

MODELING OF CELLULAR DETONATION WAVE STRUCTURE IN STOICHIOMETRIC DUAL-FUEL MIXTURE OF SYNTHESIS-GAS WITH OXIDIZER

A. V. Trotsyuk and P. A. Fomin

M. A. Lavrent'ev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, 15 Lavrent'ev Prospekt, Novosibirsk 630090, Russian Federation

Abstract: A generalized two-step chemical kinetic model of detonation of dual-fuel stoichiometric mixture of synthesis-gas with oxidizer is presented. It allows calculation of heat release in the course of chemical reaction and variation of molar mass, internal energy, and specific heat ratio of the mixture without computation of its detailed chemical composition. An algorithm for calculating the induction period of chemical reaction in the mixture under consideration according to known formulae for calculating the induction period in single-fuel mixtures of carbon monoxide and hydrogen with an oxidizer has been developed. Two-dimensional numerical calculation of the multifront detonation wave structure in the mixture under consideration at different relations between fuels is performed. Chemical transformations are described by the proposed kinetic model. Detonation cell size and qualitative wave structure (including the transformation of the cellular structure from irregular to regular with the increase in hydrogen concentration) are shown to correspond well to experimental data.

Keywords: two-fuels mixture; synthesis gas; kinetic model; detonation; cell

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Figure Captions

Figure 1 Detonation cell size in a stoichiometric mixture of syngas with air $(1 - \alpha)\text{CO} + \alpha\text{H}_2 + 0.5(\text{O}_2 + 3.76\text{N}_2)$: 1–3 and 4 – experimental data of [2] and [13], respectively; 1 — no self-sustained detonation; and 2 — detonation limit (in terms of carbon monoxide concentration) above which no self-sustaining detonation is realized

Figure 2 Calculated (1) and measured [2] detonation cell size in a stoichiometric mixture of syngas with air $(1 - \alpha)\text{CO} + \alpha\text{H}_2 + 0.5(\text{O}_2 + 3.76\text{N}_2)$: 2 — detonation; 3 — no detonation; and 4 — detonation limit

Figure 3 Detonation wave structure in a stoichiometric mixture of hydrogen with air ($\alpha = 1$): (a) flow field of normalized density; (b) numerical Schlieren-visualization; (c) temperature; and AA and BB — main transverse waves; $H = a = 1.4$ cm. Experiment [13]: $a = 1.5$ cm

Figure 4 Detonation structure in a stoichiometric mixture of syngas with air, $0.7\text{CO} + 0.3\text{H}_2 + 0.5(\text{O}_2 + 3.76\text{N}_2)$: (a) flow field of normalized density; (b) numerical Schlieren-visualization; (c) temperature; AA and BB — main transverse waves; and aa, bb, and cc — secondary transverse waves; P_1 and P_2 indicate the pockets of unburned gas; $H = a = 1.5$ cm. Experiment [2]: $a = 1.1\text{--}2.0$ cm

Figure 5 Detonation wave structure in a stoichiometric mixture of syngas with air, $0.9\text{CO} + 0.1\text{H}_2 + 0.5(\text{O}_2 + 3.76\text{N}_2)$: (a) flow field of normalized density; (b) numerical Schlieren-visualization; (c) temperature; AA and BB — main transverse waves; and aa, bb, and cc — secondary transverse waves; P_1 and P_2 indicate the pockets of unburned gas; $H = a = 2.5$ cm. Experiment [2]: $a = 2.0\text{--}4.0$ cm

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References

1. Bykovskii, F. A., S. A. Zhdan, E. F. Vedernikov, and A. N. Samsonov. 2017. Scaling factor in continuous spin detonation of syngas-air mixtures. *Combust. Explos. Shock Waves* 53(2):187–198. doi: 10.1134/S0010508217020095.
2. Austin, J. M., and J. E. Shepherd. 2003. Detonation in hydrocarbon fuel blends. *Combust. Flame* 132(1-2):73–90. doi: 10.1016/S0010-2180(02)00422-4.
3. Gamezo, V. N., D. Desbordes, and E. S. Oran. 1999. Formation and evolution of two-dimensional cellular deto-

