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I. Introduction

The knowledge of regularities of initiation of combustion processes provides the possibility of controlling combustion at its initial stages. It is obvious that conditions of initiation of a combustion wave depend on the size and shape of a reaction initial center created by an external power source in the form of heat or chemically active particles. Action of initiators (spark, heating, introduction of the active centers or additives into combustible mix) is based on the acceleration of chemical transformation both at the expense of increase in gas temperature and of increase in the number of active centers because the vast majority of gas-phase combustion processes has branched chain nature [1, 2]. Thus, controlling of local ignition demands taking into account the changes of temperature of the initial center of combustion and the quantity of active centers in it.

Dynamics of formation of the stationary flame front (FF) at spark ignition of gas mixture remains rather low-studied area of combustion physics [3-5]. One of the reasons is the difficulty of experimental investigation of ignition process, associated, first of all, with small times of stationary FF formation. A primary center of a spherical flame arising in a short period at a place of the spark discharge was experimentally observed in [6] by means of a photo register, however evolution of the center wasn't investigated. In [7] the frames of high-speed shlieren-filming of evolution of the primary combustion center at the place of a spark discharge in stoichiometric propane - air mix are presented. From the given shots it follows that stationary FF occurs within very small delays (tens of microseconds). In [5] it was shown that the use of small chemically active additives in gas mixture allows increasing the values of ignition delays.

The work is aimed at the treatment of the problem on ignition of gas combustible mix by a local source with both analytical and numerical methods. The so-called weak initiation which does not provide any noticeable gas dynamic perturbations of the environment [7] is considered. Establishment of key parameters of initiation process is carried out by the example of the model reaction of hydrogen oxidation at atmospheric pressure. Experimental data on formation of the steady spherical FF obtained with the use of high-speed color cinematography were also used.

II. Experimental

Experiments were performed in the stainless steel reactor 25 cm long and 12 cm in diameter, supplied with removable covers and an optical quartz window 12 cm in diameter at an end face (Fig.1). Electrodes of spark ignition (1 J) were placed in the center of the reactor. The distance between them was 0.5 mm. The previously prepared mixes 40%H_2 + 60% air + (0 - 2%) propene (C_3H_6) were used. For flame visualization 2% of carbon tetrachloride (CCl_4) was added to the mixes. Speed filming of ignition dynamics and FF propagation was carried out from the end face of the reactor with a color high-speed digital camera Casio Exilim F1 Pro (frames frequency –1200 s^{-1}). The filming was turned on at an arbitrary moment before initiation. A 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. Before each experiment the reactor was pumped out up to 10^{-2} Torr with a for vacuum pump 2NVR-5D. Gases H_2, C_3H_6 and liquid CCl_4, were chemically pure.

III. Results and Discussion

Influence of small chemical additive (propene, C_3H_6) on an ignition delay was investigated by the example of combustion of hydrogen in air at atmospheric pressure. In Fig. 2 (a-d) the results of high-speed filming of formation of a steady flame front in 40% H_2 + 60% air mix illuminated with 2% of CCl_4 at 1 atm in the presence of 1, 1.5 and 2% of propene are shown. We observed that without C_3H_6 additive FF reaches the edges of an optical window already at the 3rd shot after

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spark ignition. It means that the small propene additive (1-2%) leads to considerable reduction of FF velocity. It should be noted that the additive of 2% of CCl_4 under these conditions is inert and doesn't show noticeable action on hydrogen combustion in accordance with the results [3,8]. FF occurrence in the presence of 2% of propene was observed not at once, but after six initiations by the spark discharge in this mix (Fig. 2d). Fig. 2c corresponds to 3 initiations by the spark discharge. As is seen the primary center of combustion was formed, but it didn't lead to flame propagation. From Fig. 2c,d it is seen also that under conditions of three spark initiations the limit of flame initiation is observed at the size of the primary combustion center much smaller than the reactor radius. Under these conditions heat losses into reactor walls are missing. Therefore, the observed limit of flame initiation is caused by an active chemical additive in the mix. From Fig. 2e in which experimental dependencies (see Fig. 2a-c) of the diameter of the flame zone on time are shown, it is possible to estimate the smallest diameter of the primary combustion center which makes up ~ 0.3 cm.

Strong influence of small chemically active additive on the time and conditions of FF formation means that evolution of the primary center is determined by not only the thermal effect of the reaction, but also by the chemical mechanism of interaction of the active centers of combustion (atoms and radicals) with the additive.

