THREE-DIMENSIONAL MATHEMATICAL MODELING OF DETONATION IN THE AIR SUSPENSION OF N-HEXADECANE DROPLETS

V. S. Ivanov[1,2] and S. M. Frolov[1,2,3]

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

[2] Federal State Institution “Scientific Research Institute for System Analysis of the Russian Academy of Sciences,” 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation

[3] National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation

Abstract: Numerical simulation is used to study the differences and specific features of the propagation of heterogeneous detonation waves in a vertical channel filled by air suspensions of droplets of n-hexadecane and *iso*-octane — flammable liquids with very different vapor pressure under normal conditions. The difference in vapor pressure exerts a strong effect on the conditions for the existence of heterogeneous detonation in the suspensions. Thus, heterogeneous detonation in air suspensions of *iso*-octane droplets can be initiated in a channel without taking special measures. However, for the initiation of heterogeneous detonation in air suspensions of n-hexadecane droplets, there is a need in significant liquid prevaporization. For example, for the air suspension of stoichiometric composition, a degree of liquid prevaporization must exceed a certain critical value (about 40%). When the degree of liquid prevaporization is lower than this critical value, the chemical energy release behind the lead shock wave does not ensure the self-sustaining character of reaction wave propagation. When passing through the critical value of the degree of liquid prevaporization, there is a drastic change in the energy release mode in the propagating reaction wave: the energy release starts from the volumetric (kinetically controlled) self-ignition of the vapor–air mixture behind the lead shock wave accompanied with a significant increase in temperature, which accelerates subsequent processes of mixture formation and (diffusion controlled) energy release. At a subcritical value of the degree of liquid prevaporization, this starting period is weakly manifested.

Keywords: heterogeneous detonation; three-dimensional mathematical model; numerical simulation; liquid fuel droplets; n-hexadecane

DOI: 10.30826/CE24170306 **EDN:** ZPVKIA

Figure Captions

Figure 1 Calculated variation of the velocity of the lead shock wave in an air suspension of n-hexadecane droplets along the vertical channel ($d = 150$ μm, $\Phi = 1.5$, baseline values of pressure and temperature in the initiating region)

Figure 2 Comparison of the predicted profiles of pressure (*a*) and temperature (*b*) averaged over the channel cross section in the detonation wave running through the air suspension of *iso*-octane droplets at $d = 400$ μm (*1*)and in the unsteady reaction wave running through the air suspension of n-hexadecane droplets at the moment of the lead shock wave arrival in the control cross section of the channel ($L = 3.2$ m) at $d = 150$ (*2*) and 400 μm (*3*) and $\Phi = 1.8$

Figure 3 Calculated dependence of the reaction wave propagation velocity (in the control cross-section of the channel $L = 3.2$ m) in a stoichiometric ($\Phi = 1$) air suspension of n-hexadecane droplets of the initial diameter (before the start of channel fill) $d = 150$ μm on the degree of liquid prevaporization Ω under normal pressure and temperature (NPT) conditions. The dashed line connects the points at which the reaction wave still propagates unsteadily (slows down), whereas the solid line connects the points at which the steady-state propagation of heterogeneous detonation is observed

Figure 4 Predicted profiles of pressure (*a*) and temperature (*b*) in reaction waves running through air suspensions of n-hexadecane droplets with stoichiometric composition at different degrees of liquid prevaporization $\Omega = 0.1$–0.7 ($d = 150$ μm, NPT conditions). Groups of curves A and B correspond to self-sustaining ($\Omega \geq 40\%$) and unsteady ($\Omega \leq 30\%$) reaction waves. Thick lines correspond to extreme values of $\Omega = 30\%$ and 40%

Figure 5 Predicted instantaneous distributions of the fuel vapor mass fraction, pressure, and temperature in reaction waves running through air suspensions of n-hexadecane droplets with stoichiometric composition at $\Omega = 30\%$ (*a*) and 40% (*b*) ($d = 150$ μm, NPT conditions). The distributions are plotted in the symmetry plane of the channel at the moment when the lead shock front of the reaction wave arrives at the control cross section $L = 3.2$ m. The arrows show the direction of reaction wave propagation

Figure 6 Predicted instantaneous distributions of the fuel vapor mass fraction and the fuel droplet diameter in reaction waves running through air suspensions of n-hexadecane droplets with stoichiometric composition at $\Omega = 30\%$ (a) and 40% (b) ($d = 150$ μm, NPT conditions). Arrows show the direction of reaction wave propagation

Acknowledgments

The work was supported by the Russian Science Foundation (project No. 23-23-00364).

