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HEAT AND MASS TRANSFER IN COMBUSTION PROCESSES

DETONATION COMBUSTION OF A HYDROGEN–AIR MIXTURE WITH ADDITIVES OF ARGON AND OZONE

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Using a detailed kinetic mechanism of chemical interaction, the effect of adding argon and ozone to a stoichiometric hydrogen–air mixture on the detonation wave parameters was studied numerically. It has been established that the mole fractions of the used additions can be chosen so that the cell size of the detonation wave in the resulting mixture will be close to the average cell size in a pure hydrogen–air mixture, with the wave velocity and temperature of the detonation products being reduced significantly. It has been found that the detonation wave in a mixture with additives in selected concentrations is more stable against perturbations caused by multiple obstacles (barriers) located in the channel than in the initial mixture. The found specific features make it possible to consider the introduction of the indicated additives into the combustible mixture as a mechanism that lowers the temperature in the detonation wave without a significant increase in the detonation cell size and that prevents the extinction of detonation combustion in a channel with a number of barriers.

Keywords: *detonation, stoichiometric hydrogen–air mixture, cellular detonation structure, argon, ozone, multiple obstacles.*

Introduction. Determination of new mechanisms of controlling detonation is one of the main directions of studying detonation combustion. Here, of equal interest are both the mechanisms ensuring detonation damping and the methods that guarantee its preservation and make it possible to control the wave propagation. One way to control detonation is to change the composition of the mixture by introducing various additives into the combustible gas mixture or by preliminary transformation of its components. So, it was found that the addition of inert particles to the hydrogen–air mixture entering a pinched channel at a supersonic velocity can be used to stabilize the detonation wave in the flow and to control its position in order to increase the efficiency of detonation gas combustion [1–3]. On the other hand, the results of experimental study [4] indicate the possibility of using a curtain of nonreacting dust particles for complete destruction of a propagating detonation wave. In [5, 6], the possibility of preventing the suppression of detonation combustion of a stoichiometric hydrogen–air mixture in channels with obstacles by preliminary partial dissociation of molecular hydrogen and oxygen into atoms, which leads to a significant decrease in the size of the detonation cell and an insignificant increase in the wave propagation velocity, was established numerically [2, 3, 5, 6]. The refinement of the cellular structure of the detonation wave found in a numerical study with a slight increase in its velocity as a result of the indicated preliminary dissociation is confirmed by the results of experiments on the propagation of detonation in a hydrogen–oxygen mixture with addition of ozone, which decomposes rapidly behind the leading shock wave with the formation of atomic oxygen [7]. A similar refinement of the cellular detonation structure was also observed in experiments during the passage of a formed cellular detonation wave through the plasma region containing atomic oxygen along with other radicals [8]. The study of the structure of a plane one-dimensional stationary detonation wave (the Zeldovich–Neumann–Döring (ZND) detonation model) showed that both the preliminary partial dissociation of the fuel and oxidizer in a hydrogen–air mixture [6] and the addition of ozone to the mixture [7] lead to a significant decrease in the length of the induction zone, with the velocity of the Chapman–Jouguet wave and the parameters of the gas behind it varying insignificantly. However, to use detonation in various power plants, it is necessary to solve the complex problem of cooling the walls of the detonation chamber. Lowering the temperature of the combustion products greatly simplifies this task. A simple way to reduce the temperature

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behind the detonation wave is, for example, introduction of a sufficient amount of argon into the combustible mixture, however, in this case a significant increase in the detonation cell is observed [9, 10]. In [11], within the framework of the ZND detonation model, the influence of adding inert diluents and promoters (ozone and hydrogen) to the combustible mixture was considered in order to reduce the post-detonation temperature and prevent an increase in the induction zone.

In this work, within the framework of the detailed kinetics of chemical interaction, we numerically study the influence of adding argon and ozone to a stoichiometric hydrogen–air mixture on the detonation wave parameters in order to reduce the wave propagation velocity and the temperature of combustion products without a significant increase in the size of the detonation cell, which is a fundamental characteristic of the detonation ability of a mixture. This paper considers detonation combustion of the resulting mixture with additives in a flat channel, on one of the walls of which there is a region with barriers. The effect of the addition of argon and ozone to a stoihiometric hydrogen–air mixture on the parameters of a plane cellular detonation wave was first investigated in [12].

