03.1

Quenching detonation in a hydrogen-air mixture in a plane channel

© V.A. Levin, T.A. Zhuravskaya

Institute of Mechanics, Moscow State University, Moscow, Russia
E-mail: zhuravskaya@imec.msu.ru

Received June 19, 2023
Revised July 19, 2023
Accepted July 26, 2023

The paper presents the results of a numerical study of the interaction of a formed cellular detonation wave propagating in a stoichiometric hydrogen-air mixture at rest in a plane channel, with multiple obstacles (barriers) located on the inner surface of the channel. The influence of geometrical parameters of a domain with obstacles on detonation propagation has been investigated. It has been found that the location of obstacles in the deepening of the channel wall leads to a decrease in their destructive effect on the wave. The possibility of extinguishing detonation by a layer of air located along the channel well, limited by single barriers, has been studied. It has been established that filling the domain with barriers with air or argon enhances their destructive effect on the wave, thereby contributing to suppression of detonation combustion.

Keywords:: Plane channel, detonation, multiple obstacles, air layer, failure of detonation.

DOI: 10.61011/TPL.2023.09.56717.19657

The identification of new methods of quenching of detonation combustion is of great interest for explosive safety purposes. Specifically, various types of structural concepts with potential applications in a passive protection system are much needed in the atomic and hydrogen energy industry. It was found that sheets consisting of inert dust particles [1], stationary inert particles or particle clouds in gas [2,3], slit plates [4], perforated walls [5,6], and various porous inserts on the inner surface of a channel [7–9] may have a destructive effect on a propagating detonation wave. Barriers in a channel also suppress detonation combustion. It was established that the resistance of detonation in a stoichiometric hydrogen–air mixture to perturbations caused by barriers may be enhanced by preliminary partial dissociation of molecular oxygen and hydrogen into atoms or by the introduction of argon and ozone in certain specific concentrations into the mixture [10–12]. In the present study, the propagation of a detonation wave in a stoichiometric hydrogen–air mixture in a plane channel with multiple obstacles (barriers) positioned locally on one of its walls is examined numerically in order to determine the ways to enhance their destructive effect on the wave.

The propagation of a detonation wave in a stoichiometric hydrogen-air mixture at rest under normal conditions ($p_0 = 101\,325$ Pa, $T_0 = 298$ K) in a semi-infinite plane channel of width L ($L = 2$ cm) with a domain with barriers located on its inner surface was considered. Instantaneous uniform supercritical energy input into a narrow layer near the closed end of the channel was used to initiate detonation. The combustible mixture was modeled by a mixture of gaseous H_2, O_2, and N_2 in a molar ratio of 42 : 21 : 79.

The system of equations describing the plane two-dimensional nonsteady flow of a nonviscous multicomponent reacting gas mixture has the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u)}{\partial x} + \frac{\partial(\rho v)}{\partial y} = 0,$$

$$\frac{\partial(\rho u)}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial x} + \frac{\partial(\rho u v)}{\partial y} = 0,$$

$$\frac{\partial(\rho v)}{\partial t} + \frac{\partial(\rho v u)}{\partial x} + \frac{\partial(\rho v^2 + p)}{\partial y} = 0,$$

$$\frac{\partial(\rho(u^2+v^2)/2 + \rho h - p)}{\partial t} + \frac{\partial(\rho u((u^2+v^2)/2 + h))}{\partial x} + \frac{\partial(\rho v((u^2+v^2)/2 + h))}{\partial y} = 0,$$

$$\frac{\partial(\rho n_i)}{\partial t} + \frac{\partial(\rho u n_i)}{\partial x} + \frac{\partial(\rho v n_i)}{\partial y} = \rho\omega_i, \quad i = 1, \ldots, M.$$

Here, x and y are Cartesian coordinates; u and v are the corresponding velocity components; t is time; ρ, p, and h are the density, the pressure, and the specific enthalpy of the mixture; n_i and ω_i are the specific concentration and the formation rate of the ith component of the mixture; and M is the number of components. The equations of state of the combustible mixture are as follows:

$$p = \rho R_0 T \sum_{i=1}^{M} n_i, \quad h = \sum_{i=1}^{M} n_i h_i(T).$$

Here, T is temperature and R_0 is the universal gas constant. Temperature dependences $h_i(T)$ of partial enthalpies were determined based on reduced Gibbs energies of the corresponding mixture components [13]. The detailed kinetic hydrogen oxidation mechanism proposed in [14] was used to describe the chemical interaction.

