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# Flame Propagation Regimes at Combustion of Lean Hydrogen-Air Mixtures in the Presence of Additives at Central Spark Initiation at Atmospheric Pressure

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**Abstract-** By means of high-speed color cinematography it is shown that the flames in lean H<sub>2</sub>-air mixtures at an initial stage propagate symmetrically and the flame radius can be estimated from the frames of speed filming. It is shown that sufficiently strict calculation of cellular structure flame front of lean hydrogen mixes requires consideration of a 3D problem however thermal diffusion instabilities at the initial stage of combustion have no effect on the velocity of flame which can be estimated assuming unperturbed flame front in the range of 8%<H<sub>2</sub><15%. It is shown that the analysis of experimental data on flame propagation in lean mixtures does not allow taking apart results of calculation by two-dimensional model with regard to convection and without convection. It is experimentally shown, that isobutene additives in quantities below a concentration limit (up to 1.5 %) tend to increase, and CO<sub>2</sub> additives up to 15 % - to reduce the flame propagation velocity in lean H<sub>2</sub>-air mixtures. The reasons for acceleration of combustion in the presence of hydrocarbon additive are considered.

For lack of special conditions the processes of gas-phase combustion occur under non-stationary currents, density and pressure fluctuations, i.e. have non-steady character [1-3]. For example a cellular combustion front is characteristic of lean hydrogen-air mixes, caused by thermal diffusion instability [3-5]. For the first time flame cells in combustion of lean H<sub>2</sub>-air mixes were observed in [6]. In [1,7] it was shown that flame cells in lean H<sub>2</sub>-air mixes can be obtained also in microgravity conditions, i.e. the gravity field isn't essential for occurrence of cellular flames.

Investigations of flame propagation in lean H<sub>2</sub>-air mixes in narrow vertical pipes showed that flame propagation "upwards" is accompanied by the partial consumption of fuel; in this case the fuel content at concentration limit of flame propagation is less than that in a "downwards" direction [4,8].

In a 2D model of combustion of lean H<sub>2</sub>-air mixes in [9] convection and gravity were not taken into account. However, calculated velocities of flame fronts were close to their experimental values. The analytical theory of cellular flames based on representation of a flame as a dense flat structure of hexagonally packed flame balls [2], also gives a good consent with experiment at successful selection of parameters. It is important to find out limits of applicability of

the models of the hydrogen flame which do not consider convection and compressibility of the environment for calculation of flame velocities [2,4,5,7,9,10] in comparison with the models considering convection and compressibility of the environment [2, 11]. Understanding combustion of lean H<sub>2</sub>-air mixes is critical to the design of efficient, clean-burning combustion engines as well as to provide explosion safety in mines, chemical plants and engines operation.

The work is aimed at investigation of the flame structure in lean hydrogen-air mixes in a bomb of constant volume at atmospheric pressure by means of a method of high-speed cinematography; the results obtained are compared with numerical calculations and experimental data including these reported in literature.

## 1. EXPERIMENTAL

Experiments were performed with lean (5.8-15%) hydrogen-air mixes at initial atmospheric pressure and temperature  $T = 298\text{K}$  in a horizontally located stainless steel cylindrical reactor 13 cm in diameter and 15 cm long supplied with an optical quartz window at a butt-end. Spark electrodes were placed at the reactor centre; the distance between them was 0.5 mm. Experiments were performed as following. The reactor was pumped out to 10-2 Torr, than filled with CCl<sub>4</sub> (~ 4%), then with hydrogen and air up to the atmospheric pressure. The gas was maintained for 15 min for completeness of mixing, then spark initiation (1.5 J) was carried out. Notice that that the additive of CCl<sub>4</sub> is necessary for visualization of a hydrogen flame; 4% CCl<sub>4</sub> in H<sub>2</sub>-air mixture can be considered as an inert additive [12]. Speed filming of ignition dynamics and flame front (FF) propagation was carried out through an optical window by means of a color high-speed digital camera Casio Exilim F1 Pro (frames frequency, 60–1200 s<sup>-1</sup>). The video file was stored in computer memory and its time-lapse processing was performed. The pressure change in the course of combustion was recorded by means of a piezoelectric gage synchronized with the discharge. Gases were chemically pure.

The degree of expansion of combustion products  $\varepsilon_T$  was determined as follows [4] ( $P_b$  is the maximum pressure developed in the course of combustion):

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$$P_b/P_0 = 1 + \gamma (\varepsilon_T - 1) \quad (1)$$

The normal velocity  $U_n$  of FF was calculated from the equation [4]:

$$U_n = V_v / \varepsilon_T \quad (2)$$

In equations (1), (2)  $P_0$  – initial pressure,  $\gamma = 1.4$  – the ratio of specific heats,  $V_v$  – visible flame velocity.

## II. RESULTS AND DISCUSSION

As is seen in Fig. 1 (a-c), FF in lean burning mixture has a spherical form. The cells are well visualized, thus diameter of the sphere can be measured experimentally. For mixes containing < 10% of H<sub>2</sub> FF has a spherical form only at an initial stage after initiation (Fig. 1a). Further in the course of combustion the action of gravity force is shown, and FF gets a form of the hemispherical segment moving upwards (Fig. 1 a, b). For the mixes containing > 10% H<sub>2</sub> FF velocity increases so that gravity doesn't manage to be shown, and the flame propagates spherically symmetrically (Fig. 1c, d). The front of a flame remains cellular, thus with increase in hydrogen content to 15% in air the size of flame cells markedly decreases.

As is seen in Fig. 1a at an initial stage the sphericity of the combustion front (Fig. 1a, shots 2-6) is characteristic even for 8% of H<sub>2</sub> in air. High-speed filming of flame propagation in 10% H<sub>2</sub> + air is presented in Fig. 1b, also illustrating FF sphericity. The visible flame velocity  $V_v$  measured for 4% CCl<sub>4</sub> + 10%H<sub>2</sub> + 86% air mix (Fig. 1a) makes up 36 cm/s, thus the normal flame velocity  $U_n$  calculated by means of eq.(2), makes up 21 cm/s taking into account that experimental value of  $\varepsilon_T$  is 1.6 for this mix. Visible flame velocity  $V_v$  for mix 4% CCl<sub>4</sub> + 15%H<sub>2</sub> + 81% air (Fig. 1c) makes up 2.4 m/s, thus the normal velocity  $U_n$  calculated by means of eq.(2) makes up 60 cm/s taking into account the experimental value of  $\varepsilon_T = 4$ . These values of normal velocity are in good agreement with literature data, and also are close to results of numerical calculation of  $U_n$  obtained using a model of a laminar flame without convection [9], i.e. without taking into account the cellular flame structure. It means that perturbations of thermal diffusion nature observed on FF at the initial stage of combustion have no essential impact on the velocity of flame propagation of lean H<sub>2</sub>-air mixes.