Mathematical Formulation of the Problem. The paper considers the propagation of a detonation wave in a gas mixture resting under normal conditions ($p_0 = 1$ atm, $T_0 = 298$ K) in a semi-infinite flat channel of width L ($L = 1$ cm). To initiate detonation, an instantaneous uniform supercritical (sufficient for direct initiation of detonation) energy supply in a region in the form of a thin layer near the closed end of the channel is used. Deformation combustion is studied of both a pure stoichiometric hydrogen–air mixture, which is modeled as a mixture of gases H_2, O_2, and N_2 in a molar ratio 42:21:79, respectively, and a mixture with the addition of argon Ar and ozone O_3.

The system of equations describing a plane two-dimensional unsteady flow of an inviscid multicomponent reacting gas mixture has the form

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

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

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

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

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

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

where T is the temperature and R_0 is the universal gas constant. Dependences of partial enthalpies on temperature $h_i(T)$ are determined from the reduced Gibbs energies of the corresponding components of the mixture [13]. To describe the chemical interaction, use is made of the detailed kinetic mechanism of hydrogen oxidation proposed in [14].

To solve the equations of gas dynamics, an explicit second-order difference scheme based on the Godunov scheme [15–18] was used: to ensure the second order of accuracy in space, a piecewise linear reconstruction of the solution was performed over "averaged" grid quantities with a MINMOD limiter; the second order of accuracy in time was achieved using a predictor–corrector algorithm. The calculation was carried out on a grid with a partition step $\Delta = 5$ μm, which ensures the correct resolution of the structure of the detonation wave. For numerical simulation use was made of an original software module that implements hybrid parallelization of MPI/Open MP calculations. The study was carried out using the equipment of the Center for Collective Use of Ultrahigh Performance Computing Resources of the M. V. Lomonosov Moscow State University [19].

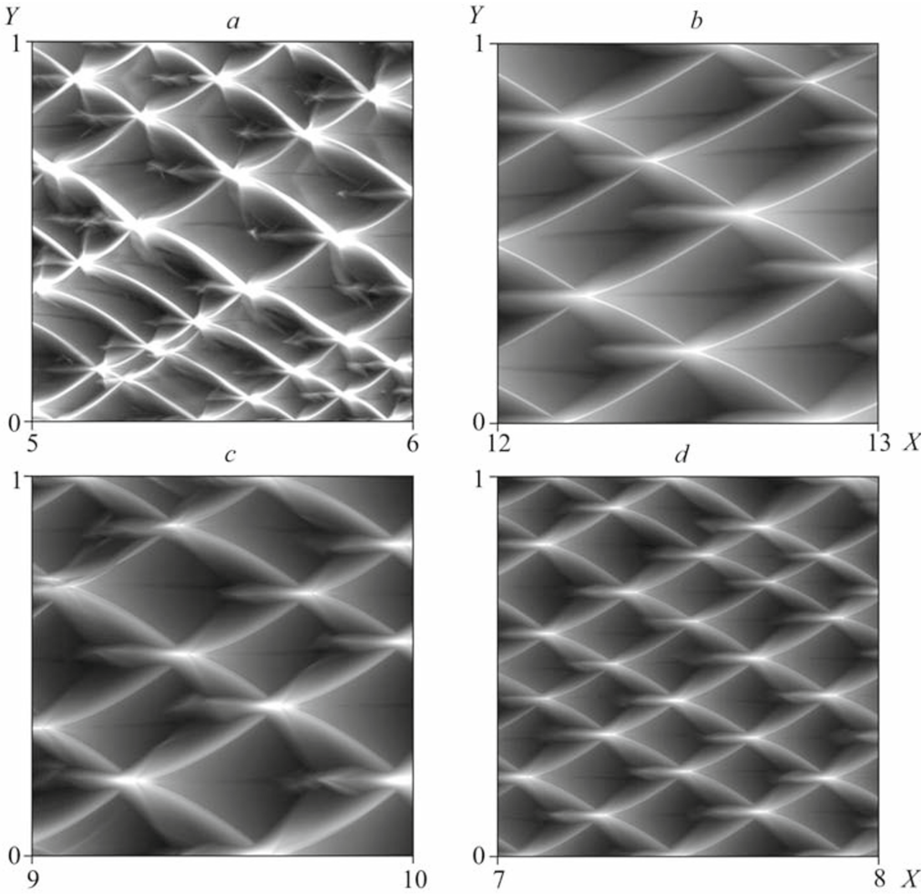

Fig. 1. Cellular structure of a detonation wave propagating in a plane channel: a) stoichiometric H_2–air mixture; b) H_2–air–80% Ar–1.5% O_3; c) H_2–air–70% Ar–0.6% O_3; d) H_2–air–70% Ar–1% O_3. Here and below, $X = x/L$, $Y = y/L$, where L is the channel width; the wave propagates from left to right.

