

DEFLAGRATION-TO-DETINATION TRANSITION IN AIR MIXTURES OF PROPANE–HYDROGEN FUEL

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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 propane–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} and the corresponding dependences should be close to linear. Contrary to expectations, the observed dependences turned out to be nonlinear and, in some cases, nonmonotonic: they exhibit local maxima. Analysis of the results suggests that the observed dependences are a manifestation of the physicochemical properties of the fuel mixtures under study. A change in the design of the flame acceleration section in the detonation tube as a whole does not affect the nature of the obtained dependences: they remain nonlinear, although the nonmonotonicity degenerates. Like other critical phenomena in chemical kinetics, nonmonotonicity can manifest itself only near critical conditions and is obscured by other effects when moving away from the critical conditions.

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

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Figure Captions

Figure 1 Three configurations of standard pulsed detonation tube with indication of measuring segments: (a) K1; (b) K2; and (c) K3; * — location of spark plug. Dimensions are in millimeters

Figure 2 Detonation velocity – distance plots for the development of DDT process in detonation tubes of configuration K1 in 5 successive shots in a stoichiometric air mixture of propane–hydrogen fuel with $x_{H_2} = 0$ (a), 0.2 (b), 0.4 (c), 0.6 (d), 0.8 (e), and 1 (f)

Figure 3 Detonation velocity – distance plots for the development of DDT process in detonation tubes of configuration K2 in 5 successive shots in a stoichiometric air mixture of propane–hydrogen fuel with $x_{H_2} = 0$ (a), 0.2 (b), 0.4 (c), 0.6 (d), 0.8 (e), and 1 (f)

Figure 4 Detonation velocity – distance plots for the development of DDT process in detonation tubes of configuration K3 in 5 successive shots in a stoichiometric air mixture of propane–hydrogen fuel with $x_{H_2} = 0$ (a), 0.2 (b), 0.4 (c), 0.6 (d), 0.8 (e), and 1 (f)

Figure 5 Detonation velocity – distance plots for the development of DDT process in detonation tubes of configuration K2 in 5 successive shots in a stoichiometric air mixture of propane–hydrogen fuel with $x_{H_2} = 0.95$ (a), 0.96 (b), 0.97 (c), 0.98 (d), and 0.99 (e)

Figure 6 Averaged over 5 successive shots dependences of flame acceleration on the traveled distance during DDT in stoichiometric air mixtures of propane–hydrogen fuel with $x_{H_2} = 1.0$ (1) and 0.99 (2) in the detonation tube of configuration K2

Figure 7 Time–distance diagram of DDT process in a stoichiometric air mixture of propane–hydrogen fuel with $x_{H_2} = 0.4$ in 5 successive shots in the detonation tube of configuration K3

Figure 8 Primary records of pressure sensors (solid curves) and ionization probes (dotted curves) in measuring sections 4 to 17 for one of the shots with a stoichiometric air mixture of propane–hydrogen fuel with $x_{H_2} = 0.2$ in the detonation tube of configuration K1

Figure 9 Measured DDT run-up distance L_{DDT} (a) and run-up time τ_{DDT} (b) as functions on hydrogen volume fraction x_{H_2} in stoichiometric air mixtures of propane–hydrogen fuel: 1 — K1; 2 — K2; and 3 — K3. Error bars correspond to the shot-to-shot scatter

Figure 10 Measured DDT run-up distance L_{DDT} (a) and run-up time τ_{DDT} (b) as functions on hydrogen volume fraction x_{H_2} in stoichiometric air mixtures of methane–hydrogen fuel: 1 — K1; 2 — K2; and 3 — K3

Figure 11 Dependences of the shock wave velocity (left scale) and the time lag of the reaction front from the shock wave (right scale) at the measuring segments upstream the helical section (6–7 (a) and 7–8 (b)) and inside the helical section (7–8 (a) and 8–9 (b)) on the hydrogen volume fraction in stoichiometric air mixtures of propane–hydrogen fuel in the detonation tube of configurations K1 (a) and K2 (b)

Figure 12 Calculated dependences of the self-ignition delays on x_{H_2} , P , and T for stoichiometric air mixtures of propane–hydrogen (solid curves) and methane–hydrogen (dashed curves) fuels