References

1. Baker, W. E., P. A. Cox, P. S. Westine, J. J. Kulesz, and R. A. Strehlow. 1983. *Explosion hazards and evaluation*. Amsterdam–Oxford–New York: Elsevier. Vol. 1. 807 p.
2. Marshall, V. C. 1987. *Major chemical hazards*. New York, NY: Ellis Horwood. 587 p.
3. Zeldovich, Ia. B., and A. S. Kompaneets. 1960. *Theory of detonation*. New York, NY: Academic Press. 284 p.
4. Nettleton, M. A. 1987. *Gaseous detonations: Their nature, effects and control*. London–New York: Chapman and Hall. 270 p.
5. Zel'dovich, Ya. B. 1980. Regime classification of an exothermic reaction with nonuniform initial conditions. *Combust. Flame* 39(2):211–214.
6. Frolov, S. M., V. Ya. Basevich, and V. S. Posvianskii. 2004. Limiting drop size and prevaporization degree required for spray detonation. *Application of detonation to propulsion*. Eds. G. D. Roy, S. M. Frolov, and J. E. Shepherd. Moscow: TORUS PRESS. 110–119.
7. Basevich, V. Ya., S. M. Frolov, and V. S. Posvyanskii. 2005. Usloviya sushchestvovaniya statsionarnoy geterogennoy detonatsii [Existence conditions for the steady-state heterogeneous detonations]. *Khim. Fiz.* 24(7):58–68.
8. Papavassiliou, J., A. Makris, R. Knystautas, J. H. S. Lee, C. K. Westbrook, and W. J. Pitz. 1993. Measurements of cellular structure in spray detonations. *Dynamic aspects of explosion phenomena*. Eds. A. L. Kuhl, J.-C. Leyer, A. A. Borisov, and W. A. Sirignano. Progress in astronautics and aeronautics ser. Washington, DC: AIAA. 154:148–69.
9. Mitrofanov, V. V. 2003. *Detonatsiya gomogennykh i geterogennykh sistem* [Detonation of homogeneous and heterogeneous systems]. Novosibirsk: Lavrentiev Institute of Hydrodynamics Publ. 200 p.
10. Borisov, A. A., B. E. Gel'fand, S. A. Gubin, S. M. Kogarko, and A. L. Podgrebenkov. 1970. The reaction zone of two-phase detonations. *Astronaut. Acta* 15(5-6):411–417.
11. Eidelman, S., and A. Burkat. 1980. Evolution of a detonation wave in a cloud of fuel droplets. Part I: Influence of ignition explosion. *AIAA J.* 18(9):1103–1109.
12. Zhdan, S. A. 1976. Calculation of a spherical heterogeneous detonation. *Combust. Explo. Shock Waves* 12(4):531–538.
13. Zhdan, S. A. 1977. Calculation of heterogeneous detonation taking into account deformation and breakdown of fuel droplets. *Combust. Explo. Shock Waves* 13(2):217–221.
14. Gubin, S. A., and M. Sichel. 1977. Calculation of the detonation velocity of liquid droplets and gaseous oxidizer. *Combust. Sci. Technol.* 17(3-4):109–117.
15. Borisov, A. A., B. E. Gelfand, and A. V. Gubanov. 1981. The effect of relaxation processes on the detonation in heterogeneous mixtures. *Archivum Combustionis* 1(3/4):243–249.
16. Voronin, D. V., and S. A. Zhdan. 1984. Calculation of heterogeneous detonation initiation for a hydrogen–oxygen mixture in an explosion tube. *Combust. Explo. Shock Waves* 20(4):461–465. doi: 10.1007/BF00782401. EDN: NGBTKZ.
17. Sichel, M. 1991. Numerical modeling of heterogeneous detonations. *Numerical approaches to combustion modeling*. Eds. E. S. Oran and J. P. Boris. Progress in astronautics aeronautics ser. New York, NY: AIAA Inc. 135:447–458.
18. Sreznevsky B. I. 1882. Ob isparenii zhidkostey [On the evaporation of liquids]. *Zh. Russkogo fiziko-khimitcheskogo obshchestva*[J. Russian Physical-Chemical Society] 14(8):420–442.
19. Nigmatulin, R. I. 1987. *Dinamika mnogofaznykh sred* [Dynamics of multiphase]. Moscow: Nauka. Part I. 464 p.
20. Frolov, S. M., V. Ya. Basevich, V. S. Posvianskii, and V. A. Smetanyuk. 2004. Isparenie i gorenie kapli uglevodorodnogo topliva. IV. Isparenie kapli s uchetom kollektivnykh effektov [Vaporization and combustion of a hydrocarbon fuel drop. Part IV: Drop vaporization with regard for spray effects]. *Khim. Fiz.* 23(7):41–50.
21. Frolov, S. M., and V. A. Smetanyuk. 2006. Teplo- i massoobmen kapli s gazovym potokom [Heat and mass transfer of liquid drop with gas flow]. *Khim. Fiz.* 25(4):42–54.
22. Ranz, W. E., and W. R. Marshall, Jr. 1952. Evaporation from drops, part I. *Chem. Eng. Prog.* 48:141–146.
23. Borisov, A. A., S. M. Frolov, V. A. Smetanyuk, S. A. Polikhov, and C. Segal. 2005. Vzaimodeystvie kapli goryuchego s gazovym potokom [Interaction of fuel drop with gas flow]. *Khim. Fiz.* 24(7):50–57.
24. Ju, Y., and C. K. Law. 2002. Propagation and quenching of detonation waves in particle laden mixtures. *Combust. Flame* 129(4):356–364.
25. Lu, T. F., and C. K. Law. 2004. Heterogeneous effects in the propagation and quenching of spray detonations. *J. Propul. Power* 20(5):820–827.
26. Frolov S. M., and V. S. Posvyanskii. 2008. Struktura i predely geterogennoy detonatsii [Structure and limits of heterogeneous detonation]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 1:1–5.