TABLE 1. Detonation Wave Parameters in Mixtures under Normal Conditions: Average Velocity of Propagation of a Self-Sustaining Plane Cellular Detonation D, Velocity of Chapman–Jouguet Detonation Wave D_{CJ}, Pressure p_{CJ}, and Temperature T_{CJ} behind the Wave

Mixture	D, m/s	D_{CJ}, m/s	p_{CJ}, atm	T_{CJ}, K
H_2–air	1964	1975	15.82	2964
H_2–air–1% O_3	1975	1979	15.96	2991
H_2–air–80% Ar–1.5% O_3	1171	1172	8.44	1623
H_2–air–70% Ar–0.6% O_3	1293	1329	10.52	1998
H_2–air–70% Ar–1% O_3	1300	1333	10.62	2011

Influence of Argon and Ozone Additives on the Detonation Combustion of the Mixture. Initial uniform supply of energy initiates a plane detonation wave in the channel, the front of which is distorted with time, transverse waves arise, resulting in the formation of a self-sustaining detonation wave with a stable cellular structure [20, 21]. In the case of a pure hydrogen–air mixture, the self-sustaining wave obtained in the calculations has an irregular structure. Thus, the maximum value of the relative deviation of the cell size from the average is quite large and amounts to more than 60%. A numerical

