

# DETONATION WAVE STRUCTURE IN A TWO-PHASE SYSTEM CONTAINING GASEOUS OXIDIZER AND LIQUID FUEL DROPLETS

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**Abstract:** The results of three-dimensional simulation of the propagation of detonation waves in suspensions of liquid isooctane droplets in air are presented. The calculation technique is based on solving mass, momentum, and energy conservation equations for the two-phase compressible turbulent reacting flow taking into account the movement, aerodynamic breakup, heating and evaporation of droplets, the finite-rate mixing of fuel components, and chemical transformations. The reliability of the method is verified by comparing the calculated and measured propagation velocities of two-phase detonations in a vertical channel of square cross section. The influence of the prehistory of the formation of a two-phase combustible mixture on the propagation velocity and structure of detonation waves in the channel is considered. New data have been obtained on the structure of the detonation waves in two-phase systems.

**Keywords:** heterogeneous detonation; *iso*-octane droplets; three-dimensional mathematical simulation; detonation structure; detonation velocity

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## Figure Captions

**Figure 1** Calculated distributions of the gas velocity ( $U$ ) and the mass fraction of fuel vapor ( $Y$ ) when filling the channel with a gas suspension of *iso*-octane droplets with an initial diameter (before the start of filling the channel) of  $400\ \mu\text{m}$

**Figure 2** Calculated dependences of the detonation wave propagation velocity along a vertical channel filled with a gas suspension of *iso*-octane droplets with an initial diameter (before the start of filling the channel) of  $400\ \mu\text{m}$  at a fuel-to-air equivalence ratio of  $\Phi = 0.7$  ( $1$ ),  $1.0$  ( $2$ ), and  $1.8$  ( $3$ ). Horizontal dotted lines correspond to the Chapman–Jouguet detonation velocity for homogeneous *iso*-octane–air mixtures of the same compositions. The vertical dash-and-dotted line corresponds to the cross section of the channel (monitoring location) in which the structure of the self-sustained detonation wave is studied

**Figure 3** Comparison of the calculated profiles of pressure ( $a$ ) and temperature ( $b$ ) along the center line of the vertical channel for self-sustained detonation waves traveling through a stoichiometric gas suspension of *iso*-octane droplets with an initial diameter (before the start of filling the channel) of  $150$  ( $1$ ) and  $400\ \mu\text{m}$  ( $2$ ); cross section  $X = 0$  corresponds to the leading front of the detonation wave upon its arrival at the monitoring location ( $3.37\ \text{m}$ )

**Figure 4** Calculated profiles of pressure ( $a$ ) and temperature ( $b$ ) along the center line of the vertical channel for self-sustained detonation waves traveling through gas suspensions of *iso*-octane droplets with an initial diameter (before the start of filling the channel) of  $400\ \mu\text{m}$  at different values of the fuel-to-air equivalence ratio:  $1 - \Phi = 0.7$ ,  $2 - 1.0$ , and  $3 - \Phi = 1.8$ ; cross section  $X = 0$  corresponds to the leading front of the detonation wave upon its arrival at the monitoring location ( $3.37\ \text{m}$ )

**Figure 5** Calculated instantaneous distributions of *iso*-octane droplet sizes and energy release zones with (upper frames) and without (lower frames) superposition of the corresponding fields behind the leading front of detonation waves traveling through droplet suspensions with fuel-to-air equivalence ratio  $\Phi = 0.7$  ( $a$ ),  $1.0$  ( $b$ ), and  $1.8$  ( $c$ ) at an initial droplet diameter (before the start of filling the channel) of  $400\ \mu\text{m}$ . Energy release zones are shown by grey dots corresponding to spontaneously ignited Monte-Carlo particles

**Figure 6** Calculated instantaneous distributions of the mass fraction of fuel vapor (upper frames) and temperature (lower frames) in a detonation wave traveling through a gas suspension of *iso*-octane droplets with an initial diameter (before the start of filling the channel) of  $400\ \mu\text{m}$  at  $\Phi = 0.7$  ( $a$ ),  $1.0$  ( $b$ ), and  $1.8$  ( $c$ )

## Table Caption

Parameters of reactions (1)–(5)