We specify concentration boundaries of various modes of a cellular flame propagation in lean H<sub>2</sub>-air mixes on a basis of Fig. 1 and [1, 4, 8]:

- "anisotropic" at H<sub>2</sub> <10% that corresponds to different velocities of flame propagation "upwards" and "downwards" in vertical pipes [4,8] and spherically-symmetric on an initial stage of combustion;

- Spherically - symmetric at 10% < H<sub>2</sub> <15%, thus distinction between propagation "upwards" and "downwards" is missing.

A spherically symmetric mode of cellular flame propagation in microgravity conditions at H<sub>2</sub> concentration less than 10% is also known [1, 7]. We will note also that in the conditions of zero gravity there exists a mode of occurrence of separate isolated motionless cells of combustion [1]. Such "flame balls" can be observed in mixtures that are well outside the conventionally defined extinction limits, e.g. In 3.85% H<sub>2</sub> - 96.15% air mixture [1].

We will specify that experimental values of the lower concentration limit of flame propagation in microgravity conditions ( $C_{\mu g}$ ) have noticeable dispersion that doesn't allow reliable establishing whether the limit value is closer to a propagation limit "upwards" or "downwards". According to [7] the limit is close to "upwards" limit value in the gravity field and makes up 5.5% H<sub>2</sub> in air, however from [1]  $C_{\mu g}$  makes up 7% H<sub>2</sub> and from [5]  $C_{\mu g}$  makes up 7% H<sub>2</sub> in the presence of 2.5% of CF<sub>3</sub>Br.

It is possible to conclude that the spherical form is inherent to cellular flames propagation in lean H<sub>2</sub> -air mixes at an initial stage. The gravity field only then distorts a shape of FF for mixes in the vicinity of the lower concentration limit of the flame propagation (Fig. 1 a, b).

We will consider some results obtained at numerical modeling of cellular flames. A flat 2D problem and the model of thermal convection in Boussinesque approximation were used to analyze FF propagation in lean H<sub>2</sub>-air mixes in [10, 11, 14]. The reduced kinetic scheme of reaction of hydrogen oxidation including 13 reactions as well as thermo chemical parameters, were taken from [8]. However, for lack of gravity the cellular mode at calculation was missing. Thus, a 2D calculation in Boussinesque approximation doesn't allow modeling experimentally observed mode of the cellular flame propagation in microgravity conditions.

To establish physical processes to be considered for a 2D modeling of the cellular FF in the microgravity conditions a numerical analysis by finite elements method with use of a software package FlexPde 6.0 [15] was carried out. Thus, because it was shown in [11,14] that within Boussinesque approximation features of lean hydrogen flames do not depend on the chemical nature of the most quickly diffusing intermediate, but the features are determined by the value of diffusion coefficient of the insufficient initial component [4,8], a chemical reaction was set by a single equation in Arrhenius form (see Appendix).

In Fig. 2 results of calculation of FF propagation are presented in Boussinesque approximation a)  $g=0$  ( $g$  is acceleration of gravity); b)  $g=980$  cm<sup>2</sup>/c. The calculation of FF propagation at  $g=0$  on the basis of

Navier-Stokes equations for a viscous compressible environment [16] is shown in Fig. 2c. As is seen in Fig. 2 (a,b,c) a 2D consideration of the convection caused by expansion of gas in the course of combustion for lack of gravity in weakly compressible environment doesn't lead to occurrence of a cellular combustion; thus taking into account of compressibility in Navier-Stokes equations provides a way to obtain a 2D cellular combustion mode. Thus, for a 2D modeling of cells at "anisotropic" ( $H_2 < 10\%$ ) mode of FF propagation Boussinesque approximation is applicable [11]; for the description of a 2D-symmetric mode in the absence of external forces compressible Navier-Stokes equations should be used.

We now turn to a 3D problem. It should be noted that it was earlier shown [4] that the steady heat and mass conservation equations admit a solution corresponding to a stationary spherical flame, though the same equations in planar geometry provide a solution in the form of a propagating wave. Indeed in the simplest case of spherical geometry, the solution to steady, free convection diffusion equations for temperature  $T$  and chemical species  $C$ ,  $\nabla^2 T = 0$  and  $\nabla^2 C$ , has the form  $c_1 + c_2/r$ , where  $c_1$  and  $c_2$  are some constants. This form reflects the fact that  $T$  and  $Y$  are bounded as  $r \rightarrow \infty$ . For cylindrical and planar geometry the forms are  $c_1 + c_2 \ln(r)$  and  $c_1 + c_2 r$ , respectively, which are unbounded as  $r \rightarrow \infty$ . Therefore a spherical flame is admitted, but not (say) a "flame cylinder" solution. On the basis of this simple consideration illustrated below (see also Appendix) one should expect occurrence of cellular FF in a 3D modeling within Boussinesque approximation. The result is shown in Fig. 2d where the section of a 3D structure of the flame front is specified in the XZ plane (a 3D mesh structure is shown in Fig.2e). As is seen in Fig.2d a 3D flame front shows a cellular structure in relation to a 2D modeling (Fig.2a) which provides completely undisturbed FF.

It follows from aforesaid that sufficiently strict calculation of cellular FF structure of lean hydrogen mixes requires consideration of a 3D problem however on the other side thermal diffusion instabilities at the initial stage of combustion have no effect on FF velocity which can be estimated assuming unperturbed flame front in the range of  $8\% < H_2 < 15\%$ .

