Control of Detonation Combustion of Hydrogen-Air Mixture in Plane Channels

V.A. Levin
Institute of Mechanics, Lomonosov Moscow State University
Moscow, Russia;
Central Aerohydrodynamic Institute
Zhukovsky, Russia;
Institute of Automation and Control Processes, Far Eastern Branch of the RAS
Vladivostok, Russia

T.A. Zhuravskaya
Institute of Mechanics, Lomonosov Moscow State University
Moscow, Russia;
Central Aerohydrodynamic Institute
Zhukovsky, Russia

1 Abstract

Using a detailed kinetic model of chemical interaction, numerical modeling of detonation combustion of a stoichiometrical hydrogen-air mixture has been carried out with purpose of determination of mechanisms of detonation wave control both in a quiescent gas mixture and in a supersonic gas flow.

2 Introduction

The intention to use detonation in energy generating plants (for example, in detonation engines) requires fundamental knowledge about detonation combustion of gas mixtures. So, the determination of means of control of detonation wave propagation in a gas is of great interest. It is well known that the velocity of detonation waves in gas mixtures depends strongly on the mixture composition, the concentrations of the fuel and oxidant, and the presence of various additions in the mixture [1], [2]. This allows one to control the propagation of a detonation wave and, if necessary, to guarantee the quenching of detonation combustion. In [3], it was found numerically that when one increases the volume fraction of quiescent inert particles in a gas mixture, the cell of the detonation wave passing through the particles enlarges; and a further increase in the fraction of particles leads to detonation failure. In [4], it was established

Correspondence to: zhuravskaya@imec.msu.ru

experimentally that detonation combustion in a gas mixture can be completely quenched by the veil of inert dust particles. On the other hand, means of conservation of detonation are of great interest too.
In this research some mechanisms of detonation wave control both in a quiescent gas mixture and in a supersonic gas flow in plane channels are considered.

3 Detonation Wave Control in a Quiescent Gas Mixture

3.1 Mathematical Model

We study propagation of a detonation wave in a quiescent gas mixture under the normal condition (pressure $p_0 = 1$ atm and temperature $T_0 = 298$ K) in a plane channel of constant width L. The instantaneous supercritical energy input in a domain in the shape of a thin layer near the closed channel end is used for direct detonation initiation. We consider a pure stoichiometrical hydrogen-air mixture (mixture of the H_2, O_2, N_2 and Ar gases in the molar ratio 42 : 21 : 78 : 1, respectively), and a preliminary prepared stoichiometrical hydrogen-air mixture. Under preliminary preparation (conversion) of the stoichiometrical hydrogen-air mixture we keep in mind a preliminary decomposition of some volumes of molecular H_2 and O_2 gases into atomic H and O gases.

In describing the chemical interaction the modified detailed kinetic mechanism of hydrogen oxidation proposed in [5] was used. This mechanism consists of twenty six reversible reactions. The partial enthalpies as functions of temperature are determined by the reduced Gibbs energies of the corresponding mixture components [6]. A set of Euler gas dynamics equations, describing a plain two-dimensional nonstationary flow of the inviscid reactive multi-component gas mixture, coupled with detailed chemical kinetics equations has been solved using a numerical method based on the Godunov's scheme [7].

The size of mesh has been chosen so that further grid refinements do not lead to a change of the flow pattern and so that the flow behind the detonation front (in particular, the flow in the induction zone) is represented correctly. Thus, the computational mesh with cell size $\Delta = 0.005$ mm was used in numerical calculations. According to [8] usage of the classical first-order Godunov's scheme and a very fine computational grid makes accurate numerical modeling of the flows under consideration possible and prevents any nonphysical oscillations of solutions. The numerical modeling was performed using the software package developed by the authors. The hybrid MPI/OpenMP parallelization of the computations was applied to reduce time expenditures.

3.2 Results of Numerical Modeling

As a result of initial supercritical energy input there is detonation wave initiation. Numerical noise causes spontaneous onset of the transverse instability of initiated detonation. As a result of it the detonation wave is modified and the steady cellular detonation is formed with time [2].