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References

- Shamshin, I. O., M. V. Kazachenko, S. M. Frolov, and V. Ya. Basevich 2020. Perekhod gorenija v detonatsiyu v vozdušnykh smesyah metanovodorodnogo goryuchego [Deflagration-to-detonation transition in air mixtures of hydrogen–methane fuel]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 13(3):60–75. doi: 10.30826/CE20130306.
- Sokolik, A. S., and K. I. Shchelkin. 1933. Rasprostranenie plameni v smesyah 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.
- Sokolik, A. S. 1960. *Samovosplamenenie, plamya i detonatsiya v gazakh* [Self-ignition, flame, and detonation in gases]. Moscow: USSR AS Publs. 422 p.
- Lee, J. H. S. 2008. *The detonation phenomenon*. — New York, NY: The Cambridge University Press. 400 p.
- Frolov, S. M., and B. E. Gel'fand. 1990. O predel'nom diametre rasprostraneniya gazovoy detonatsii v trubakh [Limiting diameter for gas detonation propagation in tubes]. *Dokl. Acad. Nauk SSSR* 312(5):1177–1180.
- Frolov, S. M., I. O. Shamshin, V. S. Aksenov, M. B. Kazachenko, and P.A. Gusev. 2019. Ranzhirovanie gazovykh toplivno-vozdushnykh smesey po ikh detonatsionnoy sposobnosti s poshch'yu etaloonoy impul'sno-detonatsionnoy 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.
- Frolov, S. M., V. I. Zvegintsev, V. S. Aksenov, I. V. Bileira, M. V. Kazachenko, I. O. Shamshin, P. A. Gusev, and M. S. Belotserkovskaya. 2020. Detonability of fuel–air mixtures. *Shock Waves* 30:721–739. doi: 10.1007/s00193-020-00966-9.
- Metghalchi, M., and J. C. Keck. 1980. Laminar burning velocity of propane–air mixtures at high temperature and pressure. *Combust. Flame* 38:143–154. doi: 10.1016/0010-2180(80)90046-2.
- Bosschaart, K. J., L. P. H. de Goey, and J. M. Burgers. 2004. The laminar burning velocity of flames propagating in mixtures of hydrocarbons and air measured with the heat flux method. *Combust. Flame* 136(3):261–269.
- Marley, S. K., and W. L. Roberts. 2005. Measurements of laminar burning velocity and Markstein number using high-speed chemiluminescence imaging. *Combust. Flame* 141(4):473–477. doi: 10.1016/j.combustflame.2005.02.011.
- Huzayyin, A. S., H. A. Moneib, M. S. Shehatta, and A. M. A. Attia. 2008. Laminar burning velocity and explosion index of LPG–air and propane–air mixtures. *Fuel* 87:39–57. doi: 10.1016/j.fuel.2007.04.001.
- Akram, M., V. Ratna Kishore, and S. Kumar. 2012. Laminar burning velocity of propane/CO₂/N₂–air mixtures at elevated temperatures. *Energ. Fuel.* 26:5509–5518. doi: 10.1021/ef301000k.
- Dowdy, D. R., D. B. Smith, S. C. Taylor, and A. Williams. 1991. The use of expanding spherical flames to determine burning velocities and stretch effects in hydrogen/air mixtures. *23th Symposium (International) on Combustion Proceedings*. Pittsburgh, PA: The Combustion Institute. 23(1):325–332. doi: 10.1016/S0082-0784(06)80275-4.
- Kwon, O. C., L.-K. Tseng, and G. M. Faeth. 1992. Laminar burning velocities and transition to unstable flames in H₂/O₂/N₂ and C₃H₈/O₂/N₂ mixtures. *Combust. Flame* 90(3-4):230–246. doi: 10.1016/0010-2180(92)90085-4.
- Tse, S. D., D. L. Zhu, and C. K. Law. 2000. Morphology and burning rates of expanding spherical