It is of interest in this connection to find out the limits of applicability of the models of hydrogen flame, which do not account for convection and compressibility of the environment, for calculation of FF velocities observed experimentally [2,4,5,7,9,10,13] in comparison with the models considering convection and compressibility of the environment [2, 11]. We will examine the data on measurement and calculation of FF normal velocities of lean H<sub>2</sub>-air mixes available in literature along with our results. A considerable set of literary data is presented in [2, 13] in which results of several groups of authors are given. Comparison of

experimental and calculated normal FF velocities in lean H<sub>2</sub> - air mixes at 1 atm and initial temperature 298 K in relation to the content of fuel in mix (equivalence ratio  $\theta$  is a fraction of fuel in a mix with air:  $\theta H_2 + 0.5(O_2 + 3.76N_2)$ ) is shown in Fig. 3. In Fig. 3 a thick curve represents results of modeling within a 1D problem [2], a thin curve shows calculated values with the use of an analytical formula [2]. Points represent experimental data cited in [2] (see Fig.1 [2]), crosses represent experimental data [10], thin circles – the data of a 2D calculation without convection (Fig.2, [9]), thick circles - the data of a 2D calculation with convection taken into account (Fig 3 and Fig.4 [10]), triangles – experimental data for lack of gravity [7]. The area filled with grey color relates to a number of sets of experimental values of FF normal velocities of lean H<sub>2</sub>- air mixes [13]. Notice that there were no reasons to choose any of the data sets as the most reliable one.

As is seen in Fig.3 the results obtained in [9] with use of a 2D model without convection (crosses), lie in the area of experimental values of FF normal velocities [13]. It is evident from Fig. 3 that the experimental errors of the data on FF propagation do not allow establishing the kinetic mechanism of H<sub>2</sub> oxidation necessary for the description of lean H<sub>2</sub>-air combustion in detail; and even taking apart the results of calculation for the 2D models including convection and without it. In other words, only successful selection of parameters allows obtaining quantitative agreement with experiment. Notice that even calculations for a 1D model (a thick curve in Fig. 3) which agrees with the experimental data in the worst way also fit with experimental data.

It means from aforesaid that at the current state of experiment any comparison of experimental data on FF propagation in lean H<sub>2</sub>-air mixes with the results of numerical modeling is credible only in qualitative aspect e.g. on velocity change of movement of the boundary between initial and actively reacting gas, as well as on the shape of this border and on the degree of its "smoothness" or perturbations of its structure. Obviously, the consideration of detailed kinetic mechanism introduces additional uncertainty into calculations. The vast majority of kinetic parameters is not accurate enough to draw reliable conclusions on the basis of modeling. The question of completeness of the kinetic mechanism used is always an open question, i.e. whether any important reaction is overlooked. Moreover as there are no unicity theorems on reactive Navier-Stokes equations, the agreement between calculated quantities and experimental ones does not argue for accord between calculation and experiment as there can be other sets of the governing parameters describing the same profiles.

We will note that the discussion carried out above refers only to H<sub>2</sub>-air mixes in the absence of other





reactive additives, for example, hydrocarbons. It is known that addition of hydrogen to hydrocarbon fuels holds much promise for providing ecological safety of combustion products e.g. in engines [1]. The results of high-speed filming of FF propagation in lean H<sub>2</sub> - air mixes in the presence of isobutene (C<sub>4</sub>H<sub>8</sub>) additive (CCl<sub>4</sub> additive was not used in the experiments) are presented in Fig. 4 (a-f); the concentration of additive in all cases doesn't exceed the lower concentration limit of C<sub>4</sub>H<sub>8</sub> ignition being equal 1.8% [12]. Notice that C<sub>4</sub>H<sub>8</sub> additive in stoichiometric and rich H<sub>2</sub> - oxygen mixtures act as combustion inhibitor [16].

Combustion of lean H<sub>2</sub> mixes is considerably accelerated in the presence of C<sub>4</sub>H<sub>8</sub> additive in agreement with [17] as is evident from comparison of sequences of the video images shown in Fig. 4 (a-f); though C<sub>4</sub>H<sub>8</sub> additive in such quantities isn't combustible. Indeed as is shown in Fig. 4 (a, b) 1.5% of C<sub>4</sub>H<sub>8</sub> additive accelerates combustion of 10% H<sub>2</sub> in air several times in comparison with 10% H<sub>2</sub> - air without additive; as is seen in Fig. 4 (c, d) the increase in additive content by a factor of three accelerates combustion of 7.5% H<sub>2</sub> with air also approximately by the same factor. Even near a combustion limit isobutene additive considerably accelerates hydrogen combustion (see Fig. 4 (d- f)).

In addition (Fig. 4 (b, c, e)), gasdynamic features of FF propagation in lean H<sub>2</sub>-air mixes in the presence of a hydrocarbon additive also qualitatively change; with increase in the content of the additive flame instabilities are no longer shown in the form of cells, but in the form of "folds" on FF surface. Such instabilities aren't observed in combustion of lean H<sub>2</sub>-air mixes in the absence of the additive. It means that FF stability in the presence of hydrocarbon additive increases.

We will note that the chemical mechanism of combustion of combined fuels on the basis of lean H<sub>2</sub> - air mixes in the presence of hydrocarbons isn't considered in literature in detail. However the solution of this problem is necessary for correct numerical modeling of combustion of lean binary mixes of hydrogen and hydrocarbon with air. Dependencies of normal velocities of FF propagation in lean H<sub>2</sub> -air mixes in the presence of the isobutene and CO<sub>2</sub> additives on H<sub>2</sub> content are shown in Fig. 5. Visible velocities were measured at an initial stage of combustion process (from the very first frames of video filming when the flame front still keeps a spherical form) with use of the equations (1) and (2).

Normal combustion velocities of H<sub>2</sub>-air mixes in the absence of additives obtained in the work are in agreement with [12]. As is seen in Fig. 2 1.5% isobutene additive is the most effective; it provides increase in the normal flame velocity of combined fuel in comparison with that of lean H<sub>2</sub> -air mix more than by a factor of 5.

Chemically inert CO<sub>2</sub> additive [12] causes reduction of FF velocity (Fig. 5).

As is seen in Fig.5, 1% of C<sub>4</sub>H<sub>8</sub> or 2% of H<sub>2</sub> is required to attain the same FF velocity e.g. for 5.8% of hydrogen in air (dotted straight lines in Fig. 5). One of the reasons of observed efficiency of a hydrocarbon additive can result from the fact that thermal effect of isobutene oxidation makes up 2549, 7 kJ/mol, and hydrogen - 242, 9 kJ/mol [12], therefore heat release in combustion of isobutene is ten times greater than in hydrogen combustion. It provides increase in FF velocity at the expense of increase in adiabatic temperature of combustion. The other reason can comprise the change in kinetic mechanism of combustion in the presence of hydrocarbon additive particularly at a stage of initiation of FF propagation. By this means in lean H<sub>2</sub>-air mixes, unlike rich ones [17] hydrocarbon additive burns down completely in an excess of oxidizer (that is accompanied by luminescence, see Fig. 4 (b-d)) therefore calculation of FF velocity in the presence of hydrocarbon additive requires a consideration of the major elementary reactions of hydrocarbon oxidation along with the mechanism of hydrogen oxidation however in doing so all difficulties mentioned above are shown in full.