It was established that the preliminary preparation (conversion) of the pure stoichiometrical hydrogen-air mixture results in a small increase of the self-sustained detonation propagation velocity and essential decrease of the detonation cell rate. So, in case of detonation combustion of the mixture H_2, H, O_2, O, N_2, Ar gases in the molar ratio 41.58 : 0.84 : 20.79 : 0.42 : 78 : 1, respectively (referred to as the prepared mixture 1) the detonation cell rate is more than two times smaller than one in an unprepared stoichiometrical hydrogen-air mixture (Figure 1 *a*, *b*) and detonation velocity increases only by 0.7%. Moreover, a small increase of quantity of decomposed gases leads to small increase of detonation propagation velocity and further sufficient decrease of detonation cell rate. So in case of the mixture H_2, H, O_2, O, N_2, Ar gases in the molar ratio 41.37 : 1.26 : 20.685 : 0.63 : 78 : 1, respectively (referred to as the prepared mixture 2) the detonation cell rate is approximately three times smaller than one in the unprepared mixture (Figure 1 *c*).

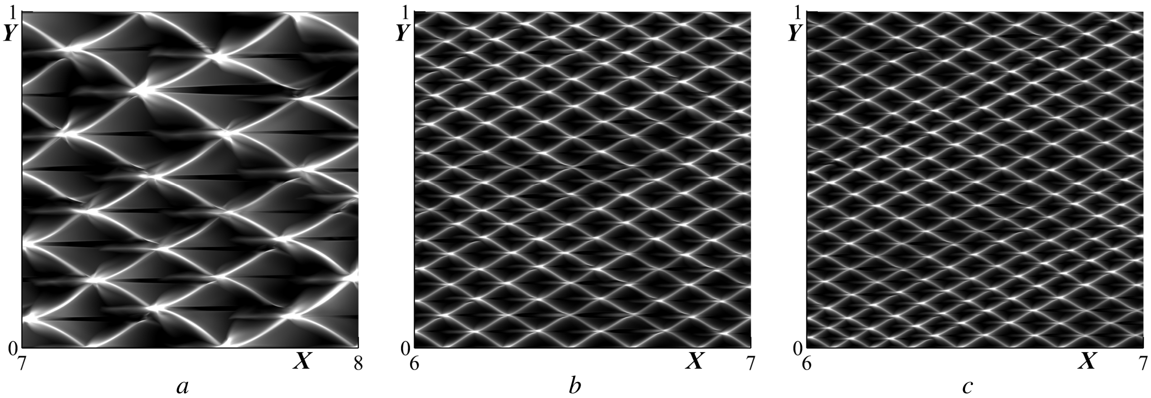

Figure 1. Numerical soot foil: *a* – the unprepared stoichiometrical hydrogen-air mixture; *b* – the preliminary prepared mixture 1 (H_2, H, O_2, O, N_2, Ar gases in the molar ratio 41.58 : 0.84 : 20.79 : 0.42 : 78 : 1), *c* – the preliminary prepared mixture 2 (H_2, H, O_2, O, N_2, Ar gases in the molar ratio 41.37 : 1.26 : 20.685 : 0.63 : 78 : 1). Here *X=x/L*, *Y=y/L*, *L* is the channel width. Detonation propagates from left to right

We examined influence of the preliminary partial gas dissociation on propagation of a detonation wave. In particular, we studied detonation propagation in a quiescent gas mixture in a plane channel of constant width with a non-destructing infinitely-thin transverse obstacle (barrier) of height smaller than the channel width *L.* The barrier is located in some distance from the closed channel end. Its location was chosen so that a detonation wave with a formed cellular structure approaches the barrier. It is known that there is a critical barrier height, dependent on the channel width, such that the detonation wave is destructed after the interaction with the barrier if its height exceeds the critical value [9]. It was established that in case of preliminary prepared mixture the critical barrier height exceeds the critical height in case of the unprepared mixture under other conditions being equal (Figure 2). Moreover, for conservation of detonation combustion in the channel in case of increasing barrier height a decomposed gases quantity has to be increased as well (Figure 3). It should be noted that in case of conservation of detonation combustion

