PYROLYSIS AND SELF-IGNITION KINETICS OF ACETONE BEHIND REFLECTED SHOCK WAVES: AN EXPERIMENT AND NUMERICAL SIMULATION

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Abstract: An experimental study of the self-ignition of a $0.5\%(CH_3)_2CO + 2\%O_2 + Ar$ stoichiometric mixture behind reflected shock waves at temperatures of 1280–1720 K and a total mixture concentration of $[M_{50}] \approx 1 \cdot 10^{-5}$ mol/cm^3 was carried out. The kinetics of the process was monitored through the absorption of CH_3 radicals ($\lambda = 216$ nm) and the emission of electronically excited OH^* radicals ($\lambda = 308$ nm). Numerical simulations were performed using various detailed kinetic mechanisms (DKM). The main reactions affecting the pyrolysis of acetone and the self-ignition of acetone–oxygen mixture were determined. It was shown that despite the significantly different descriptions of the CH_3 time profiles, various DKM closely reproduce the temperature dependence of the ignition delay time.

Keywords: self-ignition kinetics; numerical simulations; detailed kinetic mechanisms; ignition delay time, absorption and emission measurements of radicals

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References

1. Singh, H. B., D. O'Hara, D. Herlth, W. Sachse, D. R. Blake, J. D. Bradshaw, M. Kanakidou, and P. J. Crutzen. 1994. Acetone in the atmosphere: Distribution, sources, and sinks. *J. Geophys. Res. Atmos.* 99:1805–1819.
2. Yujing, M., and A. Mellouki. 2000. The near-UV absorption cross sections for several ketones. *J. Photoch. Photobio A* 134(1-2):31–36.
3. Sato K., and Y. Hidaka. 2000. Shock-tube and modeling study of acetone pyrolysis and oxidation. *Combust. Flame* 122:291–311.
4. Tsuboi, T., K. Ishii, and S. Tamura. 2001. Thermal oxidation of acetone behind reflected shock wave. *Nihon Kikai Gakkai Ronbunshu B Hen Tr. Jpn. Soc. Mech. Eng. B* 67:2797–2804.
5. Pichon, S., G. Black, N. Chaumeix, M. Yahyaoui, J. M. Simmie, H. J. Curran, and R. Donohue. 2009. The combustion chemistry of a fuel tracer: Measured flame speeds and ignition delays and a detailed chemical kinetic model for the oxidation of acetone. *Combust. Flame* 156:494–504.
6. Saxena, S., J. H. Kiefer, and S. J. Klippenstein. 2009. A shock-tube and theory study of the dissociation of acetone and subsequent recombination of methyl radicals. *32nd Symposium (International) on Combustion Proceedings.* Pittsburgh, PA: The Combustion Institute. 123–130.
7. Davidson, D. F., S. C. Ranganath, K.-Y. Lam, M. Liaw, Z. Hong, and R. K. Hanson. 2010. Ignition delay time measurements of normal alkanes and simple oxygenates. *J. Propul. Power* 26(2):280–287.
8. Chong, Ch. T., and S. Hochgreb. 2011. Measurements of laminar flame speeds of acetone/methane/air mixtures. *Combust. Flame* 158(3):490–500.
9. Akih-Kumgeh, B., and J. M. Bergthorson. 2011. Ignition of C_3 oxygenated hydrocarbons and chemical kinetic modeling of propanal oxidation. *Combust. Flame* 158(10):1877–1889.
10. Lam, K.-Y. 2013. Shock tube measurements of oxygenated fuel combustion using laser absorption spectroscopy. Stanford University. Diss.
11. Tereza, A. M., V. N. Smirnov, P. A. Vlasov, V. V. Shumova, and A. A. Garmash. 2017. Emission of OH^* and CO_2^* during the high-temperature oxidation of acetone in reflected shock waves. *J. Phys. Conf. Ser.* 496:012071. 8 p.
12. Yua, D., Zh.-Y. Tian, Z. Wang, Yu.-X. Liu, and L. Zhou. 2018. Experimental and theoretical study on acetone pyrolysis in a jet-stirred reactor *Fuel* 234:1380–1387.

13. Vlasov, P. A., N. V. Nazarova, V. N. Smirnov, and A. M. Tereza. 2018. Vosplamenenie stekhiometricheskoy smesi atsetona s kislorodom za otrazhennymi udarnymi volnami: chislennoe modelirovanie kinetiki svecheniya OH^*, CO_2^* i pogloshcheniya CO_2 [Ignition of a stoichiometric acetone–oxygen mixture behind reflected shock waves: Numerical simulation of the kinetics of luminescence of OH^*, CO_2^* and absorption of CO_2] *Goren. Vzryv (Mosk.) — Combustion and Explosion* 11(2):4–10.
14. Vlasov, P. A., V. N. Smirnov, and A. M. Tereza. 2016. Reactions of initiation of the autoignition of H_2–O_2 mixtures in shock waves. *Russ. J. Phys. Chem. B* 10(3):456–468.
15. Smirnov, V. N., A. M. Tereza, P. A. Vlasov, and I. V. Zhiltsova. 2017. Luminescent characteristics of the shock-wave ignition of an ethylene–oxygen mixture. *Combust. Sci. Technol.* 189(5):854–868.
16. Kee, R. J., F. M. Rupley, E. Meeks, and J. A. Miller. 1996. CHEMKIN III. Livermore, CA: Sandia National Laboratories. Technicl Report No. SAND96-8216.
17. Westbrook, C. K., W. J. Pitz, O. Herbinet, H. J. Curran, and E. J. Silke. 2008. A detailed chemical kinetic reaction mechanism for n-alkane hydrocarbons from n-octane to n-hexadecane. *Combust. Flame* 156(1):181–199.
18. Wang, H., S. J. Warner, M. A. Oehlschlaeger, R. Bounaceur, J. Biet, and P. A. Glaude. 2010. An experimental and kinetic modeling study of the autoignition of α-methylnaphthalene/air and α-methylnaphthalene/n-decane/air mixtures at elevated pressures. *Combust. Flame* 157:1976–1978.
19. Metcalfe, W. K., S. M. Burke, S. S. Ahmed, and H. J. Curran. 2013. A hierarchical and comparative kinetic modeling study of C_1–C_2 hydrocarbon and oxygenated fuels. *Int. J. Chem. Kinet.* 45:638–675.
20. Wang, H., A. B. Dempsey, M. Yao, M. Jia, and R. D. Reitz. 2014. Kinetic and numerical study on the effects of di-tert-butyl peroxide additive on the reactivity of methanol and ethanol. *Energ. Fuel.* 28(8):5480–5488.
21. Frenklach, M. 1984. Modeling. *Combustion chemistry*. Ed. W. C. Gardiner, Jr. New York, NY: Springer-Verlag. 423–473.
22. Gardiner, W. C., Jr., and J. Troe. 1984. Rate coefficients of thermal dissociation, izometrization, and recombination reactions. *Combustion chemistry*. Ed. W. C. Gardiner, Jr. New York, NY: Springer-Verlag. 173–196.

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