EXPERIMENTAL AND MODELING STUDY OF CHEMICAL IONIZATION IN THE OXIDATION OF ACETYLENE AND METHANE MIXTURES BEHIND REFLECTED SHOCK WAVES

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Abstract: Chemical ionization during the oxidation of methane and acetylene is experimentally and theoretically studied behind reflected shock waves over a wide temperature range and atmospheric pressure. The results of experimental measurements of the concentration of free electrons by microwave interferometry and electric probe method during the oxidation of acetylene and methane behind reflected shock waves are presented. A detailed kinetic model of the process of chemical ionization was developed. The results of experimental measurements and kinetic simulations are in good qualitative and quantitative agreement. The kinetic model of chemical ionization makes it possible to improve the kinetic description of the experimentally measured time histories of free electrons for the hydrocarbons studied.

Keywords: chemical ionization; free electrons; microwave interferometer; electric probes; shock waves; kinetic modeling

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References

1. Gaydon, A. G., and H. G. Wolfhard. 1960. *Flames, their structure, radiation and temperature*. London: Chapman and Hall. 383 p.
2. Calcote, H. F. 1949. Electric properties of flames: Burner flames in transverse electric fields. *Proc. Combust. Inst.* 3:245–253.
3. Aravin, G. S. 1951. Ionizatsiya plameni i plamennykh gazov v usloviyakh bomby i dvigatelya [Ionization of flames and flame gases in a combustion bomb and in an engine]. Moscow: N. N. Semenov Institute of Chemical Physics. PhD Diss. 300 p.

4. Kern, R. D., H. J. Singh, and K. Xie. 1990. Identification of chemi-ions formed by reactions of deuterated fuels in the reflected shock zone. *J. Phys. Chem.* 94:3333–3335.
5. Calcote, H. F. 1962. Ion production and recombination in flames. *Proc. Combust. Inst.* 8:184–199.
6. Schofield, K. 2008. The enigmatic mechanism of the flame ionization detector: Its overlooked implications for fossil fuel combustion modeling. *Prog. Energ. Combust. Sci.* 34:330–350.
7. Fialkov, A. B. 1997. Investigation on ions in flames. *Prog. Energ. Combust. Sci.* 23:399–528.
8. Lawton, J., and F. J. Weinberg. 1969. *Electrical aspects of combustion*. Oxford: University of London, Clarendon Press. 355 p.
9. Docquier, N., and S. Candel. 2002. Combustion control and sensors: A review. *Prog. Energ. Combust. Sci.* 28:107–150.
10. Ballester, J., and T. Garcia-Armingol. 2010. Diagnostic techniques for the monitoring and control of practical flames. *Prog. Energ. Combust. Sci.* 36(4):375–411.
11. Cheung, A. Y., and D. W. Koopman. 1972. A Lecher wire microwave interferometer for measurements of electron density and electron temperature in a flowing transient plasma. *Rev. Sci. Instrum.* 43(10):1444–1450.
12. Tudisco, O., A. L. Fabris, C. Falcetta, L. Accatino, R. De Angelis, M. Manente, F. Ferri, M. Florean, C. Neri, C. Mazzotta, D. Pavarin, F. Pollastrone, G. Rocchi, A. Selmo, L. Tasinato, F. Trezzolani, and A. A. Tuccillo. 2013. A microwave interferometer for small and tenuous plasma density measurements. *Rev. Sci. Instrum.* 84:033505-1–033505-7.
13. Smy, P. R. 1976. The use of Langmuir probes in the study of high pressure plasmas. *Adv. Phys.* 25(5):517–553.
14. Vlasov, P. A. 2000. Probe methods of diagnostics of chemically reacting dense plasma. *Plasma diagnostics*. Eds. A. A. Ovsyannikov and M. F. Zhukov. Cambridge International Science Publs., CISP. Ch. 12. P. 299–337.
15. Becker, K. H., D. Kley, and R. J. Norstrom. 1969. OH^* chemiluminescence in hydrocarbon atom flames. *Proc. Combust. Instit.* 12:405–411.
16. Agafonov, G. L., I. V. Bilera, P. A. Vlasov, Yu. A. Kolbanovskii, V. N. Smirnov, and A. M. Tereza. 2015. Obrazovanie sazhi pri pirolize i okislenii atsetilena i etilena v udarnykh volnakh [Soot formation during the pyrolysis and oxidation of acetylene and ethylene in shock waves]. *Kinet. Catal.* 56(1):12–30.
17. Agafonov, G. L., V. N. Smirnov, and P. A. Vlasov. 2010. Shock tube and modeling study of soot formation during pyrolysis of propane, propane/toluene and rich propane/oxygen mixtures. *Combust. Sci. Technol.* 182:1645–1671.
18. Agafonov, G. L., V. N. Smirnov, and P. A. Vlasov. 2011. Shock tube and modeling study of soot formation during the pyrolysis and oxidation of a number of aliphatic and aromatic hydrocarbons. *Proc. Combust. Inst.* 33:625–632.
19. Vlasov, P. A., Yu. K. Karasevich, I. L. Pankrat'eva, and V. A. Polyanskii. 2008. Metody issledovaniya kinetiki ionizatsii v udarnykh volnakh [Research technique of the ionization kinetics in shock waves]. *Physical-Chemical Kinetics in Gas Dynamics* 6. 32 p. Available at: www.chemphys.edu.ru/pdf/2008-12-25-001.pdf (accessed February 24, 2016).
20. Karasevich, Yu. K. 2009. Kinetics of chemical ionization in shock waves: IV. Kinetic model of ionization in acetylene oxidation. *Kinet. Catal.* 50(5):617–626.

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