Before performing analysis of the process of local ignition of hydrogen-air mix it is important to illustrate the features of development of the primary center by the example of a problem on local thermal explosion of a flat Π-shaped warming-up center in which a zero order chemical reaction occurs. According to [9, 10] the problem is described by the equation:

$$\partial\theta/\partial\tau = \partial^2\theta/\partial\xi^2 + \exp\{\theta/(1+\beta\theta)\}, \tag{1}$$

$$\tau = 0, \quad \theta = 0 \quad at \quad \xi \le R_0, \quad \theta = -\theta_н \quad at \quad \xi > R_0,$$
$$\xi = 0, \quad \xi = \infty, \quad \partial\theta/\partial\xi = 0.$$

where, $\theta = (T - T_0)E/RT_0^2$,

$$\xi = r\{\lambda RT_0^2/(Q\rho k_a E)\exp(E/RT_0)\}^{-0.5}$$

$$\tau = tQk_a E/(cRT_0^2)\exp(-E/RT_0),$$

$$R_0^2 = Fk = Q\rho k_a E/(\lambda RT_0^2)\exp(-E/RT_0)r_0^2 = r_0{}^2/at_{del}$$
$$\theta_n = (T_н - T_0)E/RT_0^2$$

Here T_0 is the initial temperature of the center, T_n- environment temperature, r_0- the initial size of the center, t - time, E, k_a, Q - energy of activation, a pre exponent and the thermal effect of a zero order reaction respectively, λ - heat conductivity, C - thermal capacity, ρ - density, *a* – heat diffusivity, t_{del} – the delay period of ignition.

The analysis of results of numerical investigation of the problem leads to the following conclusions:

a) The dimensionless delay period of thermal explosion has an order of unit, i.e. an order of the adiabatic delay period of thermal explosion. The time of thermal relaxation of the primary center is equal to Fk value in chosen scales. Critical Fk value is about 10 — 20 (depending on the shape of the center). Therefore, for local ignition it is characteristic that t_{del} is much less than the time of a thermal relaxation of the primary center τ_T:

$$\tau_{del} << \tau_T$$

It means that during development of thermal explosion in the primary center only the layer at the surface of the center (in which the whole temperature gradient is concentrated) is considerably cooled down, and the substance in the central part of the center isn't practically cooled.

b) For local ignition initial temperatures in the center and in its environment are markedly different ($\theta_n > 4$). Therefore at high activation energy a chemical heat source is localized in a narrow temperature interval in the vicinity of the maximum temperature. Therefore it is possible to allocate two zones in the center: 1) a reaction zone, where $\theta > -1$, in the central part of the primary center; 2) a zone of inert cooling, where $\theta < -1$, settling down at a border of a surface of the primary center ($\theta = (T - T_0)E/RT_0^2$), T_0 is the temperature of the center.

As is stated above, the whole temperature gradient is practically concentrated in the zone of inert cooling inside the center. Eventually substance cools down at the primary center surface and the border of the reaction zone moves to the middle of the center. Therefore critical condition is the equality of heat losses and thermal emission in the reaction zone by the time of the termination of the delay period. From here we will estimate the critical size of reaction zone $\Delta\xi_p^{cr}$:

$$\partial^2\theta/\partial\xi^2 = \exp\{\theta/(1+\beta\theta)\}; \quad 1/(\Delta\xi_p^{cr})^2 \approx 1, \quad \Delta\xi_p^{cr} \approx 1.$$

Thus, for ignition of the center it is necessary that the size of the reaction zone exceeds the critical one during the delay period.

The heat flux which is aimed away from the reaction zone is more than the thermal flux which chemical reaction can provide during a delay period. They become equal only under critical conditions at the moment of the termination of the delay period. Therefore the law of movement of the border of a reaction zone can be found from the solution of a problem on plate cooling in infinite environment [9, 10]:

$$\theta = -(\theta_n/2)\left\{ erfc\left[\frac{R_0 - \xi}{2\tau^{0.5}}\right] + erfc\left[\frac{R_0 + \xi}{2\tau^{0.5}}\right]\right\} \tag{2}$$

Temperature profile in a zone of inert cooling is approximately described by the first term of expression (2) [11]:

$$\theta = -(\theta_n/2)\left\{ erfc\left[\frac{R_0 - \xi}{2\tau^{0.5}}\right]\right\}.$$

As the border of the reaction zone is the point in which $\theta = -1$, we get the law of its movement:

$$2/\theta_n = \left\{ erfc\left[\frac{R_0 - \Delta\xi_p}{2\tau^{0.5}}\right]\right\}.$$

Thus, if the independent calculation or definition of the adiabatic delay period of the reaction in the primary center for exothermic self-accelerated reaction (for example, branched chain reaction) is possible, the use of the equation (3) will allow calculating the center radius R_0^{cr}; as according to [9,10] adiabatic delay period is related to the critical size of a reaction zone by a ratio $\Delta\xi_p^{cr} = \sqrt{\tau_{del}}$ because under critical conditions at the time of τ=1 $\Delta\xi_p = \Delta\xi_p^{cr} \approx 1$ [9]. Then the expression for the critical size of the primary center takes the form:

$$2/\theta_n = \left\{ erfc\left[\frac{R_0^{cr} - \tau_{del}^{0.5}}{2\tau_{del}^{0.5}}\right]\right\}$$

in which $\theta = (T_0 - T_n)E / RT_0^2$, then we get:

$$2/\theta_n = erfc\frac{R_0^{cr} - 1}{2} = erfc\left[\frac{(Fk)^{1/2} - 1}{2}\right] = erfc\left[\frac{r_0^{cr} \big/ a\sqrt{t_{del}} - 1}{2}\right] \tag{4}$$

Thus, the value of the adiabatic delay period t_{del} is one of the key parameters of the process of local ignition. Observed marked influence of small chemically active additive on the time of FF formation (see Fig. 2) according to eq.(4) means that the additive has strong impact on the value of t_{del}.