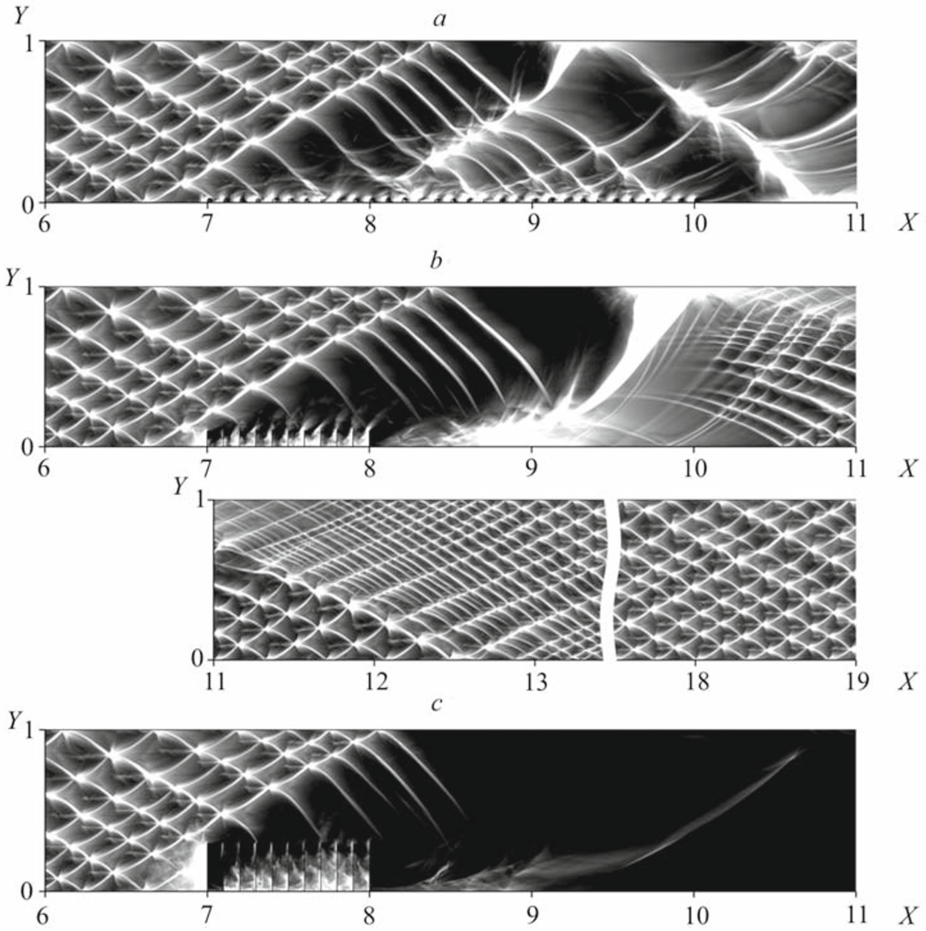

Fig. 2. Propagation of a detonation wave in a pure stoichiometric hydrogen–air mixture in a plane channel with multiple barriers: a) preservation of detonation at L_b = 3 cm, ΔL_b = 0.1 cm, H_b = 0.02 cm; b) recovery at L_b = 1 cm; ΔL_b = 0.1 cm, H_b = 0.1 cm; c) quenching of detonation combustion at L_b = 1 cm, ΔL_b = 0.1 cm, H_b = 0.3 cm.

analog of the trace left by a wave propagating in a plane channel on a sooty plate located along the wall is shown in Fig. 1a. The irregularity of the structure of the wave obtained by numerical simulation corresponds to the results of an experimental study of detonation in mixtures diluted with nitrogen [9]. The average velocity of propagation of a self-sustaining plane cellular detonation wave (D), as well as the wave velocity in the Chapman–Jouguet regime (D_{CJ}) and the parameters of the gas behind it obtained when considering the ZND detonation model for both a pure moisture and mixtures with additives are presented in Table 1. According to the calculations, the deficit of the self-sustaining wave velocity with respect to the Chapman–Jouguet detonation rate for the considered mixtures does not exceed 2.8%.

A numerical study of the effect of ozone addition on the detonation wave showed that the cellular detonation structure becomes substantially finer, while the wave velocity increases insignificantly, which corresponds to the experimental results [7]. So, in the case of x_{O_3} = 1% (x_{O_3} is the mole fraction of O_3), the detonation cell decreases by 3.2 times, while the velocity of the cellular detonation wave increases by only 0.56% (Table 1). Moreover, the addition of ozone makes the cellular structure of the detonation wave more regular, which was also observed in [7]. Note that the temperature of the combustion products, when ozone is added to the mixture, changes insignificantly and is close to 3000 K.

It is known that the dilution of the mixture with Ar leads to a decrease in the temperature in the detonation products and to a significant increase in the size of the detonation cell. However, the introduction of ozone into a hydrogen–air mixture diluted with argon will reduce the size of the detonation cell without significantly increasing the temperature in the detonation wave. The calculations performed showed that the mole fractions of Ar and O_3 can be chosen so that the size of the detonation wave cell in the resulting mixture will be close to the average cell size in a pure hydrogen–air mixture, while