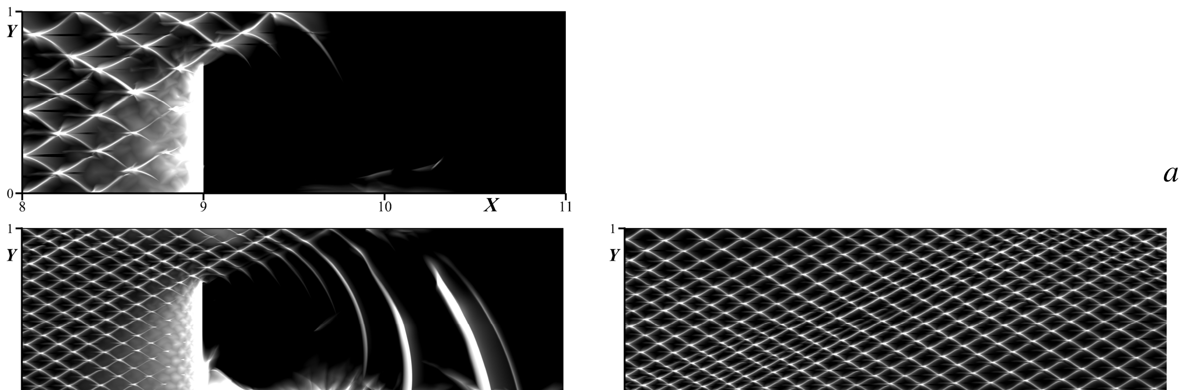

Figure 2. Numerical soot foil in case of detonation propagation in a plane channel with a barrier (barrier height h_b=0.7 *L*): *a* – detonation destruction in case of the unprepared stoichiometrical hydrogen-air mixture, *b* – detonation conservation in case of the preliminary prepared mixture 1. Here *X=x/L*, *Y=y/L*, *L* is the channel width. Detonation propagates from left to right

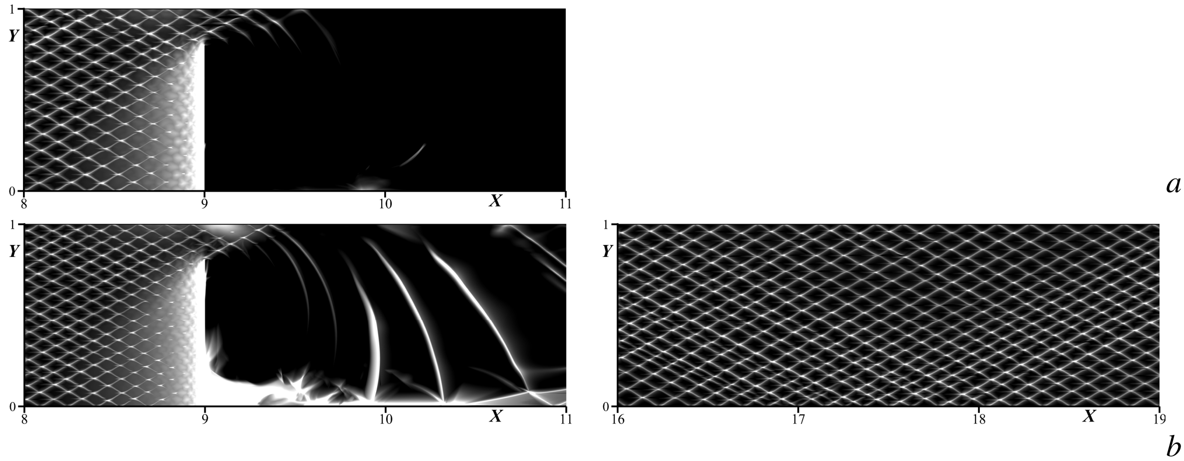

Figure 3. Numerical soot foil in case of detonation propagation of the preliminary prepared mixture in a plane channel with a barrier (barrier height h_b=0.8 *L*): *a* – detonation destruction in case of the preliminary prepared mixture 1, *b* – detonation conservation in case of the preliminary prepared mixture 2. Here *X=x/L*, *Y=y/L*, *L* is the channel width. Detonation propagates from left to right

after passing the obstacle the detonation wave structure is temporarily modified and is restored with time (Figures 2 *b*, 3 *b*).

So, the preliminary conversion of the gas can be used to prevent destruction of the detonation wave by the transverse obstacle (barrier) located in the channel.