We will illustrate influence of the chemical mechanism of combustion reaction on critical conditions of local ignition by the example of the branched chain process of hydrogen oxidation which is considered to be well-known [1, 3, 4].

To describe hydrogen oxidation we will take into account only main stages of the process of chemical transformation: chain origination $H_2 + O_2 \rightarrow 2OH$ (k_0), chain propagation (k_1, k_3) and chain branching (k_2), tri molecular chain termination (k_6, k_{11}), termination of hydrogen atom on the additive in the reaction H + In → products (k_5) [4]. Nonlinear reactions of chain propagation and chain branching during the delay period are ignored [3, 4].

In a chain unit of hydrogen oxidation

$OH + H_2 \rightarrow H_2O + H$ (k_1),
$H + O_2 \rightarrow OH + O$ (k_2),
$O + H_2 \rightarrow OH + H$ (k_3)

heat isn't practically released [1]. Here k_i are velocity constants of the corresponding reactions. The heat of reaction of hydrogen oxidation is released in recombination of the active centers. In rich mixes these are hydrogen atoms which concentration markedly exceeds concentrations of atoms O and radicals OH [1]. Atoms of hydrogen recombine with each other and with oxidizer molecules with participation of the third particle M with thermal effects Q_2 and Q_1 respectively in the following reactions:

$H + H + M \rightarrow H_2 + M$ (k_{11}) + Q_2,
$H + O_2 + M \rightarrow HO_2 + M$ (k_6) + Q_1 .

We will qualitatively analyse influence of various factors (initial gas temperature, initial concentration of atoms of hydrogen and concentration of additive) on the delay period of thermal ignition of a stoichometric hydrogen – oxygen mix. The system of the equations describing adiabatic process of thermal ignition was analyzed in dimensionless variables. The characteristic time scale was chosen as $t_0 = 1/(k_2^0 [O_2]_0)$, where k_2^0 is the reaction pre exponent of (2). In the chosen scale of dimensionless time 1 second corresponds approximately ~ 10^5 dimensionless units along the τ axis in Fig. 3. Dimensionless variables and parameters were defined as follows: τ = t/t_0, Y_0, Y_1, Y_3 = [concentration of atoms of hydrogen, molecular oxygen and an additive respectively] / [initial concentration of molecular oxygen], T – temperature (K)

$$\begin{aligned}
dY_0/d\tau &= 3k_0/ k_2^0 + 2\exp(-8380/T)\, Y_0Y_1 - k_5/k_2^0 Y_0Y_3 - k_6/k_2^0 MY_0Y_1 - k_{11}/ k_2^0 (Y_0)^2M \\
dY_1/d\tau &= -3k_0/k_2^0 - \exp(-8380/T)\, Y_0Y_1 - k_6/k_2^0 MY_0Y_1 \\
dT/d\tau &= 1/ (C_p\rho)[Q_1 k_6/ k_2^0 MY_0Y_1 + Q_2 k_{11}/ k_2^0 (Y_0)^2M] \\
dY_3/d\tau &= - k_5/ k_2^0 Y_0Y_3
\end{aligned} \tag{5}$$

The equations of the set (5) were integrated using a Runge-Kutta fourth order method with an adaptive step of integration and the following initial conditions, $Y_0 = 1$, $Y_1 = 1$, $Y_3 = 0 \div 0.03$, $T_0 = 1000$ (K) is the measured temperature value in gas in a zone of spark ignition [12]. The values of other parameters were the following: **$\rho = 10^{-3}$ g/cm^3** [13], $C_p = 0.88$ kal /g. grad [13], $M = 750.\ 10^{19}/T_0$ cm^{-3} (atmospheric pressure), $k_2 = k_2^0 \exp(-8380/T)$ cm^3/ molec. s $= 0.30.10^{-9} \exp(-8380/T)$ cm^3/ molec. s [14], $k_{11} = 0.14.10^{-31} (T/300)^{-0.4}$ cm^6/ molec^{2}s [15], $k_6 = 10^{-32}$ cm^6/ molec^{2}s [16], $k_5 = 10^{-11} \exp(-1500/T)$ cm^3/molec. s [8], $k_0 = 0.33.10^{-9} \exp(-22000/T)$ cm^3/ molec. s [17], $Q_1 = 45$ kcal/ mol [1], $Q_2 = 100$ kcal/ mol [1], $[O_2]_0 = 760\ (0.13\ 10^{19}/T_0)$ cm^3.

