoctane. *Russ. J. Phys. Chem. B* 10(5):801–809.
12. <http://ru.combex.org/lab1313.htm> (accessed December 25, 2017).
13. Sarathy, S. M., C. K. Westbrook, M. Mehl, *et al.* 2011. Comprehensive chemical kinetic modeling of the oxidation of 2-methylalkanes from C₇ to C₂₀. *Combust. Flame* 158(12):2338–2357.
14. Belyaev, A. A., and V. S. Posvyanskiy. 1985. Algoritmy i programmy [Algorithms and programs]. *Inform. byull. Gos. fonda algoritmov i programm SSSR* [Inform. Bull. of the State Fund of Algorithms and Programs of the USSR] 3:35.

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