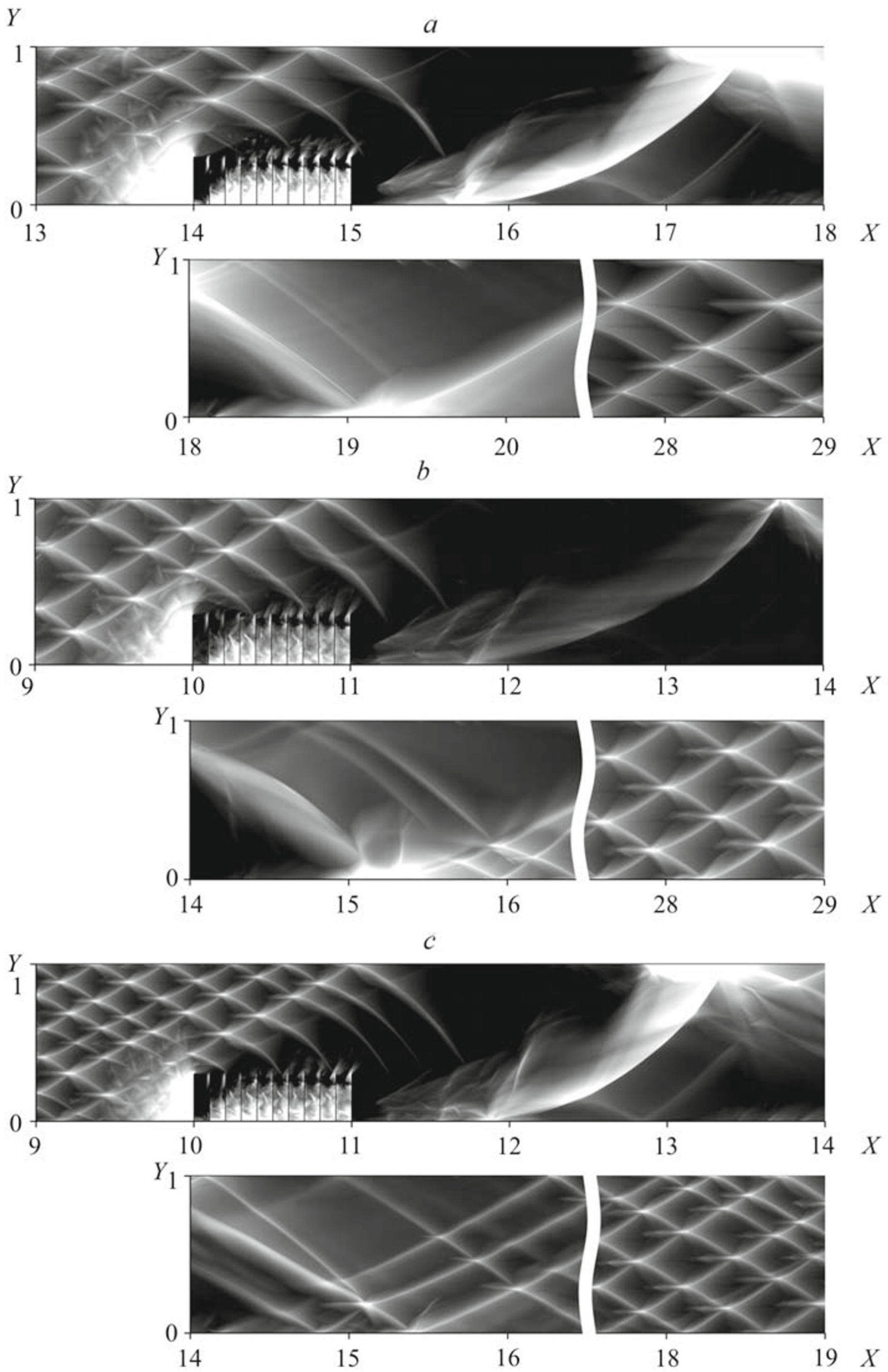

Fig. 3. Recovery of detonation in a plane channel with barriers L_b = 1 cm, ΔL_b = 0.1 cm, H_b = 0.3 cm; a) H_2–air–80% Ar–1.5% O_3; b) H_2–air–70% Ar–0.6% O_3; c) H_2–air–70% Ar–1% O_3. Here and below, $X = x/L$, $Y = y/L$, where L is the channel width; the wave propagates from left to right.

the wave velocity and temperature of the detonation products will be reduced significantly. For example, it was found that the cell size of a detonation in a hydrogen–air mixture on addition of 80% Ar and 1.5% O_3 is slightly more than in a pure mixture (Fig. 1b), with the temperature in the detonation wave not exceeding 1800 K with the velocity of the self-sustaining wave being 1.68 times lower than the detonation velocity in a pure mixture (Table 1). The amount of argon introduced