We summarize shortly the results obtained. It is established that cellular flames of lean H<sub>2</sub>-air mixtures at an initial stage propagate spherically symmetrically. Therefore combustion velocity can be estimated from the change of visible radius of a flame front. It is shown that Boussinesque approximation is applicable for the description of cells occurrence in the field of gravity at H<sub>2</sub> <10% within a 2D problem; in the conditions of microgravity it is necessary to invoke compressible Navier-Stokes equations within a 2D problem or Boussinesque approximation within a 3D problem. It is shown that the error of experimental data on FF propagation in lean H<sub>2</sub> -air mixes doesn't allow carrying out reliable verification of various numerical models as well as establishing the kinetic mechanism of H<sub>2</sub> oxidation necessary for the description of lean H<sub>2</sub>-air combustion in detail. With use of a method of color high-speed filming it is shown that isobutene additives in quantities below lower concentration limit of ignition increase FF velocity of lean H<sub>2</sub>-air mixes. The increase in adiabatic temperature of combustion can be one of the reasons of increase in flame propagation velocity; the other reason is change in kinetic mechanism of combustion in the presence of additive. It was shown that the most effective concentration of isobutene additive which provides increase in the normal flame velocity of the combined fuel in comparison with H<sub>2</sub>-air mix more than by a factor of 5 amounts to 1.5%.

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## APPENDIX

A qualitative 3D modeling for microgravity conditions was performed as follows. Chemical process is presented by a single reaction in Arrhenius form. In Boussinesque approximation, we assume that the fluid is almost incompressible, except for thermal expansion effects which generate a buoyant force. The incompressible form of the Navier-Stokes equations can be written:

$$\text{grad}(U) = 0 \quad (3)$$

$$\partial U / \partial t + U \text{grad}(U) + \text{grad}(p) = \nu \text{div}(\text{grad}(U)) + F \quad (4)$$

Where  $U$  represents the velocity vector,  $p$  is the pressure,  $\nu$  is the kinematic viscosity,  $F=0$  - is the vector of body forces.

Eq. (3) is continuity equation while eq. (4) expresses the conservation of momentum. Dimensionless form of reactive Navier-Stokes equations ( $T$ -temperature,  $C$ -concentration) is according to [11]:

$$p = \rho T \text{ (state equation)}$$

$$\rho = \rho_0 (1 - \alpha (T - T_0)) \text{ (Boussinesque approximation)}$$

$$\text{grad}(U) = 0$$

$$\partial U / \partial t + U \text{grad}(U) + \text{grad}(p) = \nu / \text{Re} (\text{div}(\text{grad}(U)))$$

$$\partial T / \partial t + U \text{grad}(T) = 1 / \text{Re} * \text{Pr}_T (\text{div}(\text{grad}(T))) + \beta_2 \cdot RC$$

$$\partial C / \partial t + U \text{grad}(C) = 1 / \text{Re} * \text{Pr}_C (\text{div}(\text{grad}(C))) + \beta_1 \cdot RC$$

$\text{Re} = 10^5$ ,  $\text{Pr}_T = \mu C_p / \lambda = 0.72$  [18]  $\text{Pr}_C = \mu C_p / D = 0.5 \text{ Pr}_T$  ( $\lambda$  - heat conductivity,  $D = 2\lambda$  - diffusivity in lean mixture,  $D > \lambda$  for a lean  $H_2$  mixture [8]). Reaction of the first order is set by Arrhenius's law  $RC(C, T) = (1-C) \exp[\zeta(1-1/T)]$ , Temperature of walls of the external sphere is  $T_0$ , concentration  $C$  on the wall of the sphere is zero. The flame was initiated with a heated internal cube (Fig 2d). Temperature of flame initiation on an internal cube surface is  $5T_0$ , temperature in volume -  $T_0$ , initial concentration  $C_0$  is 0; other parameters are put equal  $T_0 = 1$ ,  $\alpha = 9 \cdot 10^{-3}$ ,  $\rho_0 = 6 \cdot 10^{-3}$ ,  $\zeta = 10$ ,  $\beta_2 = 0.3$ ,  $\beta_1 = 0.2$ ,  $g = 0$ . Software package of a finite elements method FlexPde 6.0 [15] was used.

For qualitative consideration of conditions of occurrence of cellular structures we followed BUOYANT.PDE example from FlexPde 6.0 [15] for the solution of a 2D problem. The reactor of circular section with ignition by a step on a horizontal axis was considered. Calculations were performed in the top half of area (Fig. 2 a-c). Using  $\text{grad}(U) = 0$  and  $\text{grad}(\text{rot}(U)) = 0$  ratios, and  $w$  definition =  $\text{rot}(U)$ , we get the momentum conservation equation in the form:

$$\partial w / \partial t + u \partial w / \partial x + v \partial w / \partial y = \nu \text{div}(\text{grad}(w)) - g \partial \rho / \partial x$$

Taking into account that in two dimensions velocity has only two components, say  $u$  and  $v$ , and the vorticity has only one, which we shall write as  $w$ .

Let us consider now continuity equation. If we define a scalar function  $\phi$  such that

That  $u = \partial \phi / \partial y$ ,  $v = -\partial \phi / \partial x$ , then  $\text{grad}(U) = \partial^2 \phi / \partial x \partial y - \partial^2 \phi / \partial y \partial x = 0$ , and the continuity equation is satisfied exactly, then  $\text{div}(\text{grad}(\phi)) = -w$

If  $F$  is a gravitational force, then  $F = (0, -g\rho)$  and  $\text{rot}(F) = -g \partial \rho / \partial x$  where  $\rho$  is the density, and  $g$  is the acceleration of gravity. If we assume linear expansion of the gas with temperature, then

$$\rho = \rho_0 (1 + \alpha (T - T_0)) \text{ and } \text{rot}(F) = -g \rho_0 \alpha \partial T / \partial x$$

For temperature we have  $\text{div}(\lambda \text{grad}(T)) = \rho_0 C_p (\partial T / \partial t + u \partial T / \partial x + v \partial T / \partial y)$ ,  $C_p$  - the thermal capacity at a constant pressure.