4 Detonation Wave Control in a Supersonic Gas Flow

The ability of detonation control in the stoichiometrical hydrogen-air mixture flowing at a supersonic velocity into a symmetrical plane channel with a constriction by means of inert dust particles addition in the gas was studied.

The scheme of a part of the channel above the symmetry plane is shown in Figure 4 *a*. A combustible mixture under the normal condition flows at a supersonic velocity into the channel parallel to its symmetry plane through the boundary $x = x_4$ and flows out through the boundary x =0. To initiate detonation at the initial time, we used an instantaneous supply of supercritical energy to a thin layer near the section $x = x_1$ (the shaded region in Figure 4 *a*). The detailed statement of the problem has been given in [10]. The numerical simulation of detonation combustion of a dust-laden gas mixture was carried out within the framework of the multicomponent mixture extension [11] of the one-temperature one-velocity model [12] describing the flow of a gas with small inert particles.

We considered a gas flow in channels with the following geometric parameters: x_1 = 0.125 m, x_3 = 0.375 m, x_4 = 0.5 m, l_2 = 0.0175 m, l_3 = 0.035 m, $l > l_3$, and different values of parameter α=$(x_2-x_1)/(x_3-x_1)$, which determines the position of the channel neck $x = x_2$.

In case of a channel geometric parameters of which do not guarantee detonation stabilization in a flow (the detonation wave moves through the channel and leaves it in the counterflow direction) it has been established that the addition of fine dust particles into the gas flow may be used for detonation stabilization due to decrease of detonation velocity in the dusty gas mixture. So, in case of the pure combustible mixture incoming into the channel (l =0.04 m and α = 0.5) with M_0 = 4.9 the detonation wave propagates into the converging part and leaves the channel against the flow. However, the addition of

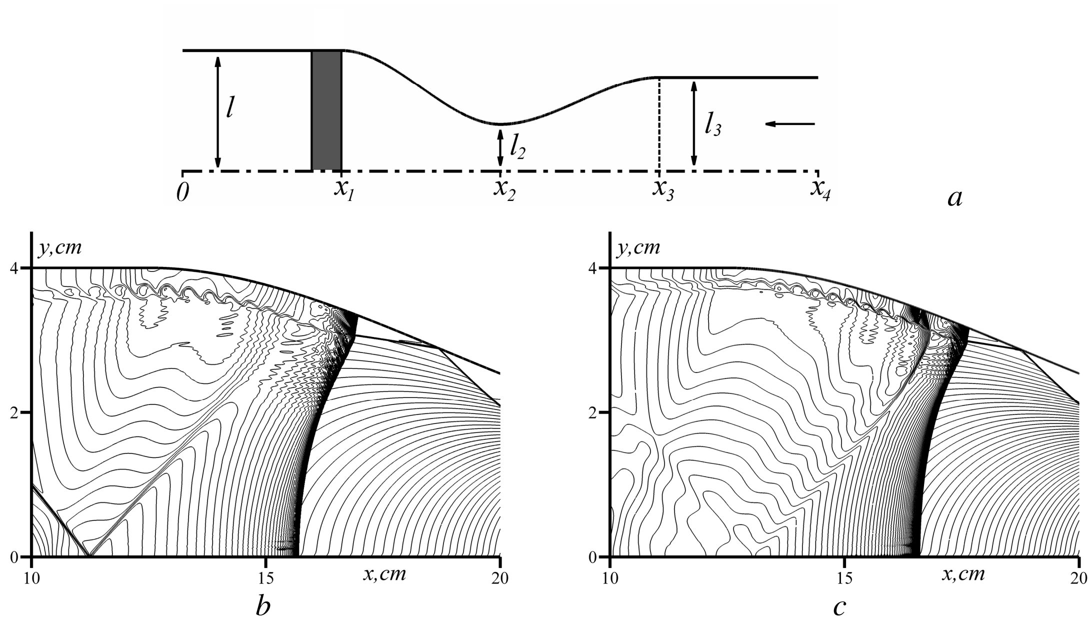

Figure 4. a – the schematic of the upper channel part (the arrow shows to flow direction); b, c – density contours in case of stabilization of a detonation wave in the channel with constriction for the dusty gas mixture, $\mathrm{M}_0 = 4.9$, α=0.5, and $l = 0.04$ m in case of dust mass fraction $Y_S = 0.104$ (b), 0.065 (c). A computational grid of Δ=0.02÷0.03 mm was used

small dust particles (dust mass fraction $Y_S = 0.104$) in the mixture flowing into the channel with $\mathrm{M}_0 = 4.9$ provides detonation wave stabilization in the diverging part of the channel (Figure 4 *b*).