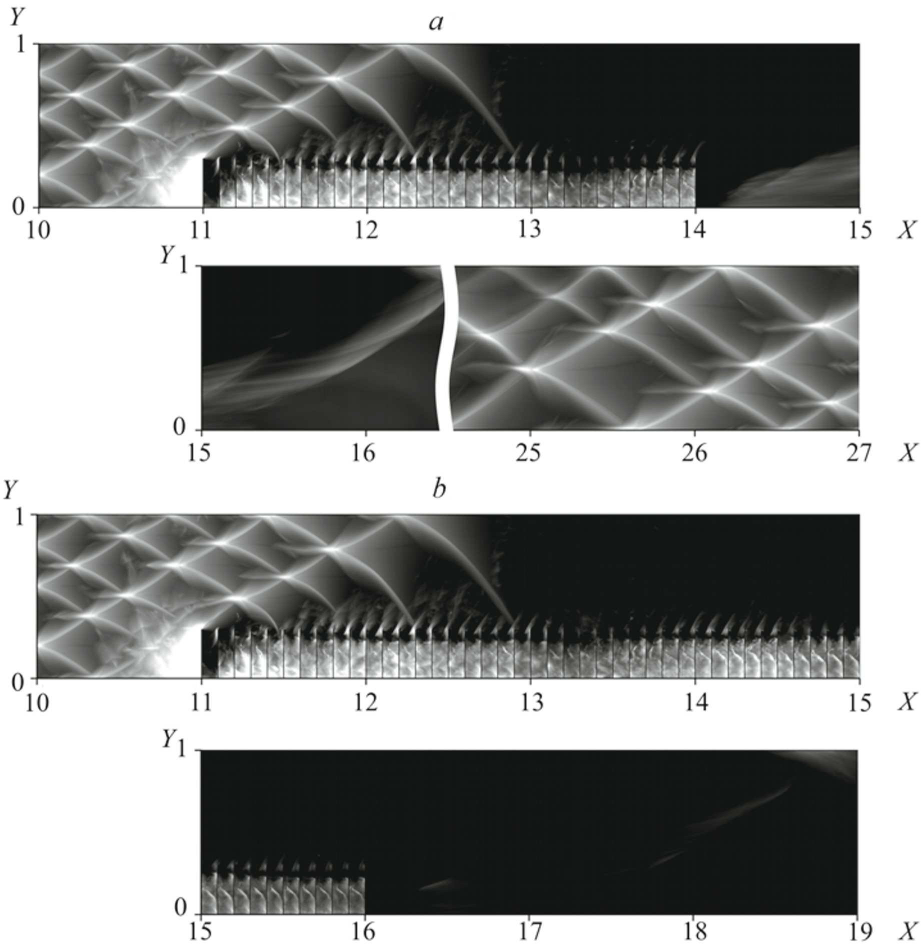

Fig. 4. Propagation of a detonation wave in an H_2–air–70% Ar–0.6% O_3 mixture at $\Delta L_b = 0.1$ cm, $H_b = 0.3$ cm: a) recovery of detonation at $L_b = 3$ cm; b) quenching of detonation combustion at $L_b = 5$ cm.

into the mixture can be reduced. It was found that in the case of 70% Ar and 0.6% O_3, a detonation wave is formed in the mixture, the cell size of which slightly exceeds the average size of a detonation cell in a pure mixture (Fig. 1c), and an increase in the fraction of ozone to1% leads to the formation of a detonation wave with a finer (compared to a pure mixture) cellular structure (Fig. 1d). In this case, the temperature of the combustion products changes insignificantly on increase of the fraction of ozone and is close to 2000 K, and the wave velocity in both considered cases is less than the detonation velocity in a pure mixture by more than 1.5 times (Table 1). Moreover, in contrast to the detonation combustion of a pure mixture, the detonation wave in the mixture, diluted simultaneously with Ar and O_3, has a regular cellular structure. So, the maximum relative deviation of the transverse dimension of the detonation cell from the average in the considered mixtures does not exceed 25%.

Propagation of Detonation in a Channel with Multiple Barriers. To investigate the stability against strong perturbations of detonation combustion of a mixture obtained after addition of Ar and O_3 into a stoichiometric hydrogen–air mixture, the interaction of a cellular detonation wave with a barriers-containing region located on one of the channel walls, which is a simple model of an insert with a porous coating on the inner surface of the channel (for example, covered with steel wool) [22], was considered. Porous coatings of walls are taken to be tool for suppressing detonation combustion [23–25]. On the other hand, experimental studies of wave propagation in a channel filled with a porous material showed that porous media can be used to facilitate reinitiation of detonation when a wave enters the volume of a reacting mixture [26, 27].

