KINETIC MODEL OF OXIDATION AND SELF-IGNITION OF TRIETHYL ALUMINUM IN AIR

N. M. Kuznetsov[1], S. M. Frolov[1,2,3], P. A. Storozhenko[4], and I. O. Shamshin[1,3]

[1]N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation
[2]National Research Nuclear University MEPhI, 31 Kashirskoe Sh., Moscow 115409, Russian Federation
[3]Scientific Research Institute of System Studies, Russian Academy of Sciences, 36-1 Nakhimovsky Prosp., Moscow 117218, Russian Federation
[4]State Research Center "State Scientific Research Institute of Chemistry and Technology of Organo-Element Compounds," 38 Entuziastov Shosse, Moscow 105118, Russian Federation

Abstract: A model for the heterogeneous interaction of air oxygen with fuel (triethyl aluminum) microdroplets is proposed. It is assumed that the main reaction responsible for the self-ignition of a stoichiometric mixture of fuel with air is the reaction of the intrusion of oxygen molecules into fuel molecules with the subsequent monomolecular decomposition of the intrusion product and the release of light hydrocarbon radicals into the gas phase. The rate of release was determined depending on the size of the microdroplets and the activation energy of the intrusion reaction rate constant. In the gas phase, the radicals interact with oxygen, generating other sequential and parallel reactions, the same as in the gas-phase kinetics of oxidation, ignition, and combustion of light alkanes (methane, ethane, and butane) and their derivatives. Chemical kinetic schemes and the corresponding kinetic equations as well as algorithms and codes relevant to such gas-phase processes exist and are intended to be used for the numerical solution of the problem of triethyl aluminum self-ignition.

Keywords: triethyl aluminum; implantation reaction; rate constant; activation energy; microdroplet; ignition delay (induction period); direct and inverse problems

DOI: 10.30826/CE19120310

Acknowledgments

This work was supported by the subsidy given to the N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences to implement the state assignment on the topic No. 0082-2016-0011 "Fundamental studies of conversion processes of energetic materials and development of scientific grounds for controlling these processes" (Registration No. AAAA-A17-117040610346-5) and to the Scientific Research Institute for System Analysis to implement the state assignment on the topic No. 0065-2019-0005 "Mathematical modeling of dynamic processes in deformed and reactive media using multiprocessor computational systems" (Registration No. AAAA-A19- 119011590092-6), and partly by the Russian Foundation for Basic Research (project 16-29-01065ofi-m).

References

1. Kuznetsov, N. M., S. M. Frolov, and P. A. Storozhenko. 2019. Raschet standartnoy ental'pii obrazovaniya i teploty polnogo sgoraniya trietilalyuminiya v vodyanom pare i vozdukhe [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.
2. Kondratiev, V. N., ed. 1974. *Energii razryva khimicheskikh svyazei, potentsialy ionizatsii i srodstvo k elektronu: Spravochnik* [Energy of breaking chemical bonds. Ionization potentials and electron affinity: The handbook]. Moscow: Nauka. 352 p.
3. Dean, J. A. *Lange's handbook of chemistry*. 15th ed. McGraw-Hill. 1292 p.
4. Mischenko, K. P., and A. A. Ravdel', eds. 1967. Kratkiy spravochnik fiziko-khimicheskikh velichin [Short handbook of phisico-chemical values]. 5th ed. Leningrad: Khimiya Publs. 184 p.
5. Robinson, P. J., and K. A. Holbrook. 1972. *Unimolecular reactions*. London: Wiley-Interscience. 388 p.
6. Kuznetsov, N. M. 1982. *Kinetika monomolekulyarnykh reaktsii* [Kinetics of monomolecular reactions]. Moscow: Nauka. 221 p.
7. Kondratiev, V. N., E. E. Nikitin, A. O. Reznikov, and S. Ya. Umanskii. 1976. *Termicheskie bimolekulyarnye reak-*

tsii v gazakh [Thermal bimolecular reactions in gases]. Moscow: Nauka. 191 p.

8. Semenov, N. N. 2005. *Izbrannye trudy. T. 3: O nekotorykh problemakh khimicheskoy kinetiki i reaktsionnoy sposobnosti* [Selected works. Vol. 3: On some problems of chemical kinetics and reactivity]. Moscow: Nauka. 499 p.

Received June 27, 2019

Contributors

Kuznetsov Nikolay M. (b. 1929) — Doctor of Science in physics and mathematics, professor, 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; N-M-Kuznetsov@yandex.ru

Frolov Sergey M. (b. 1959) — Doctor of Science in physics and mathematics, head of department, 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; professor, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; senior research scientist, Scientific Research Institute for System Analysis, Russian Academy of Sciences, 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; smfrol@chph.ras.ru

Storozhenko Pavel A. (b. 1950) — Doctor of Science in chemistry, professor, Academician of the Russian Academy of Sciences, director, State Research Center "State Scientific Research Institute of Chemistry and Technology of Organo-Element Compounds," 38 Entuziastov Shosse, Moscow 105118, Russian Federation; bigpastor@mail.ru

Shamshin Igor O. (b. 1975) — Candidate of Science in physics and mathematics, 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; research scientist, Scientific Research Institute for System Studies, Russian Academy of Sciences, 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; igor_shamshin@mail.ru