- flames in H₂/O₂/inert mixtures up to 60 atmospheres. *P. Combust. Inst.* 28(2):1793–1800. doi: 10.1016/S0082-0784(00)80581-0.
- 16. Penyazkov, O. G., K. A. Ragotner, A. J. Dean, and B. Varatharajan. 2005. Autoignition of propane–air mixtures behind reflected shock waves. *P. Combust. Inst.* 30:1941–1947. doi:10.1016/j.proci.2004.08.122.
 - 17. Gallagher, S. M., H. J. Curran, W. K. Metcalfe, D. Healy, J. M. Simmie, and G. Bourque. 2008. A rapid compression machine study of the oxidation of propane in the negative temperature coefficient regime. *Combust. Flame* 153:316–333. doi: 10.1016/j.combustflame.2007.09.004.
 - 18. Cheng, R. K., and A. K. Oppenheim. 1984. Autoignition in methane–hydrogen mixtures. *Combust. Flame* 58:125–139. doi: 10.1016/0010-2180(84)90088-9.
 - 19. Kéromnès, A., W. K. Metcalfe, K. A. Heufer, N. Donohoe, A. K. Das, C.-J. Sung, J. Herzler, C. Naumann, P. Griebel, O. Mathieu, M. C. Krejci, E. L. Petersen, W. J. Pitz, and H. J. Curran. 2013. An experimental and detailed chemical kinetic modeling study of hydrogen and syngas mixture oxidation at elevated pressures. *Combust. Flame* 160(6):995–1011. doi: 10.1016/j.combustflame.2013.01.001.
 - 20. Milton, B. E., and J. C. Keck. 1984. Laminar burning velocities in stoichiometric hydrogen and hydrogen–hydrocarbon gas mixtures. *Combust. Flame* 58(1):13–22. doi: 10.1016/0010-2180(84)90074-9.
 - 21. Yu, G., C. K. Law, and C. K. Wu. 1986. Laminar flame speeds of hydrocarbon–air mixtures with hydrogen addition. *Combust. Flame* 63(3):339–347.
 - 22. Law, C. K., and O. C. Kwon. 2004. Effects of hydrocarbon substitution on atmospheric hydrogen–air flame propagation. *Int. J. Hydrogen Energ.* 29(8):867–79. doi: 10.1016/j.ijhydene.2003.09.012.
 - 23. Tang, C., Z. Huang, C. Jin, J. He, J. Wang, X. Wang, and H. Miao. 2008. Laminar burning velocities and combustion characteristics of propane–hydrogen–air premixed flames. *Int. J. Hydrogen Energ.* 33:4906–4914. doi: 10.1016/j.ijhydene.2008.06.063.
 - 24. Zhen, H. S., C. S. Cheung, C. W. Leung, and Y. S. Choy. 2012. Effects of hydrogen concentration on the emission and heat transfer of a premixed LPG-hydrogen flame. *Int. J. Hydrogen Energ.* 37(7):6097–6105. doi: 10.1016/j.ijhydene.2011.12.130.
 - 25. Titova, N. S., P. S. Kuleshov, O. N. Favorskii, and A. M. Starik. 2014. The features of ignition and combustion of composite propane–hydrogen fuel: Modeling study. *Int. J. Hydrogen Energ.* 39(12):6764–6773. doi: 10.1016/j.ijhydene.2014.01.211.
 - 26. Man, X., C. Tang, L. Wei, L. Pan, and Z. Huang. 2013. Measurements and kinetic study on ignition delay times of propane/hydrogen in argon diluted oxygen. *Int. J. Hydrogen Energ.* 38:2523–2530. doi: 10.1016/j.ijhydene.2012.12.020.
 - 27. Sevrouk, K. L., P. N. Krivosheyev, O. G. Penyazkov, S. A. Torohov, N. S. Titova, and A. M. Starik. 2016. Numerical and experimental analysis of propane–hydrogen mixture ignition in air. *J. Phys. Conf. Ser.* 774:012083. doi: 10.1088/1742-6596/774/1/012083.
 - 28. Schwer D. A., Kailasanath K. Towards an assessment of rotating detonation engines with fuel blends. AIAA Paper No. 2017-4942. doi: 10.2514/6.2017-4942.
 - 29. Basevich, V. Ya., S. N. Medvedev, F. S. Frolov, and S. M. Frolov. 2015. Promotion of the high-temperature autoignition of hydrogen–air and methane–air mixtures by normal alkanes. *Russ. J. Phys. Chem. B* 9(2):250–254. doi: 10.1134/S1990793115020025.
 - 30. 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.
 - 31. Semenov, N. N. 1934. *Tsepyne reaktsii* [Chain reactions]. Leningrad: Goskhimizdat Publ.
 - 32. Lee, J. H. S., R. Knystautas, and A. Freiman. 1984. High speed turbulent deflagrations and transition to detonation in H₂–air mixtures. *Combust. Flame* 56:227–239.
 - 33. Shchelkin, K. I. 1949. *Bystroe gorenie i spinovaya detonatsiya gazov* [Fast combustion and spinning detonation of gases]. Moscow: Voenizdat Publ. 196 p.
 - 34. 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 C₁–C₁₀ to C₁₁–C₁₆. *Russ. J. Phys. Chem. B* 7(2):161–169. doi: 10.1134/S1990793113020103.

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