Taking into account diffusion the system of the equations takes the form:

$$\partial w / \partial t + u \partial w / \partial x + v \partial w / \partial y = \nu \text{div}(\text{grad}(w)) - g \partial \rho / \partial x$$

$$\text{div}(\text{grad}(\phi)) = -w$$

$$\text{div}(\lambda \text{grad}(T)) + \beta_2 RC = \rho_0 C_p (\partial T / \partial t + u \partial T / \partial x + v \partial T / \partial y)$$

$$\text{div}(D \text{grad}(C)) + \beta_1 RC = \partial C / \partial t + u \partial C / \partial x + v \partial C / \partial y$$

and the equation of state  $p = \rho T$

The temperature of the walls of the external cylinder is  $T_0$ , the concentration  $C$  on the wall is zero. Newmann's boundary condition for temperature, concentration and density are set on a part of abscissa axis dividing the top and bottom half of the cylinder. The initiation temperature of a flame on a step was  $5T_0$ , the temperature in volume is  $T_0$ , initial concentration is 0; other parameters are the following:  $T_0 = 1$ ,  $D = 2$ ,  $\lambda = 0.01$ ,  $\alpha = 0.009$ ,  $\rho_0 = 10^{-2}$ ,  $\zeta = 16$ ,  $\nu = 0.001$ ,  $\beta_2 = 0.3$ ,  $\beta_1 = 0.2$ ,  $g = 0$  (Fig. 2a),  $g = 980$  (Fig. 2b).

Compressible Navier-Stokes equations in the absence of gravity forces have the form [18]:

$$\partial U / \partial t + U \text{grad}(U) + \text{grad}(p) = \nu \text{div}(\text{grad}(U)) + \mu \sigma (\sigma \times U) + F \text{ (momentum conservation)}$$

$$\partial \rho / \partial t + \text{grad}(\rho U) = 0 \text{ (continuity equation)}$$

We enter function  $w$  into the moment equation with regard to the identity

$$\text{rot}(\text{rot}(w)) = \sigma (\sigma \times w) - \text{div}(\text{grad}(w)) \text{ the equation takes the form :}$$

$$\partial w / \partial t + u \partial w / \partial x + v \partial w / \partial y = \nu \text{div}(\text{grad}(w)) + \mu (\text{rot}(w) - \text{div}(\text{grad}(w)))$$

Along with the equations of continuity, temperature and concentration we have also:

$$\partial \rho / \partial t + \text{grad}(\rho U) = 0$$

$$\begin{aligned} &Cp/(\rho Re Pr) \operatorname{div}(\operatorname{grad}(T)) + \beta_2 RC - (\partial T/\partial t + u \partial T/\partial x + v \\ &\partial T/\partial y) = Cp(Cp-1)/(\rho Re) ((\partial u/\partial y + \partial v/\partial x)^2 + \frac{1}{2} ((\partial u/\partial x + \\ &\partial v/\partial y)^2 + (\partial v/\partial y)^2 + (\partial u/\partial x)^2)) \operatorname{div}(D \operatorname{grad}(C)) + \beta_1 RC = \partial C/\partial t \\ &+ u \partial C/\partial x + v \partial C/\partial y \end{aligned}$$

The initial and boundary conditions given above were used in calculations used. Dimensionless scales were chosen as follows [18]:  $L$  – length,  $T_0$  – temperature, pressure –  $R\rho_0 T_0$ , velocity –  $(\gamma R T_0)^{1/2}$ , time –  $L/(\gamma R T_0)^{1/2}$ . The dimensionless parameters  $\gamma = Cp/Cv$ ,  $Pr = \mu Cp / \lambda = 0.72$  [18],  $Re = \rho_0 (\gamma R T_0)^{1/2} L/\nu$ ,  $\mu = \nu/3$  (Fig. 2c).

