DEFLAGRATION-TO-DETONATION TRANSITION IN AIR MIXTURES OF HYDROGEN–METHANE FUEL

I. O. Shamshin[1], M. V. Kazachenko[1], S. M. Frolov[1,2], and V. Ya. Basevich[1]

[1]N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation

[2]A. G. Merzhanov Institute of Structural Macrokinetics and Materials Science of the Russian Academy of Sciences, 8 Acad. Osipyan Str., Chernogolovka, Moscow Region 142432, Russian Federation

Abstract: The previously proposed experimental method for evaluating the detonability of fuel–air mixtures, based on measuring the run-up distance L_{DDT} and/or run-up time τ_{DDT} of deflagration-to-detonation transition (DDT) in a standard pulsed detonation tube, was applied to study the DDT in stoichiometric air mixtures of blended methane–hydrogen fuel with a volume fraction of hydrogen x_{H_2} ranging from 0 to 1 under the fixed thermodynamic and gasdynamic conditions. Based on the known data on combustion and self-ignition of such a fuel, it was expected that the DDT run-up distance and time should gradually decrease with hydrogen concentration x_{H_2}. Contrary to expectations, the dependences of L_{DDT} and τ_{DDT} on x_{H_2} in the range $0.25 < x_{\mathrm{H}_2} < 0.65$ turned out to be irregular: instead of a monotonic decrease, L_{DDT} and τ_{DDT} reach local maxima.

Keywords: methane–hydrogen fuel; fuel–air mixture; detonability; standard pulsed detonation tube; deflagration-to-detonation transition

DOI: 10.30826/CE20130306

Figure Captions

Figure 1 Schematic of standard pulsed detonation tube with indication of measuring segments: * — location of spark plug; **0** — location of a special probe; **1**–**15** — cross-sections of ionization probes; and **8**–**9** and **11**–**15** — cross sections of pressure sensors. Dimensions are in millimeters

Figure 2 Detonation velocity–distance plots for the development of the DDT process in 10 successive shots in a stoichiometric air mixture of methane–hydrogen fuel with $x_{\mathrm{H}_2} = 0$ (*a*), 0.2 (*b*), 0.25 (*c*), 0.3 (*d*), 0.35 (*e*), 0.4 (*f*), 0.45 (*g*), 0.5 (*h*), 0.55 (*i*), 0.6 (*j*), 0.65 (*k*), 0.7 (*l*), 0.8 (*m*), 0.9 (*n*), 0.95 (*o*), and 1 (*p*)

Figure 3 Time–distance diagram for the development of the DDT process in a stoichiometric air mixture of methane–hydrogen fuel with $x_{\mathrm{H}_2} = 0.3$ in 10 successive shots

Figure 4 Primary records of pressure sensors (solid curves) and ionization probes (dashed curves) in measuring sections **5** (*a*), **6** (*b*), **7** (*c*), and **8** (*d*) in one of 10 shots for a fuel mixture with $x_{\mathrm{H}_2} = 0.4$

Figure 5 Primary records of pressure sensors (solid curves) and ionization probes (dashed curves) in measuring sections **5** (*a*), **6** (*b*), **7** (*c*), and **8** (*d*) in one of 10 shots for a fuel mixture with $x_{\mathrm{H}_2} = 0.8$

Figure 6 Measured DDT run-up distance L_{DDT} (*a*) and run-up time τ_{DDT} as functions on hydrogen volume fraction x_{H_2} in a stoichiometric air mixture of methane–hydrogen fuel. Dashed lines correspond to the DDT at $x_{\mathrm{H}_2} \geq 0.8$ in the flame acceleration section of the standard pulsed detonation tube

Figure 7 Measured dependences of the reaction front propagation velocities at two measuring segments **3**–**4** and **4**–**5** before entering the screw (focusing) section of the detonation tube and at measuring segment **8**–**9** at the exit from the screw section

Figure 8 Calculated dependences of the self-ignition delay on temperature, pressure (*1* — 1 MPa; *2* — 2; and *3* — 3 MPa), and volume fraction of hydrogen x_{H_2} in a stoichiometric air mixture of methane–hydrogen fuel: A — $T_0 = 1000$ K; B — 1200; and C — $T_0 = 1400$ K

Table Captions

Table 1 Composition of natural gas (%(vol.))