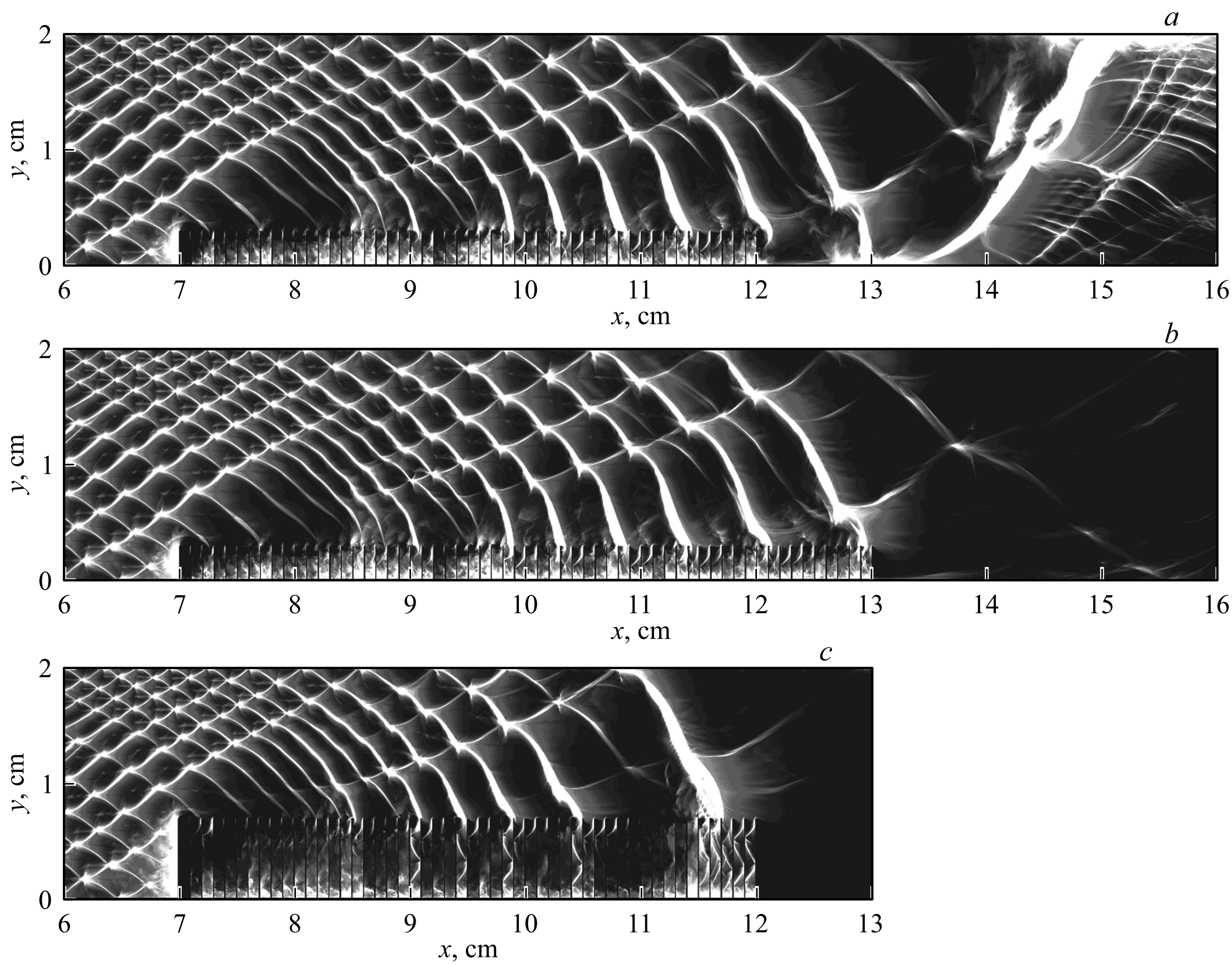

Figure 1. Numerical soot foils in case of detonation interaction with multiple barriers ($\Delta L_b = 1$ mm). *a* — Reinitiation of detonation at $L_b = 5$ cm and $H_b = 3$ mm; *b, c* — quenching of detonation combustion at $L_b = 6$ cm, $H_b = 3$ mm and $L_b = 5$ cm, $H_b = 7$ mm, respectively. Here and elsewhere, a wave propagates from left to right.