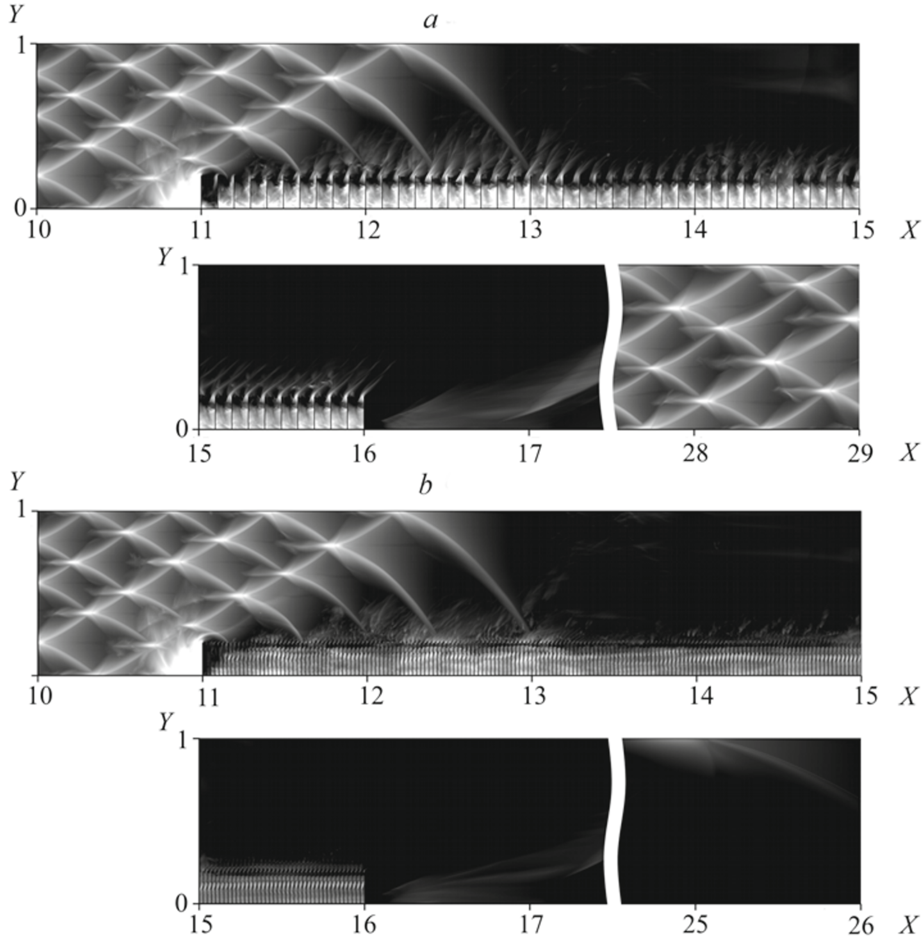

Fig. 5. Propagation of a detonation wave in an H_2–air–70% Ar–0.6% O_3 mixture of $L_b = 5$ cm, $H_b = 0.2$ cm: a) recovery of detonation at $\Delta L_b = 0.1$ cm; b) quenching of detonation combustion at $\Delta L_b = 0.025$ cm.

In the case of a region with barriers, the result of interaction of a wave with obstacles is determined by the length of the region L_b, barrier height H_b, and by the distance between adjacent barriers ΔL_b. It is known that both in the case of a single barrier [28], and of multiple obstacles [6] (at fixed values of L_b and ΔL_b), the detonation wave is suppressed, if the height of barriers exceeds a certain critical value, which depends on the channel width. Numerical traces illustrating the preservation, recovery, and quenching of detonation in a hydrogen–air mixture in a channel with multiple barriers are shown in Fig. 2.

As a result of the numerical simulation, it was found that the critical height of obstacles in the cases of mixtures with additions of Ar and O_3 (at the concentrations indicated above, see Table 1) is higher than in the case of a pure mixture with other constant parameters. The numerical trace prints illustrating the detonation recovery in a mixture with additions of Ar and O_3 after passing the region with barriers that quench the detonation combustion in a pure mixture (Fig. 2c) are presented in Fig. 3. The calculations showed that an increase in the length of the region with barriers or a decrease in the distance between adjacent obstacles in a number of cases significantly reduce the critical height (Figs. 4 and 5). So, in a mixture of H_2–air–70% Ar–0.6%O_3 at $\Delta L_b = 0.1$ cm the height of obstacles $H_b = 0.3$ cm is subcritical if the length of the region $L_b = 3$ cm (Fig. 4a) and becomes supercritical (obstacles destroy detonation) when L_b increases up to 5 cm (Fig. 4b). When $L_b = 5$ cm and $\Delta L_b = 0.1$ cm, the height of the barriers $H_b = 0.2$ cm (Fig. 5a) is subcritical, however, an increase in the frequency of their location to $\Delta L_b = 0.025$ cm leads to the suppression of detonation by obstacles (Fig. 5b), i.e., the height of barriers becomes supercritical. Note that when detonation combustion is reinitiated after the interaction with barriers, the size of the detonation cell of the self-sustianing wave being formed in a number of cases differs from the size of the