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## FIGURES

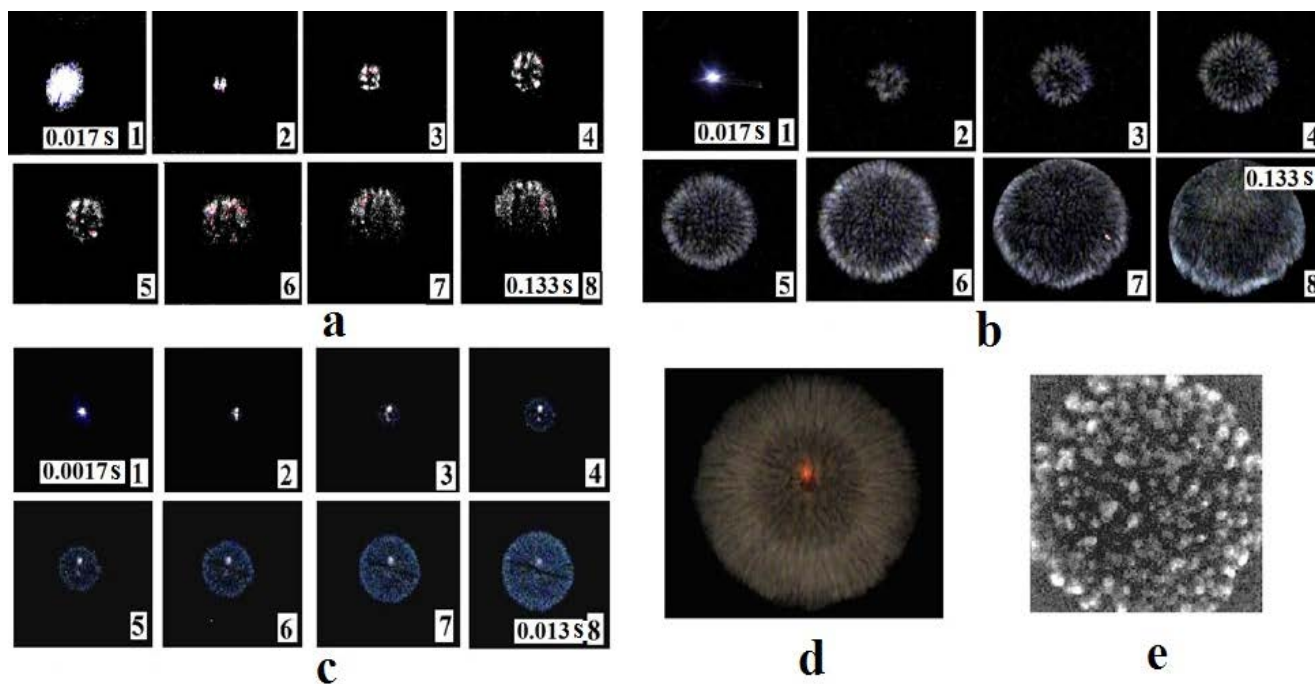
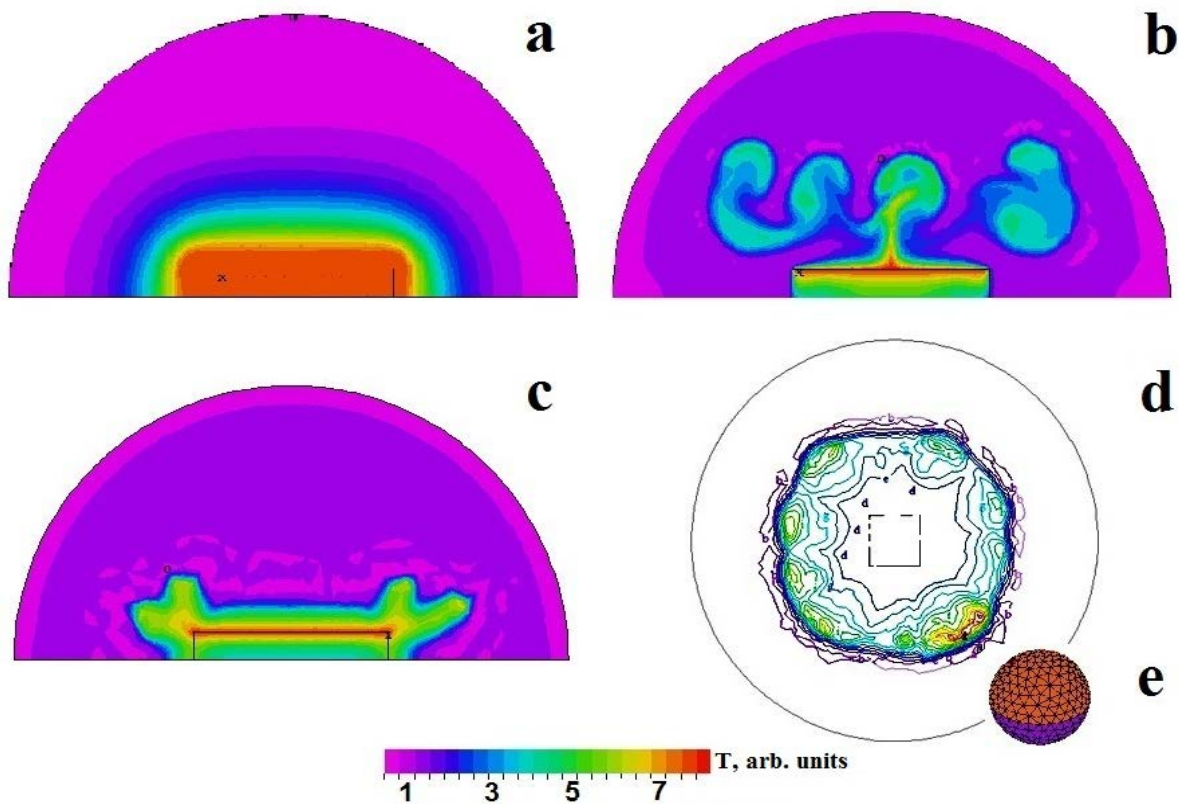