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## References

- Roy, G. D., S. M. Frolov, A. A. Borisov, and D. W. Netzer. 2004. Pulse detonation propulsion: Challenges, current status, and future perspective. *Prog. Energ. Combust.* 30(6):545–672.
- Frolov, S. M., V. S. Aksenov, V. S. Ivanov, I. O. Shamshin, and S. A. Nabatnikov. 2019. Broskovye ispytaniya bespilotnogo letatel'nogo apparata s pryamotochnym vozdušno-reaktivnym impul'sno-detonatsionnym dvigatelem [Catalapult launching tests of an unmanned aerial vehicle with a ramjet pulsed-detonation engine]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 12(1):63–72. doi: 10.30826/CE19120108.
- Bykovsky, F. A., and S. A. Zhdan. 2013. *Nepreryvnaya spinovaya detonatsiya* [Continuous spin detonation]. Novosibirsk: Institute of Hydrodynamics SB RAS Publ. 422 p.
- Frolov, S. M., V. S. Ivanov, I. O. Shamshin, V. S. Aksenov, M. Yu. Vovk, I. V. Mokrynskiy, V. A. Bruskov, D. V. Igonkin, S. N. Moskvitin, A. A. Illarionov, and E. Yu. Marchukov. 2022. Forsazhnaya kamera s detonatsionnym gorenim kerosina [Afterburner operating on detonative combustion of liquid jet propulsion fuel]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 15(1):67–71. doi: 10.30826/CE22150108.
- Smirnov, N., V. Nikitin, V. R. Dushin, Yu. G. Filippov, V. Nerchenko, and J. Khadem. 2015. Combustion onset in non-uniform dispersed mixtures. *Acta Astronaut.* 115. doi: 10.1016/j.actaastro.2015.04.021.
- Fedorov, A. V., and T. A. Khmel. 2005. Numerical simulation of formation of cellular heterogeneous detonation of aluminum particles in oxygen. *Combust. Expl. Shock Waves* 41:435–448. doi: 10.1007/s10573-005-0054-7.
- Dabora, E. K., and L. P. Weinberger. 1974. Present status of detonations in two-phase systems. *Acta Astronaut.* 1(3-4):361–372. doi:10.1016/0094-5765(74)90103-9.
- Mitrofanov, V. V. 2003. *Detonatsiya gomogennykh i geterogennykh sistem* [Detonation of homogeneous and heterogeneous systems]. Novosibirsk: Institute of Hydrodynamics SB RAS Publ. 200 p.
- Kailasanath, K. 2003. Recent developments in the research on pulse detonation engines. *AIAA J.* 41(2):145–159.
- Tangirala, V., A. Dean, O. Perroomian, and S. Palaniswamy. 2007. Investigations of two-phase detonations for performance estimations of a pulsed detonation engine. AIAA Paper No. 2007-1173. doi: 10.2514/6.2007-1173.
- Frolov, S. M., and V. S. Posvyanskii. 2010. Detonability of liquid-fuel drop suspensions in air. *Explosion dynamics and hazards*. Eds. S. M. Frolov, F. Zhang, and P. Wolanski. Moscow: TORUS PRESS. 337–364.
- Meng, Q., M. Zhao, Y. Xu, L. Zhang, and H. Zhang. 2022. Structure and dynamics of spray detonation in *n*-heptane droplet-vapor-air mixtures. 43 p. doi: 10.48550/arXiv.2209.11913.
- Jourdain, N., N. Tsuboi, and A. K. Hayashi. 2022. Investigation of liquid *n*-heptane/air spray detonation with an Eulerian–Eulerian model. *Combust. Flame* 244:112278. doi: 10.1016/j.combustflame.2022.112278.
- Ivanov, V. S., and S. M. Frolov. 2010. Matematicheskoe modelirovanie perekhoda gorenija v detonatsiyu v trube so spiral'yu Shchelkina i fokusiruyushchim ustroystvom [Mathematical modeling of the combustion-to-detonation transition in a tube with a Schelkin spiral and a focusing device]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 3:63–70.
- Ivanov, V. S., I. O. Shamshin, and S. M. Frolov. 2023. Computational study of deflagration-to-detonation transition in a semi-confined slit combustor. *Energies* 16:7028.
- Frolov, S. M., V. S. Aksenov, and I. O. Shamshin. 2017. Perekhod gorenija v detonatsiyu v stratifitsirovannoy sisteme kislorod–plenka zhidkogo topliva [Deflagration-to-detonation transition in a stratified system oxygen–liquid fuel film]. *Khim. Fizika* 36(6):34–44. doi: 10.7868/S0207401X17060073.
- Tannehill J. C., A. A. Dale, and R. H. Pletcher. 1997. *Computational fluid mechanics and heat transfer*. Washington, DC: Taylor and Francis, 1997. 792 p.
- Versteeg, H. K., and W. Malalasekera. 2007. *An introduction to computational fluid dynamics: The finite volume method*. London: Longman Scientific and Technical. 696 p.
- Dukowicz, J. K. *Quasi-steady droplet change in the presence of convection*. Los Alamos, CA: University of California, 1979. 18 p.
- Reitz, R. D. 1987. Modeling atomization processes in high-pressure vaporizing sprays. *Atomisation Spray Technology* 3(4):309–337.
- Pope, S. B. 1985. PDF methods for turbulent reactive flows. *Prog. Energ. Combust.* 11(2):119–192.
- Frolov, S. M., and V. S. Ivanov. 2010. Combined flame tracking particle method for numerical simulation of deflagration-to-detonation transition. *Deflagrative and detonative combustion*. Eds. G. Roy and S. Frolov. Moscow: TORUS PRESS. 133–156.
- Frolov, S. M., V. S. Ivanov, B. Basara, and M. Suffa. 2013. Numerical simulation of flame propagation and localized

- pre-flame autoignition in enclosures. *J. Loss Prevent. Proc.* 26:302–309.
24. Basevich, V. Ya., A. A. Belyaev, S. N. Medvedev, V. S. Posvyansky, and S. M. Frolov. 2015. Kineticheskie detal'nyy i global'nyy mekhanizmy dlya surrogatnogo topliva [Detailed and global kinetic mechanisms for surrogate fuel]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 8(1):21–28.
25. Benmahammed, M. A., B. Veysiére, B. A. Khasainov, and M. Mara. 2016. Effect of gaseous oxidizer composition on the detonability of isooctane–air sprays. *Combust. Flame* 165:198–207.
26. Ivanov, V. S., and S. M. Frolov. 2024. Three-dimensional mathematical simulation of two-phase detonation in the system of a gaseous oxidizer with fuel droplets. *Russ. J. Phys. Chem. B* 18(5):1341–1349. doi: 10.1134/S1990793124701112.
27. Frolov, S. M., A. N. Polenov, B. E. Gel'fand, and A. A. Borisov. 1986. Features of detonation in systems with arbitrary losses. *Sov. J. Chem. Phys.* 5(7):1641–1668.

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