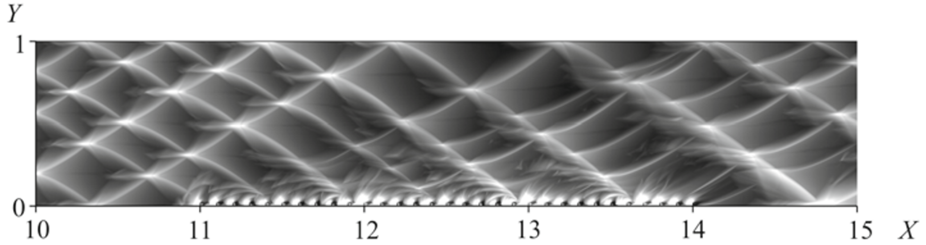

Fig. 6. Preservation of detonation combustion in an H_2–air–70% Ar–0.6% O_3 mixture at L_b = 3 cm, ΔL_b = 0.1 cm, and H_b = 0.02 cm.

cell of the detonation wave approaching the obstacles. This is associated with the existence of the range of the cell size of self-sustaining detonation, which was noted during numerical simulation [28] and was observed in experiments for various mixtures, including those with a large amount of argon [29].

In cases where the height of obstacles is substantially less than the critical value, detonation combustion persists across the channel as the wave propagates along the region with barriers. The size of detonation cells increases, while [in contrast to a pure mixture (Fig. 2a)] the structure of detonation is close to a regular one (Fig. 6), which was observed in experiments with mixtures with a large content of argon [25]. On the other hand, when the wave propagates in a mixture with additives along the region with obstacles, a number of characteristic features are revealed typical of mixtures with an irregular cellular structure. Thus, along with the suppression of transverse waves, new transverse waves are generated on the barriers from local perturbations in the zone of reaction (Fig. 6), and with increase in the height of obstacles (the height is still lower than the critical), local quenching of detonation combustion is observed.

When a wave propagates along a series of barriers in a mixture with additives of argon and ozone, a more intense (compared to a pure mixture) formation of diverging shock waves near obstacles is observed, which is a consequence of the decomposition of ozone behind reflected shocks between the barriers, which is accompanied by energy release. This leads to more intense formation of transverse waves on the detonation front, as well as to enhancement of the leading shock wave, which increase the resistance of detonation against perturbations caused by the obstacles located in the channel.

When detonation is recovered in a mixture with additives after passing the region with obstacles, a detonation with a larger cell is initially formed, the size of which gradually decreases (Fig. 3). This character of detonation combustion recovery is typical of mixtures with a regular cellular structure of detonation [30] and differs qualitatively from the character of detonation recovery in a pure mixture (Fig. 2b) corresponding to gases with irregular wave structure [30].

Conclusions. Using the detailed kinetic mechanism of chemical interaction, the effect of additions of argon and ozone to a stoichiometric hydrogen–air mixture on the parameters of the detonation wave is studied numerically.

It has been established that the molar fractions of introduced additives can be chosen so that the size of the detonation wave cell in the mixture obtained will be close to the average size of the cell in a pure mixture, while the wave velocity and temperature of the detonation products will be lowered considerably. It was found that the detonation combustion of the mixture obtained after the introduction of argon and ozone in selected concentrations is more stable to perturbations caused by multiple obstacles located in the channel than in a pure gas. It is shown that introduction of indicated additives makes the structure of the detonation wave regular and qualitatively changes the mechanism of reinitiation of detonation after the region with obstacles is passed.

The established characteristic features of detonation combustion of a mixture with additives of argon and ozone make it possible to use the introduction of these additives both to decrease the temperature in detonation products without a significant increase in the size of the detonation cell and to present destruction of detonation in a channel with barriers.

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NOTATION

D, propagation velocity of a self-sustaining plane cellular detonation wave, m/s; D_{CJ}, velocity of Chapman–Jouguet detonation wave, m/s; H_b, height of barriers, cm; L_b and ΔL_b, length of the region with barriers and the distance between adjacent barriers, cm; *L*, channel width, cm; *M*, number of components in a mixture; p_0, initial pressure of a gas mixture, atm; p_{CJ}, pressure behind the Chapman–Jouguet wave, atm; T_0, initial temperature of the mixture, K; T_{CJ}, temperature behind the Chapman–Jouguet wave, K; x_{O_3}, molar fraction of O_3; *X* and *Y*, dimensionless longitudinal and transverse Cartesian coordinates, respectively.

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