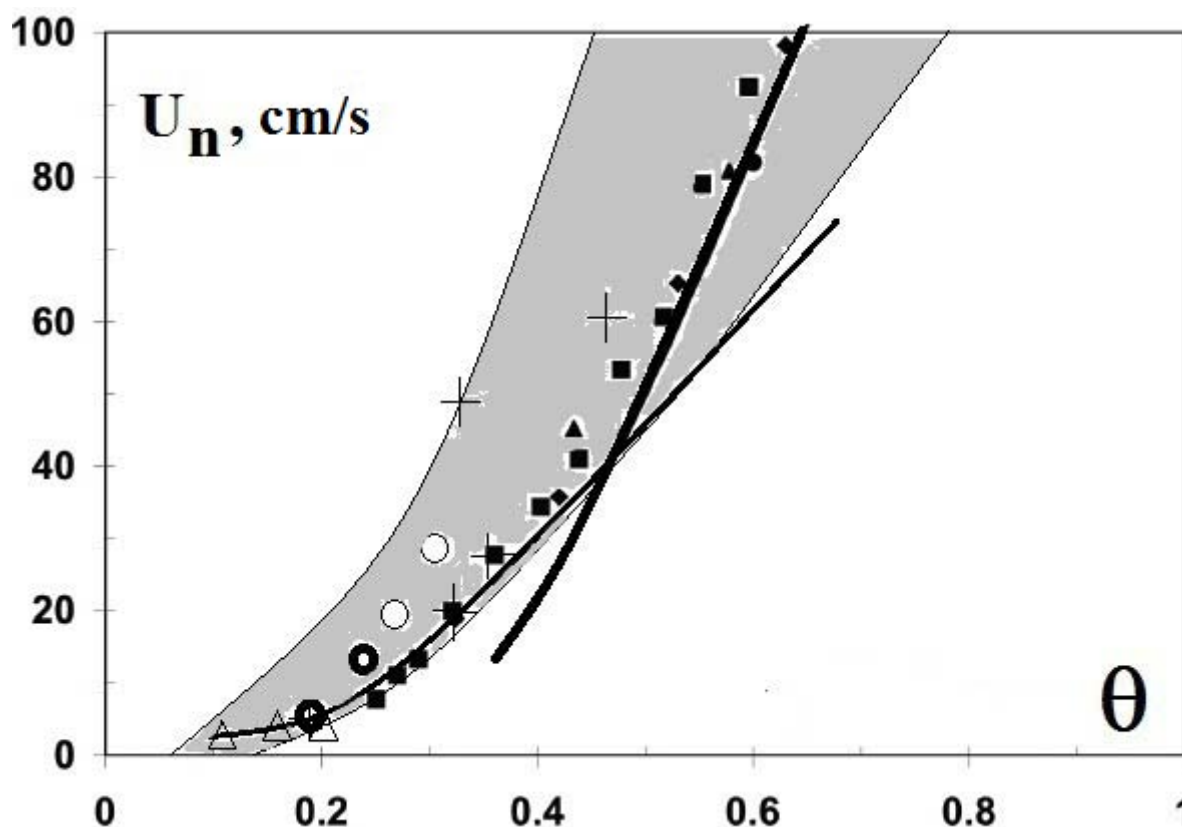
Figure 1 : High-speed filming

- Of process of FF propagation illuminated with 4%  $\text{CCl}_4$  + 8%  $\text{H}_2$  + 88% air,  $T_0 = 298\text{K}$ ,  $E_0 = 1.5\text{ J}$ . Speed of filming is 60 frames/s [9];
- Of process of FF propagation illuminated with 4%  $\text{CCl}_4$ , in 10% $\text{H}_2$  + 86% air at initial pressure of 1 atm. Speed of filming is 60 frames/s;
- Of process of FF propagation illuminated with 4%  $\text{CCl}_4$ , in 15% $\text{H}_2$  + 81% air at initial pressure of 1 atm. Speed of filming is 600 frames/s. The figure on a shot corresponds to a shot number when shooting. The first shot corresponds to occurrence of the spark discharge;
- The shot from high-speed filming of FF propagation illuminated with 2% for  $\text{CCl}_4$ , in mix 12.5% $\text{H}_2$  + 87.5% air with an atmospheric pressure [8]. Speed of filming is 60 frames / s;
- The shot from high-speed filming of FF propagation illuminated in the conditions of a microgravity, 7.0% of  $\text{H}_2$  in air, an additive of 0.4% of  $\text{CF}_3\text{Br}$ , 1.18 s after initiation [7].





**Figure 2 :** Calculation by a finite elements method [15] (see Appendix) of a combustion zone propagation (temperature field) at a certain moment in a 2D Boussinesque approximation a)  $g=0$ , b)  $g=980 \text{ cm/s}^2$ , c) of a combustion zone propagation (temperature field) at a certain moment at  $g=0$ , the solution of a 2D compressible Navier-Stokes equations; d) of a combustion zone propagation (temperature field) at a certain moment in a 3D Boussinesque approximation where the section of a 3D structure of the flame front is specified in the XZ plane, e) a 3D mesh structure. A scale of dimensionless  $T$  in arbitrary units is shown in the bottom



**Figure 3 :** Comparison of experimental and calculated normal FF velocities in lean  $\text{H}_2$  - air mixes at 1 atm and initial temperature 298 K in relation to the content of fuel in mix (equivalence ratio  $\theta$  is a fraction of fuel in mix with air:  $\theta\text{H}_2 + 0.5(\text{O}_2 + 3.76\text{N}_2)$ ). Thick curve represents results of modeling within a 1D problem [2], a thin curve shows calculated values with the use of analytical formula [2]. Points represent experimental data cited in [2] (see Fig.1 [2]), crosses represent experimental data [10], thin circles – the data of a 2D calculation without convection (Fig.2, [9]), thick circles - the data of a 2D calculation with convection taken into account (Fig 3 and Fig.4 [10]), triangles – experimental data for lack of gravity [7]. The area filled with grey color relates to experimental values of FF normal velocities of lean  $\text{H}_2$ - air mixes [13]

