

KINETIC MODEL AND CALCULATION OF SELF-IGNITION OF TRIETHYL ALUMINUM MICRODROPLETS IN AIR

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Abstract: Based on the model of heterogeneous interaction of oxygen with microdroplets of triethyl aluminum (TEA) resulting in the release of light hydrocarbon radicals into the gas phase, a computer code is developed and used for parametric calculations of the ignition delay of a spatially uniform mixture of TEA microdroplets in air. The calculations are performed with a variation of the kinetic parameters of the rate limiting reaction and are intended for further comparison with experiments.

Keywords: triethyl aluminum; interstitial reaction; rate constant; activation energy; microdroplets; ignition delay; radical formation; detailed kinetics; computer code

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References

1. Marsel, J., and L. Kramer. 1958. Spontaneous ignition properties of metal alkyls. *Symposium (International) on Combustion* 7(1):906–912. doi: 10.1016/S0082-0784(58)80135-6.
2. Gonçalves, R. F. B., K. Iha, J. A. F. F. Rocco. 2018. Reactive molecular dynamics simulation and chemical kinetic evaluation of combustion of triethylaluminum (TEA). *Quim. Nova* 41(5):507–511 doi: 10.21577/0100-4042.20170200.
3. Sydora, O. L. 2019. Selective ethylene oligomerization. *Organometallics* 38:997–1010. doi: 10.1021/acs.organomet.8b00799.
4. Davis, S. M., and N. Yilmaz. 2014. Thermochemical analysis of hypergolic propellants based on triethylaluminum/nitrous oxide. *Int. J. Aerospace Eng.* 2014:269836. 5 p. doi: 10.1155/2014/269836.
5. Kuznetsov, N. M., S. M. Frolov, P. A. Storozhenko, and I. O. Shamshin. 2019. Kineticheskaya model' oksleniya i vosplamneniya $\text{Al}(\text{C}_2\text{H}_5)_3$ v vozdukh [Kinetic model of oxidation and self-ignition of triethyl aluminum in air]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 12(3):91–97.
6. Kuznetsov, N. M., S. M. Frolov, and P. A. Storozhenko. 2019. Raschet standartnoy ental'pii obrazovaniya i teploty polnogo sgoraniya trietilaluminiiya v vodyanom pare i v vozdukh [Calculation of the standard enthalpy of formation and heat of complete combustion of triethylaluminum in water vapor and in air]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 12(2):10–13. doi: 10.30826/CE19120202.
7. Zel'dovich, Ya. B., G. I. Barenblatt, V. B. Librovich, and G. M. Makhviladze. 1980. *Matematicheskaya teoriya goreniiya i vzryva* [Mathematical theory of combustion and explosion]. Moscow: Nauka. 478 p.
8. Basevich, V. Ya., A. A. Belyaev, and S. M. Frolov. 2007. The mechanisms of oxidation and combustion of normal alkane hydrocarbons: The transition from C_1 – C_3 to C_4H_{10} . *Russ. J. Phys. Chem. B* 2(5):477–484.
9. Williams, F. A. 1965. *Combustion theory*. Addison-Wesley Publishing Co. 447 p.

10. Burcat, A. 2005. Thermodynamic data at the Web site of the Laboratory for Chemical Kinetics. Ideal gas thermodynamic data in polynomial form for combustion and air pollution use. Available at: <http://garfield.chem.elte.hu/Burcat/burcat.html> (accessed November 29, 2019).
11. Azatyan, V. V., A. M. Kogan, M. G. Neigauz, A. I. Poroi-kova, and E. N. Aleksandrov. 1975. Rol' samorazogreva pri gorenii vodoroda vblizi pervogo predela vosplamleniya [The role of self-heating during the combustion of hydrogen near the first ignition limit]. *Kinet. Catal.* 16(3):577–585.

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