The results of calculations are presented in Fig. 3. For estimation of the value of temperature increase at the expense of recombination of hydrogen atoms introduced into an initial mix calculations for lack of chain branching ($k_2 = 0$, the reaction of hydrogen oxidation doesn't occur, Fig. 3 a, b) were carried out. It follows from the calculations that due to heat which is released in recombination of hydrogen atoms introduced into initial mix, the temperature of gas mix increases (Fig. 3a). The additive of propene to the same mix leads to reduction of the maximum temperature (Fig. 3b). Propene influence for lack of the branching reaction shows itself as warming- up reduction. This is reached at the expense of smaller thermal emission in reaction of the active center with propene in comparison with recombination of hydrogen atoms with each other and with oxygen molecules.

From Fig. 3c, in which change in time of concentration of hydrogen atoms, oxygen and propene (**$k_2 \neq 0$**) molecules is given for absence and for presence of propene, it is seen that propene additive provides increase in τ_{del}. In calculations the delay period was estimated as the time of achievement of maximum concentration of hydrogen atoms.

We will apply the results obtained to the explanation of influence of active chemical additives on the process of spark initiation. As in the area of discharge not only temperature increases, but also super equilibrium concentration of active particles [7] is attained, then at the expense of their recombination (after discharge) temperature will additionally increase, and τ_{del} will respectively decrease (see Fig. 3c - calculation for dimensionless initial concentration of atoms of hydrogen 0.1, Fig. 3d - 0.017).

Propene additive leads, on the contrary, to increase in τ_{del}; as the active centers of combustion including those formed at an initiating impulse, are terminated on propene molecules and don't lead to chain branching until propene is consumed. In addition, influence of propene on the value of τ_{del} shows itself also in warming-up reduction. It is due to smaller heat release in reaction of the active center with propylene in comparison with recombination of hydrogen atoms with each other and with oxygen molecules.

It is necessary to tell apart two cases. If initial concentration of active particles is more than concentration of additive, the additive is quickly consumed due to interaction with these active particles and has no impact on the further development of ignition process. In this case τ_{del} **slightly** depends on additive concentration (see Fig. 3d) and is determined by the time of the development of ignition process without additive.

If initial concentration of active particles is less than concentration of additive, the delay period strongly depends on concentration of additive (see Fig. 3 d, e). This result is a consequence of slow consumption of additive in the reaction of chain origination.

It is known from literature on ignition and combustion that the velocity of oxidation reaction is a sharp function of initial temperature [1-4, 7]. Such dependence is determined by the high activation energy of the chain branching reaction. This fact is a necessary condition of occurrence of critical phenomena of local ignition and application of the approach developed above for their calculation. To estimate the critical size of the primary center we can use analytical expression for τ_{del} **in** hydrogen-air mix, obtained in *Appendix* (equation (11)).

Let us substitute the following values of parameters in the equation (4) for the critical size of the primary ignition center: Tn = 300K, E = 16.7 kcal/mol, ***a*** **≈ 0.8 cm^2/s** (for rich H_2-air mix [13]). Its solution for t_{del} is:

$$t_{del} = \frac{1.56\left(r_0^{cr}\right)^2}{1 + 2\Omega^2} \tag{6}$$

Where Ω is the root of the equation- **$4175T_0\, \mathrm{erfc}\,\Omega + 1252500\, \mathrm{erfc}\,\Omega + T_0^2 = 0$,** and T_0 is the temperature of the primary center. Dependencies of τ_{del} on the critical radius of the primary center for temperatures of the center 800K, 1000K, 1500K, 2000K, calculated by (6), are shown in Fig. 4.

We will apply the obtained results to estimate the value of initial concentration of hydrogen atoms in the primary center. We will use for this purpose both the experimental data shown in Fig. 2e, and expressions for calculation of τ_{del}, obtained in the *Appendix* (equations (9), (11)), which describe well experimental data from literature. Experimental values of t_{del} given in Fig. 5 are taken from [19] and calculated by equation (11). As is seen the results of calculations by eq. (11) for temperatures <1500K adequately agree with experimental data [19] even for the mix H_2: O_2 = 1: 1.

The smallest diameter of the primary center from which a combustion wave develops, makes up 0.3 cm according to Fig. 2e. The value of $\tau_{del} \approx 0.02$ s at T_0=1000 K (experimental value of gas temperature in spark ignition zone [12]) corresponds to this critical radius according to Fig. 4.

On the other hand the delay period τ_{del} can be calculated directly by equation (9) for various initial concentrations of hydrogen atoms and in=2 %. Results of the calculations are shown in Fig. 6a. In this case the delay period was considered as time interval for which the warming up of mix becomes equal to a characteristic interval $\frac{RT_0^{\,2}}{E}$. This interval for E = 16.7 kcal/mol and T_0=1000K equals 120^0. As follows from Fig. 6a the delay period ($t_{del} = 0.02$ c) corresponds to initial concentration of hydrogen atoms $\sim 7.10^{17}$ cm^3, i.e. the value has a reasonable order. This result is evidence that the developed approach for the analysis of critical conditions of local ignition is applicable.