Table 2 Results of thermodynamic calculations of mean molecular mass, specific heat ratio, sound velocity, and Chapman–Jouguet detonation velocity for stoichiometric air mixtures of methane–hydrogen fuel with different x_{H_2} at $T_0 = 300$ K and $P_0 = 0.1$ MPa

Acknowledgments

The 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 (Registration No. AAAA-A17-117040610346-5) and to the A. G. Merzhanov Institute of Structural Macrokinetics and Materials Science of the Russian Academy of Sciences to implement the state assignment on the topic 45.2. The authors are grateful to Dr. I. V. Bilera for help with the chromatographic analysis of natural gas composition.

References

1. Sokolik, A. S., and K. I. Shchelkin. 1933. Rasprostranenie plameni v smesyakh metana s kislorodom v zakrytykh trubakh [Flame propagation in mixtures of methane with oxygen in closed tubes]. *Zh. Fiz. Khim.* [Russ. J. Phys. Chem. A] 4(1):109–128.
2. Sokolik, A. S. 1960. *Samovosplamenenie, plamya i detonatsiya v gazakh* [Self-ignition, flame, and detonation in gases]. Moscow: USSR AS Publs. 422 p.
3. Lee, J. H. S. 2008. *The detonation phenomenon*. New York, NY: The Cambridge University Press. 400 p.
4. Frolov, S. M. and B. E. Gel'fand. 1990. O predel'nom diameter rasprostraneniya gazovoy detonatsii v trubakh [On the limiting diameter of propagation of gas detonation in tubes]. *Dokl. Akad. Nauk* 312(5):1177–1180.
5. Frolov, S. M., I. O. Shamshin, V. S. Aksenov, M. V. Kazachenko, and P. A. Gusev. 2019. Ranzhirovanie gazovykh toplivno-vozdushnykh smesey po ikh detonatsionnoy sposobnosti s pomoshch'yu etalonnoy impul'snodetonatsionnoy truby [Ranking of gaseous fuel–air mixtures according to their detonability using a standard pulsed detonation tube]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 12(3):78–90. doi: 10.30826/CE19120309.
6. Frolov S. M., V. I. Zvegintsev., V. S. Aksenov, I. V. Bilera, M. V. Kazachenko, I. O. Shamshin, P. A. Gusev, and M. S. Belotserkovskaya. 2000. Detonability of fuel–air mixtures. *Shock Waves*. doi: 10.1007/s00193-020-00966-9.
7. Karim, G. A., I. Wierzba, and Y. Al-Alousi. 1996. Methane–hydrogen mixtures as fuels. *Int. J. Hydrogen Energ.* 21(7):625–631.
8. Kozlov, V. E., I. V. Chechet, S. G. Matveev, N. S. Titova, and A. M. Starik. 2016. Modeling study of combustion and pollutant formation in HCCI engine operating on hydrogen rich fuel blends. *Int. J. Hydrogen Energ.* 41:3689–3700. doi: 10.1016/j.ijhydene.2015.12.078.
9. Halter, F., C. Chauveau, N. Djebaiily-Chaumeix, and I. Goekalp. 2005. Characterization of the effects of pressure and hydrogen concentration on laminar burning velocities of methane–hydrogen–air mixtures. *P. Combust. Inst.* 30:201–208. doi: 10.1016/j.proci.2004.08.195.
10. Ilbas, M., A. P. Crayford, I. Yilmaz, P. J. Bowen, and N. Syred. 2006. Laminar-burning velocities of hydrogen–air and hydrogen–methane–air mixtures: An experimental study. *Int. J. Hydrogen Energ.* 31:1768–1779. doi: 10.1016/j.ijhydene.2005.12.007.
11. Boushaki, T., Y. Dhue, L. Selle, B. Ferret, and T. Poinsot. 2012. Effects of hydrogen and steam addition on laminar burning velocity of methane–air premixed flame: Experimental and numerical analysis. *Int. J. Hydrogen Energ.* 37:9412–9422. doi: 10.1016/j.ijhydene.2012.03.037.
12. Donohoe, N., A. Heufer, W. K. Metcalfe, H. J. Curran, M. L. Davis, O. Mathieu, D. Plichta, A. Morones, E. L. Petersen, and F. Guethe. 2014. Ignition delay times, laminar flame speeds, and mechanism validation for natural gas/hydrogen blends at elevated pressures. *Combust. Flame* 161:1432–1443. doi: 10.1016/j.combustflame.2013.12.005.
13. Miao, Haiyan, Lin Lu, and Zuohua Huang. 2011. Flammability limits of hydrogen-enriched natural gas. *Int. J. Hydrogen Energy* 36:6937–6947. doi: 10.1016/j.ijhydene.2011.02.126.
14. Troshin, K. Ya., A. A. Belyaev, A. V. Arutyunov, A. A. Tsarenko, A. V. Nikitin, and V. S. Arutyunov. 2020. Vliyanie davleniya na samovosplamenenie metanovodorodnykh smesey s vozdukhom [The influence of pressure on the self-ignition delay of methane–hydrogen–air mixtures] *Goren. Vzryv (Mosk.) — Combustion and Explosion* 13(1):18–32. doi: 10.30826/CE20130102.
15. Zhang, Y., Z. Huang, L. Wei, J. Zhang, and C. K. Law. 2019. Experimental and modeling study on ignition delays of lean mixtures of methane, hydrogen, oxygen, and argon at elevated pressures. *Combust. Flame* 159:918–931. doi: 10.1016/j.combustflame.2011.09.010.
16. Herzler, J., and C. Naumann. 2009. Shock-tube study of the ignition of methane/ethane/hydrogen mixtures with hydrogen contents from 0% to 100% at different pressures. *P. Combust. Inst.* 32:213–220. doi: 10.1016/j.proci.2008.07.034.
17. Medvedev, S. P., A. N. Polenov, S. V. Khomik, and B. E. Gel'fand. 2010. Deflagration-to-detonation transition in air-binary fuel mixtures in an obstacle laden channel. *Russ. J. Phys. Chem. B* 4(1):70–74. doi: 10.1134/S1990793110010112.
18. Meyer, J. W., P. A. Urtiew, and A. K. Oppenheim. 1970. On the inadequacy of gasdynamic processes for triggering the transition to detonation. *Combust. Flame* 14:13–20.
19. Lee, J. H. S., R. Knystautas, and A. Freiman. 1984. High speed turbulent deflagrations and transition to detonation in H_2–air mixtures. *Combust. Flame* 56:227–239.
20. Cantera. Available at: www.cantera.org (accessed August 12, 2020).
21. Azatyan, V. V., A. M. Kogan, M. G. Neuhaus, A. I. Poroikova, and T. N. Aleksandrov. 1975. Rol' samorazogreva pri gorenii vodoroda vblizi pervogo predella vosplameneniya [The role of self-heating in combustion of

