

# THREE-DIMENSIONAL DIRECT NUMERICAL SIMULATION OF TURBULENT COMBUSTION OF HYDROGEN–AIR AND METHANE–AIR MIXTURES IN THE FIELD OF SYNTHETIC TURBULENCE

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**Abstract:** The technique of three-dimensional direct numerical simulation of turbulent flame propagation in gaseous reaction mixtures under conditions of stationary, homogeneous, and isotropic synthetic turbulence is proposed. The technique is based on a detailed kinetic mechanism of combustion of a multicomponent mixture. The technique is applied to the calculation of the turbulent combustion of mainly fuel-lean hydrogen–air and methane–air mixtures. The calculated propagation speeds of a turbulent flame are in satisfactory agreement with the measured values. The calculated concentrations of the active reaction centers — OH, H, and O — are shown to be less in a turbulent flame than in the laminar flame which also agrees with experiment.

**Keywords:** direct numerical simulation; synthetic turbulence; turbulent combustion; detailed kinetic mechanism; hydrogen; methane

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## References

1. Bell, J. B., M. S. Day, and J. F. Grac. 2002. Numerical simulation of premixed turbulent methane combustion. *P. Combust. Inst.* 29:1987–1993.
2. Echekki, T., and J. H. Chen. 2003. Direct numerical simulation of autoignition in nonhomogeneous hydrogen–air mixtures. *Combust. Flame* 134(3):169–191.
3. Bell, J. B., R. K. Cheng, M. S. Day, and I. G. Shepherd. 2006. Numerical simulation of Lewis number effects on lean premixed turbulent flames. *P. Combust. Inst.* 31:1309–1317.
4. Aspden, A. J., M. S. Day, and J. B. Bell. 2016. Three-dimensional direct numerical simulation of turbulent lean premixed methane combustion with detailed kinetics. *Combust. Flame* 166:266–283.
5. Basevich, V. Ya., V. P. Volodin, S. M. Kogarko, and N. I. Peregudov. 1982. Raschety turbulentnogo plameni v dvumernom priblizhenii [Calculations of turbulent flame in two-dimensional approximation]. *Khim. Fiz.* 1(8):1130–1137.
6. Basevich, V. Ya., A. A. Belyaev, S. M. Frolov, and B. Basara. 2017. Pryamoe chislennoe modelirovanie turbulentnogo gorenija gazov v dvumernom priblizhenii [Direct numerical simulation of turbulent combustion of gases in two-dimensional approximation]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 10(1):4–10.
7. Basevich, V. Ya., A. A. Belyaev, S. M. Frolov, and F. S. Frolov. 2019. Direct numerical simulation of turbulent combustion of hydrogen–air mixtures of various compositions in a two-dimensional approximation. *Russ. J. Phys. Chem. B* 13(1):75–85.

8. Karpov, V. P., and E. S. Severin. 1980. Effects of molecular-transport coefficients on the rate of turbulent combustion. *Combust. Explos. Shock Waves* 16(1):41–46.
9. Williams, F. A. 1994. *The combustion theory*. Boca Raton, FL: CRC Press. 708 p.
10. Loitsyanskii, L. G. 2003. *Mekhanika zhidkosti i gaza* [Mechanics of liquids and gases]. Moscow: Drofa Publ. 840 p.
11. Godunov, S. K., and V. S. Ryaben'kiy. 1977. *Raznostnye skhemy* [Finite-difference schemes]. Moscow: Nauka. 440 p.
12. 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.
13. Burcat, A. Ideal gas thermodynamic data in polynomial form for combustion and air pollution use. Laboratory for Chemical Kinetics. Available at: <http://garfield.chem.elte.hu/Burcat/burcat.html> (accessed May 24, 2019).
14. Reid, C., J. Prausnitz, and T. Sherwood. 1977. *The properties of gases and liquids*. 3rd ed. London: McGraw Hill. 688 p.
15. Basevich, V. Ya., and S. M. Kogarko. 1985. Hydrocarbon formation in turbulent combustion of a methane–air mixture. *Combust. Explos. Shock Waves* 21(5):514–518.

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