As is seen in Fig. 6a, it is possible to allocate two stages at initial concentration of hydrogen atoms more than 10^{16} cm^3 in the course of warming-up: the fast stage when the velocity of heat release is determined by recombination with participation of hydrogen atoms in initial mix, and the slow one, related to heat release in the reaction of hydrogen oxidation.

For investigation of influence of initial concentration of additive on the critical size of the primary center and, respectively, on the value of critical energy of ignition, the calculation of change of a warming up in time by equation (9) was carried out at various initial concentration of additive (*In*) and given concentration of hydrogen atoms $[H]_0 = 10^{14}$ cm^3. Concentration of the additive was chosen in such a way that the inequality $[In] > [H]_0$ was fulfilled. Results of these calculations are shown in Fig. 6b. As well as for Fig. 6a t_{del} was considered as the time interval for which the warming up of mix becomes equal to one characteristic interval.

As is seen in Fig. 6b, increase in concentration of an additive from 0.5% to 1% leads to increase in t_{del} from 0.02 s to 0.12 s, and from 1% to 2% from 0.12 s to 0.32 s. However such small amouns of additive (from 0.5% to 2%) correspond to change of the critical size of the center and respectively, the minimum energy of ignition by ~ 6.25 times.

We summarize shortly the results obtained.

The approximate analytical method is applied for analysis of the problem on local chain- thermal explosion by the example of the branched chain reaction of hydrogen oxidation in the presence of chemically active additive. It is shown that key parameters defining the critical size of the primary center of ignition, are the temperature in the local ignition center; quantity of the active centers of combustion created with the local source; and the presence of active chemical additives in combustible mixture. Comparison to the experiment has shown applicability of the developed approach for the analysis of critical conditions of local ignition in combustible gas mixtures.

APPENDIX

Analytical definition of τ_{del} of hydrogen-air mix at atmospheric pressure

We will consider the branched chain mechanism of hydrogen oxidation, described above. We will neglect consumption of initial reagents during τ_{del}. Then we have:

$$\frac{dH(t)}{dt} = l_0 + l_1 H(t) - 2k_{11} M H(t)^2$$

$$C_p \rho \frac{dT(t)}{dt} = Q_1 k_6 O_{20} M H(t) + Q_2 k_{11} M H(t)^2 \qquad (7)$$

where $l_0 = k_i H_{20} O_{20}$ и $l_1 = 2k_2 O_{20} - k_5 In_0 - k_6 O_{20} M$, H_{20}, O_{20} и In_0 – initial concentration of initial components and an additive, C_p is molar thermal capacity at a constant pressure, ρ - density. Into the first equation of system (7) we will put $H(t) = \frac{1}{k_{11} M y(t)^2} \frac{dy(t)}{dt}$, then we get:

$$\frac{d^2 y(t)}{dt^2} = l_0 k_{11} M y(t) + l_1 \frac{dy(t)}{dt}$$

Its solution under initial condition H (0) = H_0 (the local source generates only hydrogen atoms) is:

$$H(t)=\frac{-\xi_1\exp(\xi_1 t)m+n\xi_2\exp(\xi_2 t)}{k_{11}M(-\exp(\xi_1 t)m+n\exp(\xi_2 t))}$$ Where

$$\xi_1=\frac{1}{2}l_1+\sqrt{l_1^{\,2}+4k_{11}Ml_0},\ \xi_2=\frac{1}{2}l_1-\sqrt{l_1^{\,2}+4k_{11}Ml_0},\quad m=\xi_1-k_{11}HoM,\ n=\xi_2-k_{11}HoM$$

Integration of the second equation of the set for T (0) = T_0 gives:

$$T(t)=To+\left(\frac{(\xi_1+\xi_2)\beta}{2\xi_1^{\,2}\xi_2^{\,2}}+\frac{Q_1k_6O_2}{k_{11}M\rho C_P}\right)\ln\left(\frac{-\exp(\xi_1 t)m+n\exp(\xi_2 t)}{n-m}\right)$$

$$-$$

$$\frac{\beta t}{2\xi_1\xi_2}-\frac{\beta mn(\xi_2-\xi_1)(\exp(\xi_1 t)+\exp(\xi_2 t))}{2(n-m)\xi_1^{\,2}\xi_2^{\,2}(-\exp(\xi_1 t)m+n\exp(\xi_2 t))}\quad \text{where}\quad \beta=\frac{Q_2}{C_P\rho k_{11}M} \tag{8}$$

According to [20] we will consider that the delay period expires when self-heating exceeds one characteristic interval, namely $\Delta T=T(t)-To=\dfrac{RTo^2}{E}$. We consider activation energy of the linear branching reaction (k_2, a limiting stage) as activation energy.