- nations. *Combust. Flame* 116(1-2):154–165. doi: 10.1016/S0010-2180(98)00031-5.
4. Takeshima, N., K. Ozawa, N. Tsuboi, A. K. Hayashi, and Y. Morii. 2020. Numerical simulations on propane/oxygen detonation in a narrow channel using a detailed chemical mechanism: formation and detailed structure of irregular cells. *Shock Waves* 30:809–824. doi: 10.1007/s00193-020-00978-5.
 5. Tang-Yuk, K. C., X. C. Mi, J. H. S. Lee, H. D. Ng, and R. Deiterding. 2022. Transmission of a detonation wave across an inert layer. *Combust. Flame*. 236:111769. doi: 10.1016/j.combustflame.2021.111769.
 6. Fomin, P. A., A. V. Trotsyuk, and A. A. Vasil'ev. 2014. Approximate model of chemical reaction kinetics for detonation processes in mixture of CH₄ with air. *Combust. Sci. Technol.* 186(10-11):1716–1735.
 7. Nikolaev, Yu. A., and D. V. Zak. 1988. Agreement of models of chemical reactions in gases with the second law of thermodynamics. *Combust. Explos. Shock Waves* 24(4):461–464. doi: 10.1007/BF00750021.
 8. Strickland-Constable, R. F. 1949. The burning velocity of gases in relation to the ignition delay. *3rd Symposium (International) on Combustion and Flame, and Explosion Phenomena* 33(1):229–235.
 9. Nikolaev, Yu. A., A. A. Vasil'ev, and V. Yu. Ul'yanitskii. 2003. Gas detonation and its application in engineering and technologies. *Combust. Explos. Shock Waves* 39(4):382–410. doi: 10.1023/A:1024726619703.
 10. Vasil'ev, A. A. 2007. Detonation properties of the synthesis gas. *Combust. Explos. Shock Waves* 43(6):703–709. doi: 10.1007/s10573-007-0095-1.
 11. Lu, P. L., E. K. Dabora, and J. A. Nicholls. 1969. The structure of H₂–CO–O₂ detonations. *Combust. Sci. Technol.* 1(1):65–74. doi: 10.1080/00102206908952191.
 12. Strehlow, R. A., A. J. Crooker, and R. E. Cusey. 1967. Detonation initiation behind accelerating shock wave. *Combust. Flame* 11(4):339–351. doi: 10.1016/0010-2180(67)90023-5.
 13. Guirao, C. M., R. Knustautas, J. H. Lee, W. Benedick, and M. Berman. 1982. Hydrogen–air detonations. *19th Symposium (International) on Combustion Processes*. Haifa, Israel. 583–590.
 14. Vasil'ev, A. A. 2007. Ignition delay in multifuel mixtures. *Combust. Explos. Shock Waves* 43(3):282–285. doi: 10.1007/s10573-007-0041-2.
 15. Starik, A. M., N. S. Titova, A. S. Sharipov, and V. E. Kozlov. 2010. Syngas oxidation mechanism. *Combust. Explos. Shock Waves* 46(5):491–506. doi: 10.1007/s10573-010-0065-x.
 16. Nikolaev, Yu. A., and M. E. Topchiyan. 1977. Analysis of equilibrium flows in detonation waves in gases. *Combust. Explos. Shock Waves* 13(3):327–338. doi: 10.1007/BF00740309.
 17. The NASA Computer program CEARUN (Chemical Equilibrium with Applications). Available at: <https://cearun.grc.nasa.gov/index.html> (accessed February 8, 2022).
 18. Trotsyuk, A. V. Numerical simulation of the structure of two-dimensional gaseous detonation of an H₂–O₂–Ar mixture. 1999. *Combust. Explos. Shock Waves* 35(5):549–558. doi: 10.1007/BF02674500.
 19. Godunov, S. K., ed. 1976. *Chislennoe reshenie mnogomernykh zadach gazovoy dinamiki* [Numerical solutions of multidimensional problems of gasdynamics]. Moscow: Nauka. 400 p.
 20. Yamamoto, S., and H. Daiguji. 1993. Higher-order-accurate upwind schemes for solving the compressible Euler and Navier–Stokes equations. *Comput. Fluids* 22(2/3):259–270. doi: 10.1016/0045-7930(93)90058-H.
 21. Daiguji, H., X. Yuan, and S. Yamamoto. 1997. Stabilization of higher-order high resolution schemes for the compressible Navier–Stokes equation. *Int. J. Numer. Method. H.* 7(2/3):250–274. doi: 10.1108/09615539710163293.
 22. Chakravarthy, S. R., and S. Osher. 1985. A new class of high accuracy TVD schemes for hyperbolic conservation laws. AIAA Paper No. 85-0363.
 23. Lin, S.-Y., and Y.-S. Chin. 1995. Comparison of higher resolution Euler schemes for aeroacoustic computations. *AIAA J.* 33:237–245.
 24. Batten, P., M. A. Leschziner, and U. C. Goldberg. 1997. Average-state Jacobians and implicit methods for compressible viscous and turbulent flows. *J. Comput. Phys.* 137(1):38–78.
 25. Coquel, F., and B. Perthame. 1998. Relaxation of energy and approximate Riemann solvers for general pressure laws in fluid dynamics. *SIAM J. Numer. Anal.* 35(6):2223–2249.
 26. Shen, J. W., and X. Zhong. 1996. Semi-implicit Runge–Kutta schemes for non-autonomous differential equations in reactive flow computations. AIAA Paper No. 96-1969.

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Contributors

- Trotsyuk Anatoliy V.** (b. 1959) — Candidate of Science in physics and mathematics, senior research scientist, M. A. Lavrent'ev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, 15 Lavrent'ev Prospekt, Novosibirsk 630090, Russian Federation; trotsyuk@hydro.nsc.ru
- Fomin Pavel A.** (b. 1958) — Doctor of Science in physics and mathematics, senior research scientist, M. A. Lavrent'ev Institute of Hydrodynamics of the Siberian Branch of the Russian Academy of Sciences, 15 Lavrent'ev Prospekt, Novosibirsk 630090, Russian Federation; pavel_fomin_new@mail.ru