Barriers in the channel were modeled as infinitely thin solid surfaces with the impermeability condition satisfied on them (and on the channel walls).

An explicit second-order scheme based on the Godunov's method [15] was used to solve the gas dynamics equations. Calculations were performed on a grid with grid step $\Delta = 5\,\mu$m that provided a correct resolution of the detonation wave structure. An original software module with MPI/OpenMP hybrid parallelizing was used for numerical modeling. The study was carried out with the use of equipment of the shared research facilities of HPC computing resources at Lomonosov Moscow State University [16].

A plane detonation wave was initiated as a result of the initial input of energy. The front of this wave gets curved in the course of time, transverse waves emerge, as result a self-sustaining detonation wave with a cellular structure is formed. Transverse waves, which propagate along the front and undergo periodic head-on collisions, couple with the front via three-shock Mach configurations. Since temperature in the vicinity of coupling points is high, a propagating detonation wave in an experiment leaves burn marks in the form of diamond-shaped cells, which are formed by trajectories of triple points, on a sooty plate positioned along the channel wall [17]. Numerical analogs of the experimentally observed detonation soot tracks (numerical soot foils) were used to illustrate the obtained results (Figs. 1–3).

Obstacles on the channel wall were positioned so that the formed cellular detonation approached them. The result of interaction of the wave with the domain with obstacles depends on length L_b of this domain, barrier height H_b, and distance ΔL_b between the neighboring barriers. In the present study, domains with obstacle spacing $\Delta L_b = 1$ mm were examined. The obtained calculated data demonstrated that detonation combustion may be quenched by increasing the barrier height or the length of the domain with barriers (with the other parameters remaining unchanged). Specifically, detonation is restored after the interaction with obstacles $H_b = 3$ mm in height positioned within a section of the channel wall with length $L_b = 5$ cm (Fig. 1, *a*). However, it is sufficient to extend the domain

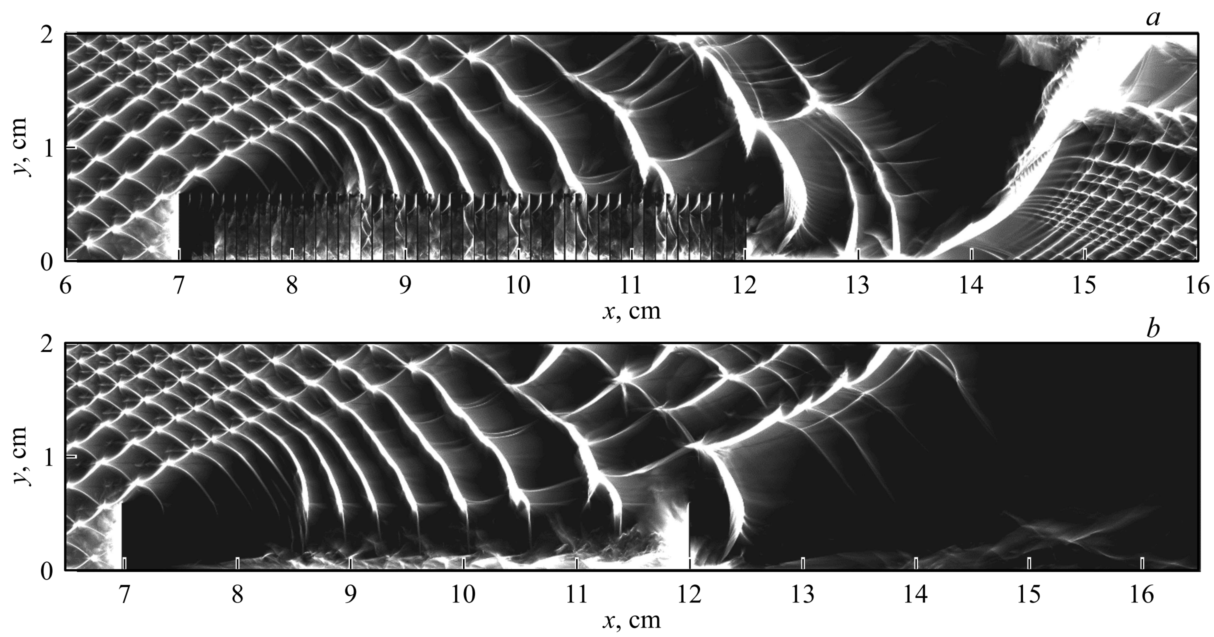

Figure 2. Numerical soot foils in case of detonation interaction with a domain with barriers ($\Delta L_b = 1$ mm) and an air layer at $L_b = 5$ cm and $H_b = 6$ mm. *a* — Reinitiation of detonation beyond the domain with barriers; *b* — quenching of detonation combustion by the air layer.