During the delay period it is possible to neglect concentration of accumulated hydrogen atoms. In addition, direct calculation shows that it is possible to ignore also the term $\dfrac{\beta t}{2\xi_1\xi_2}$. The equation (5) after substituting the values ξ_1 and ξ_2 takes a form:

$$\frac{RTo^2}{E}=\Delta T=$$

$$\left(\frac{\beta l_1}{2k_{11}^{\,2}M^2l_0^{\,2}}+\frac{Q_1k_6O_2}{k_{11}M\rho C_P}\right)\ln\left(-\frac{-\exp((l_1+\frac{k_{11}Ml_0}{l_1})t)(-\xi_2+k_{11}HoM)+(-\xi_1+k_{11}HoM)\exp(\xi_2 t)}{(l_1+\frac{2k_{11}Ml_0}{l_1})}\right) \tag{9}$$

We will simplify the equation (9) in order to get the equation for the delay period in an explicit form

$$:\ \frac{RTo^2}{E}=\Delta T=\left(\frac{\beta l_1}{2k_{11}^{\,2}M^2l_0^{\,2}}+\frac{Q_1k_6O_2}{k_{11}M\rho C_P}\right)\ln\left(\frac{\exp(l_1t)k_{11}M(Hol_1+l_0)}{l_1^{\,2}}+1-\frac{k_{11}MH_0}{l_1}-\frac{k_{11}Ml_0t}{l_1}\right) \tag{10}$$

Further we will calculate the value RT_0^2/E for the given conditions (T_0=1000K, E = 16.7 kcal/mol): $RT_0^2/E\approx$ 120. The point of intersection of the dependence (11) with a line y=120 also will give the required value of the delay period τ_{del} (Fig. 6 a, b). As is seen the value of the delay period depends both on the amount of the active centers introduced into gas mixture at initiation and on the concentration of additive in gas mixture. We solve the equation (10) for t, substituting $\dfrac{RTo^2}{E}$ instead of ΔT. Then by definition t = τ_{del} the value of the delay period. We get:

$$\tau_{del}=\frac{1}{k_{11}Ml_0l_1}\left(LambertW\left(-\frac{Hol_1+l_0}{l_0}\exp\left(\frac{-l_1\left(l_1\exp\left(\frac{RTo^2}{E\alpha}\right)-l_1-k_{11}MHo\right)}{k_{11}Ml_0}\right)\right)k_{11}Ml_0+l_1^{\,2}(\exp\left(\frac{RTo^2}{E\alpha}\right)-1)+k_{11}MHol_1\right) \tag{11}$$

In the equation (11) Lambert W (x) +exp (Lamber tW (x)) = x by definition,

$$\alpha = \left(\frac{\beta l_1}{2k_{11}{}^2 M^2 l_0{}^2} + \frac{Q_1 k_6 O_2}{k_{11} M \rho C_P} \right)$$

It is possible to show that the results of calculation by equations (9) - (11) practically coincide.