Moreover, we have established that the concentration of dust particles in the incoming flow can be considered as a control mechanism for the position of the stabilized wave. For example, a small decrease in the dust mass fraction to $Y_S = 0.065$ leads to a situation when the detonation wave propagates further into the diverging part and stabilizes closer to the neck of the channel (Figure 4 *c*).

5 Conclusions

Using a detailed kinetic model of chemical interaction, numerical modeling of detonation combustion of a stoichiometrical hydrogen-air mixture has been carried out with purpose of determination of mechanisms of control of a detonation wave. It has been established that preliminary preparation of the gas mixture (some volumes of molecular H_2 and O_2 gases has been preliminary decomposed into atomic H and O gases) and addition of fine inert dust particles into the combustible gas mixture can be applied as detonation control mechanisms.

In case of the quiescent gas mixture under the normal condition a study of possibility of detonation wave control due to preliminary conversion of the mixture was performed. In particular, we obtained that preliminary preparation of the mixture can be applied to prevent detonation combustion quenching in the channel with a transverse barrier.

Numerical investigation of detonation combustion of the gas mixture flowing with supersonic velocity into a symmetrical plane channel with a constriction reveals that the addition of fine dust particles into the gas may be used both for detonation stabilization and stabilized detonation location control in the supersonic flow of the gas mixture.

6 Acknowledgments

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References

[1] Soloukhin RI. (1966). Shock Waves and Detonations in Gases. Mono Book, Baltimore.

[2] Lee JHS. (2008). The Detonation Phenomenon. Cambridge Univ. Press, Cambridge.

[3] Bedarev IA, Fedorov AV. (2017). Mathematical modeling of the detonation wave and inert particles interaction at the macro and micro levels. J. Phys.: Conf. Ser. 894 (1), 012008.

[4] Vasil'ev AA, Pinaev AV, Trubitsyn AA, Grachev AYu, Trotsyuk AV, Fomin PA, Trilis AV. (2017). What is burning in coal mines: Methane or coal dust? Combust. Explos. Shock Waves. 53: 8.

[5] Bezgin LV, Kopchenov VI, Sharipov AS, Titova NS, and Starik AM. (2013). Evaluation of prediction ability of detailed reaction mechanisms in the combustion performance in hydrogen/air supersonic flows. Combust. Sci. Technol. 185: 62.

[6] Thermodynamic Properties of Individual Substances, Ed. by Gurvich LV, Veyts IV. (1989). Hemisphere, New York. 1(2).

[7] Godunov SK, Zabrodin AV, Ivanov MYa, Kraiko AN, Prokopov GP. (1976). Numerical Solution of Multidimensional Problems of Gasdynamics. Moscow, Nauka. 400 p.

[8] Bocharova OV, Lebedev MG. (2017). Testing the First Order Accurate Godunov Method on Some Prototype and Applied Problems. Computational Mathematics and Modeling, 28 (1): 18.

[9] Zhuravskaya TA. (2007). Propagation of Detonation Waves in Plane Channels with Obstacles. Fluid Dynamics 42(6): 987.

[10] Levin VA, Zhuravskaya TA. (2017). Controlling the position of a stabilized detonation wave in a supersonic gas mixture flow in a plane channel. Tech. Phys. Lett. 43(3): 316.

[11] Zhuravskaya TA, Levin VA. (2016). Stability of gas mixture flow with a stabilized detonation wave in a plane channel with a constriction. Fluid Dyn. 51: 544.

[12] Sedov LI. (1993). Similarity and Dimensional Methods in Mechanics. CRC Press, Boca Raton, FL.

[13] Sadovnichy V, Tikhonravov A, Voevodin Vl, Opanasenko V. (2013). "Lomonosov": Supercomputing at Moscow State University. In Contemporary High Performance Computing: From Petascale toward Exascale (Chapman & Hall/CRC Computational Science). CRC Press, Boca Raton, USA. P. 283-307.