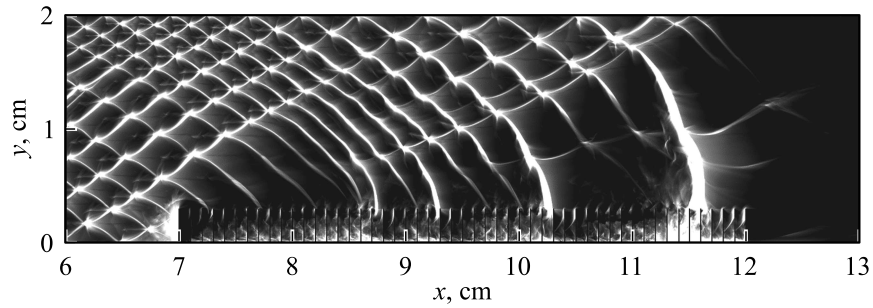

Figure 3. Numerical soot foil illustrating the quenching of detonation combustion by an air-filled domain with barriers ($L_b = 5$ cm, $H_b = 3$ mm, $\Delta L_b = 1$ mm).

to $L_b = 6$ cm or raise the barrier height to $H_b = 7$ mm to suppress detonation combustion (Figs. 1, *b* and *c*). Having analyzed the propagation of a detonation wave (Fig. 1) along the domain with barriers, we found signs of quenching of transverse waves at obstacles and emergence of new ones in the detonation wave. The cell size of the detonation wave increased gradually in the process, which is consistent with the results of experiments on detonation propagation in channels with porous walls [9].

The interaction of a wave with multiple barriers positioned in a cavity in the wall (niche) was studied alongside with its interaction with obstacles positioned on the inner channel surface, which may be regarded as an insert with a porous coating (e.g., steel wool [18]). Barriers with their height being equal to the niche depth were considered. Obstacles positioned this way modeled a porous insert in the channel wall. It was found that, although the channel expands (subcritically) in the barrier domain, thus causing local decay of a wave entering the niche, the overall destructive effect of obstacles on the wave is significantly weaker than the one induced by obstacles positioned on the inner channel surface (under otherwise equal conditions). This feature of detonation combustion in the case of barriers positioned in a niche is attributable to the formation of a flow with a propagating wave in a channel with obstacles that is wider (by the niche depth) than the initial channel.

The interaction of a detonation wave with an air layer under normal conditions (bounded by single barriers on both sides) at the channel wall was also examined. It was established that this layer acts similarly to a domain with obstacles, contributing to detonation quenching. Its destructive effect may be enhanced by increasing the height or length of this layer. In fact, an air layer is, in certain cases, a more efficient quencher of detonation combustion than a domain with obstacles of the same height and length with barrier spacing $\Delta L_b = 1$ mm (Fig. 2).

In accordance to the results of experiments on detonation combustion of mixtures with an irregular cellular structure in channels with porous inserts [9], calculated data revealed that the outcome (conservation or quenching of detonation) of interaction with barriers is governed by two competing contrary processes: weakening of transverse waves at barriers and emergence of new ones from local perturbations in the reaction zone (Fig. 1). Therefore, structural changes contributing to the first process should facilitate the decay of a detonation wave. It was found that filling the barrier domain with air is one possible way to enhance the destructive effect of obstacles on a wave. Specifically, complete detonation quenching was observed when the initial combustible mixture was substituted with air in the domain with length $L_b = 5$ cm and obstacles with height $H_b = 3$ mm (Fig. 3). The same domain with obstacles filled with a combustible mixture (Fig. 1, a) or an air layer with the same extent and height did not destroy a wave. The results of calculations demonstrated that the substitution of air in the barrier domain with argon, which has a greater molar weight, intensifies the formation of waves reflected from the domain. However, the positioning of a series of barriers in a domain filled with argon may also be regarded as a design solution contributing to detonation quenching.