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Figures

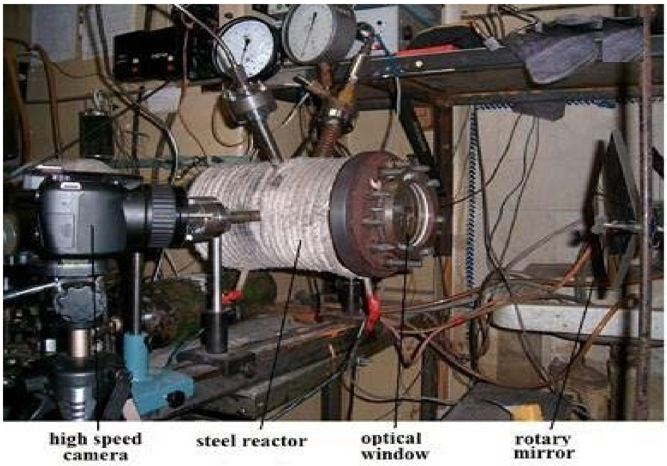

Figure 1 : Experimental installation

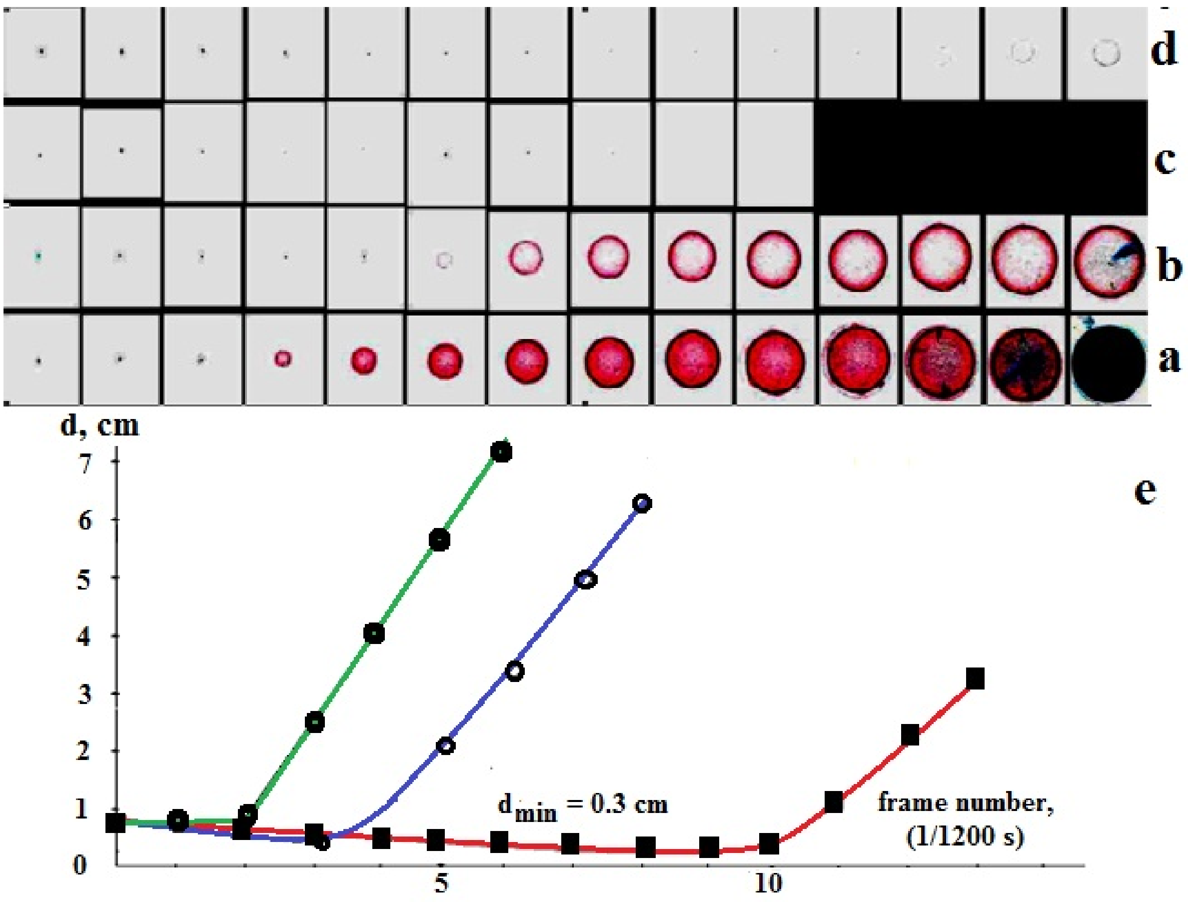

Figure 2 : Speed filming of propagation of the spherical flame front in the mix H_2 – air at atmospheric pressure in the presence of propene. The flame front is illuminated by 2% CCl_4 additive. Speed of filming is 1200 frames/s. Colors are inverted. The first frames to the left in the in the picture are the first frames after spark discharge.

a) 2% of propene, 6th initiation,
b) 2% of propene, 3rd initiation,
c) 1.5 % of propene,
d) 1% of propene,
e) Dependencies of the diameter of flame zone on time for Fig. 1a (points), b (circles), d (squares).