hydrogen in the vicinity to the first ignition limit]. *Kinet. Catal.* 16(3):577–585.

22. Basevich, V. Ya., A. A. Belyaev, V. S. Posvyanskii, and S. M. Frolov. 2013. Mechanisms of the oxidation and combustion of normal paraffin hydrocarbons: Transition from C_1–C_{10} to C_{11}–C_{16}. *Russ. J. Phys. Chem. B* 7(2):161–169. doi: 10.1134/S1990793113020103.
23. 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 isooctane. *Russ. J. Phys. Chem. B* 10(5):801–809. doi: 10.1134/S199079311605016X.
24. Slack, M. W. 1977. Rate coeeficient for $H + O_2 + M = HO_2 + M$ evaluated from shock tube measurements of induction times. *Combust. Flame* 28:241–249.

Received August 14, 2020

Contributors

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; igor_shamshin@mail.ru

Kazachenko Maxim V. (b. 1997) — junior research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; maksx71997@gmail.com

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; head of laboratory, A. G. Merzhanov Institute of Structural Macrokinetics and Materials Science of the Russian Academy of Sciences, 8 Acad. Osipyan Str., Chernogolovka, Moscow Region 142432, Russian Federation; smfrol@chph.ras.ru

Basevich Valentin Ya. (b. 1926) — Doctor of Science in technology, 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; basevichv@yandex.ru