Thus, the results of numerical modeling of interaction between a formed cellular detonation wave, which propagates along a plane channel filled with a stoichiometric hydrogen–air mixture at rest, and multiple obstacles (barriers) positioned on the inner channel surface demonstrated that, under otherwise equal conditions, an increase in the barrier height or the length of the domain with obstacles contributes to the suppression of detonation combustion. In contrast, the positioning of barriers in a cavity in the channel wall weakens their destructive effect on this wave. It was found that an air layer (bounded by single barriers) positioned along the channel wall may be used to quench detonation. It was established that filling the domain with barriers with air or argon enhances their destructive effect on a detonation wave.

Funding

This study was carried out at the Institute of Mechanics of the Moscow State University and was supported financially by the Russian Science Foundation (project No. 21-11-00307).

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] A.A. Vasil'ev, A.V. Pinaev, A.A. Trubitsyn, A.Yu. Grachev, A.V. Trotsyuk, P.A. Fomin, A.V. Trilis, Combust. Explos. Shock Waves, **53** (1), 8 (2017). DOI: 10.1134/S0010508217010026.

[2] I.A. Bedarev, A.V. Fedorov, J. Phys.: Conf. Ser., **894** (1), 012008 (2017). DOI: 10.1088/1742-6596/894/1/012008

[3] D.A. Tropin, Int. J. Hydrogen Energy, **47** (66), 28699 (2022). DOI: 10.1016/j.ijhydene.2022.06.169

[4] T. Obara, J. Sentanuhady, Y. Tsukada, S. Ohyagi, Shock Waves, 18 (2), 117 (2008). DOI: 10.1007/s00193-008-0147-9

[5] S.P. Medvedev, S.V. Khomik, B.E. Gel'fand, Russ. J. Phys. Chem. B, 3 (6), 963 (2009). DOI: 10.1134/S1990793109060165.

[6] H. Qin, J.H.S. Lee, Z. Wang, F. Zhuang, Proc. Combust. Inst., **35** (2), 1973 (2015). DOI: 10.1016/j.proci.2014.07.056

[7] O.V. Sharypov, Y.A. Pirogov, Comb. Explos. Shock Waves, **31** (4), 466 (1995). DOI: 10.1007/BF00789368.

[8] A. Teodorczyk, J.H.S. Lee, Shock Waves, **4** (4), 225 (1995). DOI: 10.1007/BF01414988

[9] M.I. Radulescu, J.H.S. Lee, Combust. Flame, **131** (1−2), 29 (2002). DOI: 10.1016/S0010-2180(02)00390-5

[10] V.A. Levin, T.A. Zhuravskaya, Tech. Phys. Lett., **46** (2), 189 (2020). DOI: 10.1134/S1063785020020248.

[11] T.A. Zhuravskaya, V.A. Levin, Fluid Dyn., **55** (4), 488 (2020). DOI: 10.1134/S0015462820040138.

[12] V.A. Levin, T.A. Zhuravskaya, Dokl. Phys., **66** (12), 320 (2021). DOI: 10.1134/S1028335821110057.

[13] Thermodynamic properties of individual substances, ed. by L.V. Gurvich, I.V. Veyts (Hemisphere, N.Y., 1989), vol. 1, pt 2.

[14] L.V. Bezgin, V.I. Kopchenov, A.S. Sharipov, N.S. Titova, A.M. Starik, Combust. Sci. Technol., **185** (1), 62 (2013). DOI: 10.1080/00102202.2012.709562

[15] A.V. Rodionov, USSR Comput. Math. Math. Phys., **27** (2), 175 (1987). DOI: 10.1016/0041-5553(87)90174-1.

[16] Vl. Voevodin, A. Antonov, D. Nikitenko, P. Shvets, S. Sobolev, I. Sidorov, K. Stefanov, Vad. Voevodin, S. Zhumatiy, Supercomput. Front. Innov., **6** (2), 4 (2019). DOI: 10.14529/jsfi190201

[17] R.I. Soloukhin, *Udarnye volny i detonatsiya v gazakh* (GIFML, M., 1963), pp. 150−152 (in Russian).

[18] G.Yu. Bivol, S.V. Golovastov, V.V. Golub, Shock Waves, **28** (5), 1011 (2018). DOI: 10.1007/s00193-018-0831-3

Translated by Ego Translating