27. 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.
28. Frolov, S. M., and V. Ya. Basevich. 2006. Gorenie kapel' [Combustion of droplets. *Zakony goreniya* [Laws of combustion]. Ed. Yu. V. Polezhaev. Moscow: UNPC "Energomash." 130–159.
29. Ivanov, V. S., S. M. Frolov, and A. E. Zangiev. 2024. Struktura detonatsionnoy volny v dvukhfaznoy sisteme gazoobraznyy okislitel' – kapli zhidkogo goruchego [Structure of detonation wave in a two-phase system of gaseous oxidizer – liquid fuel droplets]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 17(3):49–61.
30. *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.
31. Benmahammed, M. A., B. Veyssiere, B. A. Khasainov, and M. Mara. 2016. Effect of gaseous oxidizer composition on the detonability of isooctane–air sprays. *Combust. Flame* 165:198–207.
32. Reitz, R. D. 1987. Modeling atomization processes in high-pressure vaporizing sprays. *Atomization Spray Technology* 3(4):309–337.
33. Dukowicz, J. K. 1979. *Quasi-steady droplet change in the presence of convection*. Los Alamos, CA: University of California, 1979. 18 p.
34. Pope, S. B. 1985. PDF methods for turbulent reactive flows. *Prog. Energ. Combust.* 11(2):119–192.
35. 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.
36. Frolov, S. M., V. S. Ivanov, B. Basara, and M. Suffa. 2013. Numerical simulation of flame propagation and localized preflame autoignition in enclosures. *J. Loss Prevent. Proc.* 26:302–309.
37. 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 [Kinetic detailed and global mechanisms for surrogate fuel]. *Goren. Vzryv (Mosk.) — Combustion and Explosion* 8(1):21–28.

Received July 3, 2024

Contributors

Ivanov Vladislav S. (b. 1986) — Doctor of Science in physics and mathematics, leading research scientist, N. N. Semenov Federal Research Center for Chemical Physics of the Russian Academy of Sciences, 4 Kosygin Str., Moscow 119991, Russian Federation; research scientist, Federal State Institution "Scientific Research Institute for System Analysis of the Russian Academy of Sciences," 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; ivanov.vls@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; professor, National Research Nuclear University MEPhI (Moscow Engineering Physics Institute), 31 Kashirskoe Sh., Moscow 115409, Russian Federation; leading research scientist, Federal State Institution "Scientific Research Institute for System Analysis of the Russian Academy of Sciences," 36-1 Nakhimovskii Prosp., Moscow 117218, Russian Federation; smfrol@chph.ras.ru