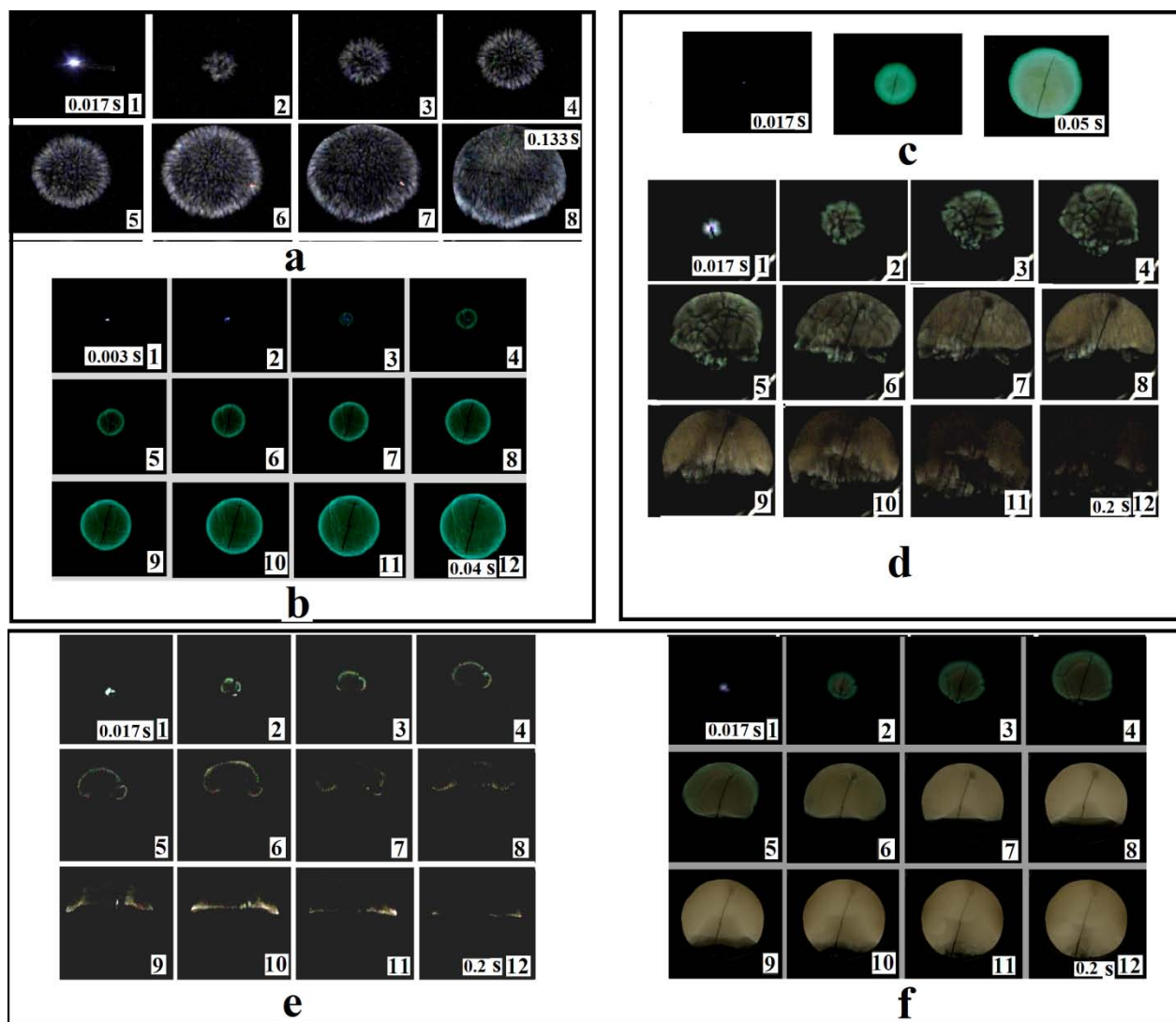


Figure 4 : High-speed filming

- Of process of FF propagation illuminated with 4%  $\text{CCl}_4$ , in 10%  $\text{H}_2$  + 86% air at initial atmospheric pressure. Speed of filming is 60 frames/s;
- Of process of FF propagation in 1.5%  $\text{C}_4\text{H}_8$  + 10%  $\text{H}_2$  + 88.5% air at initial atmospheric pressure. Speed of filming is 300 frames/s.
- Of process of FF propagation in 1.5%  $\text{C}_4\text{H}_8$  + 7.5%  $\text{H}_2$  + 91% air at initial atmospheric pressure. Speed of filming is 60 frames/s;
- Of process of FF propagation in 0.5%  $\text{C}_4\text{H}_8$  + 7.5%  $\text{H}_2$  + 92% air at initial atmospheric pressure. Speed of filming is 60 frames/s
- Of process of FF propagation in 1%  $\text{C}_4\text{H}_8$  + 5.8%  $\text{H}_2$  + 93.2% air at initial atmospheric pressure. Speed of filming is 60 frames/s.
- Of process of FF propagation in 1%  $\text{C}_4\text{H}_8$  + 6.5%  $\text{H}_2$  + 92.5% air at initial atmospheric pressure. Speed of filming is 60 frames/s. The figure on a shot corresponds to a shot number when shooting. The first shot corresponds to occurrence of the spark discharge.

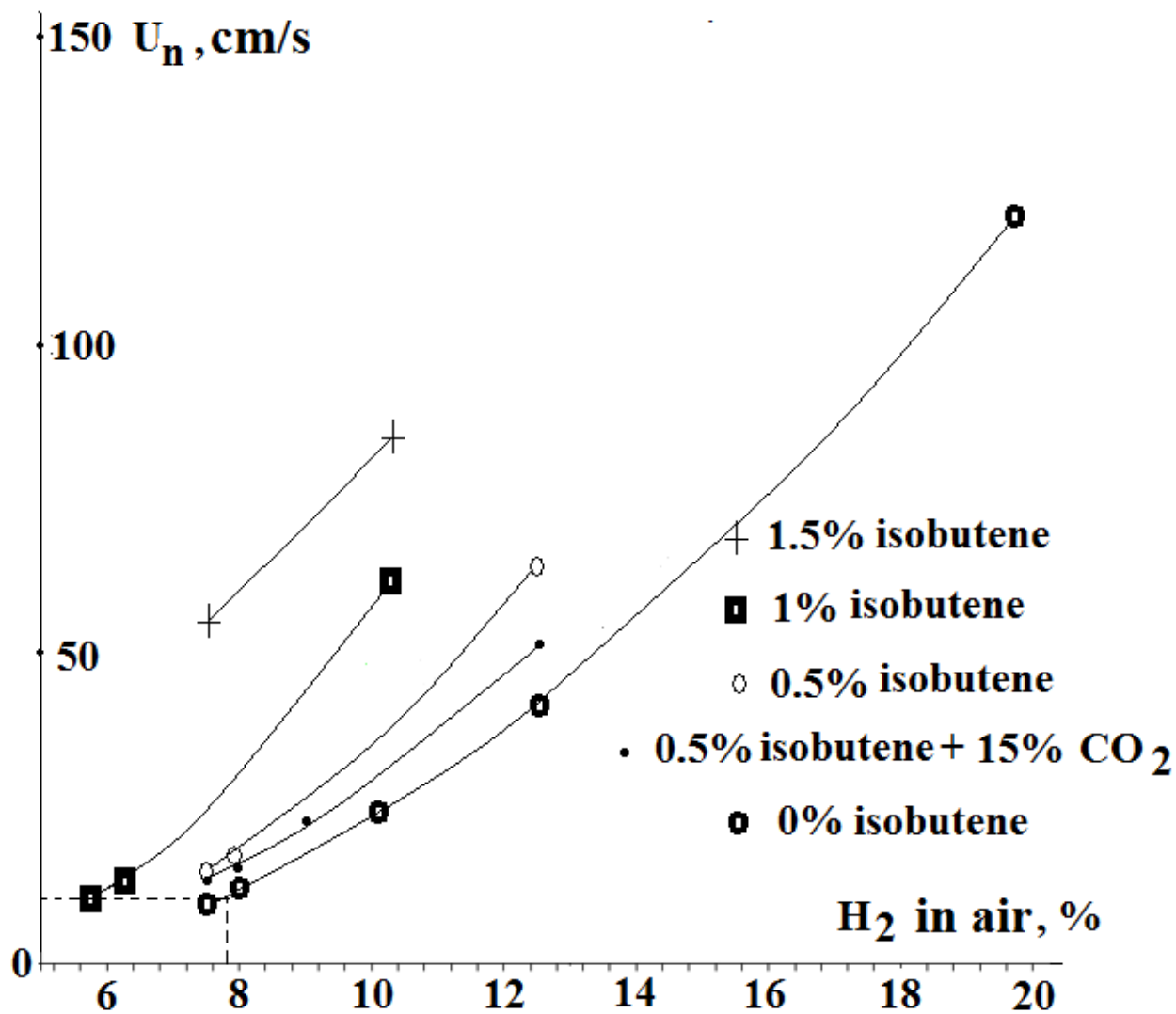


Figure 5 : Normal velocities of combustion of lean  $H_2$ -air mixes in the presence of isobutene and  $CO_2$  additives