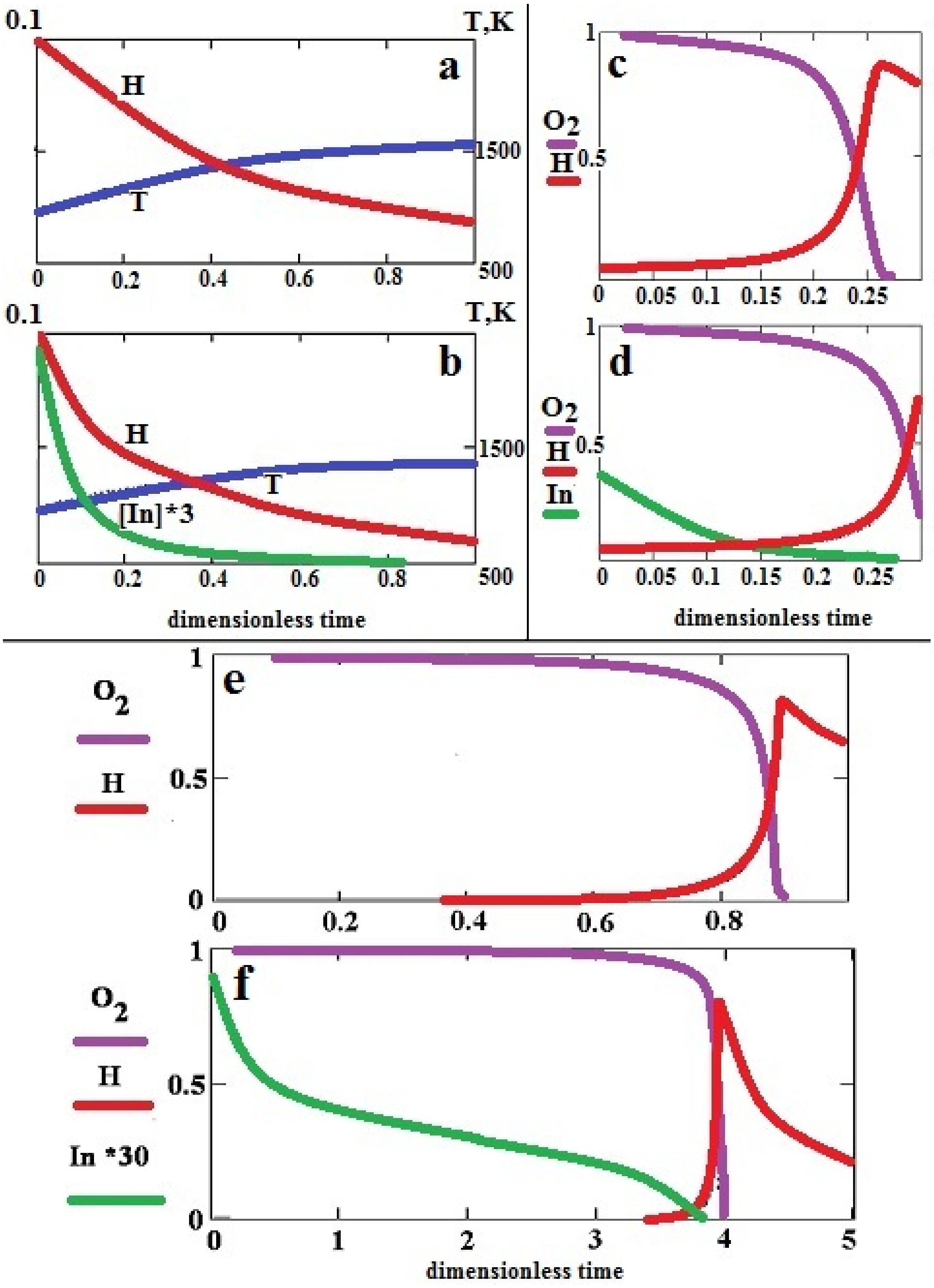

Figure 3 : Calculated dependencies of concentration of hydrogen atoms, molecular oxygen, temperature and additive at initiated combustion of hydrogen in air at atmospheric pressure.

a) $k_2 = 0$, the additive in the mix is missing;
b) $k_2 = 0$, concentration of additive in the mix is 3%;
c) the additive in the mix is missing, dimensionless concentration $[H]_0 = 0.1$;
d) concentration of additive in the mix is 3%, dimensionless concentration $[H]_0 = 0.1$;
e) the additive in the mix is missing, dimensionless concentration $[H]_0 = 0.017$;
f) Concentration of an the additive in mix is 3%, dimensionless concentration $[H]_0 = 0.017$.

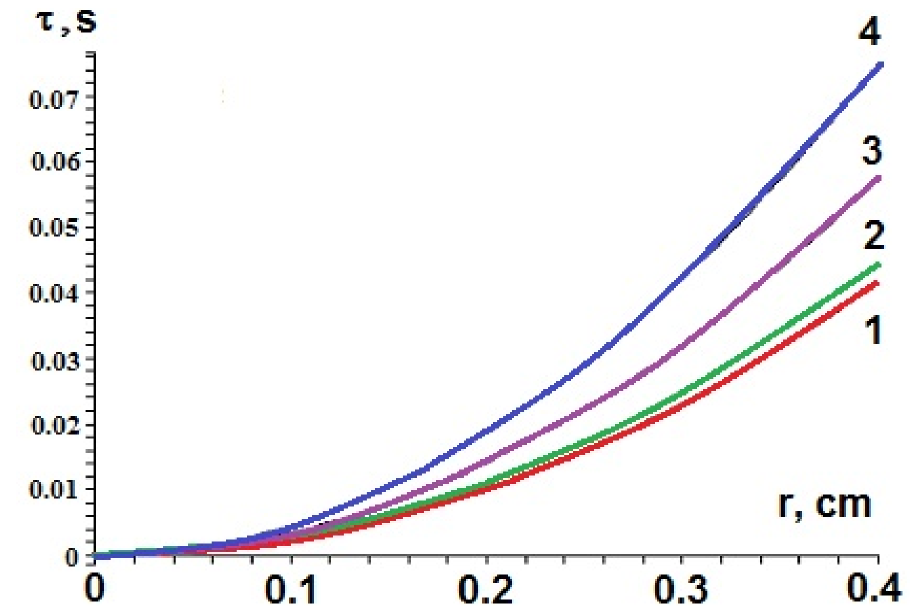

Figure 4 : Values of critical radius calculated by equation (6) depending on the delay period τ_{del} for various temperatures of the primary center: 1 – 800K, 2 - 1000K, 3 - 1500K, 4 - 2000K.

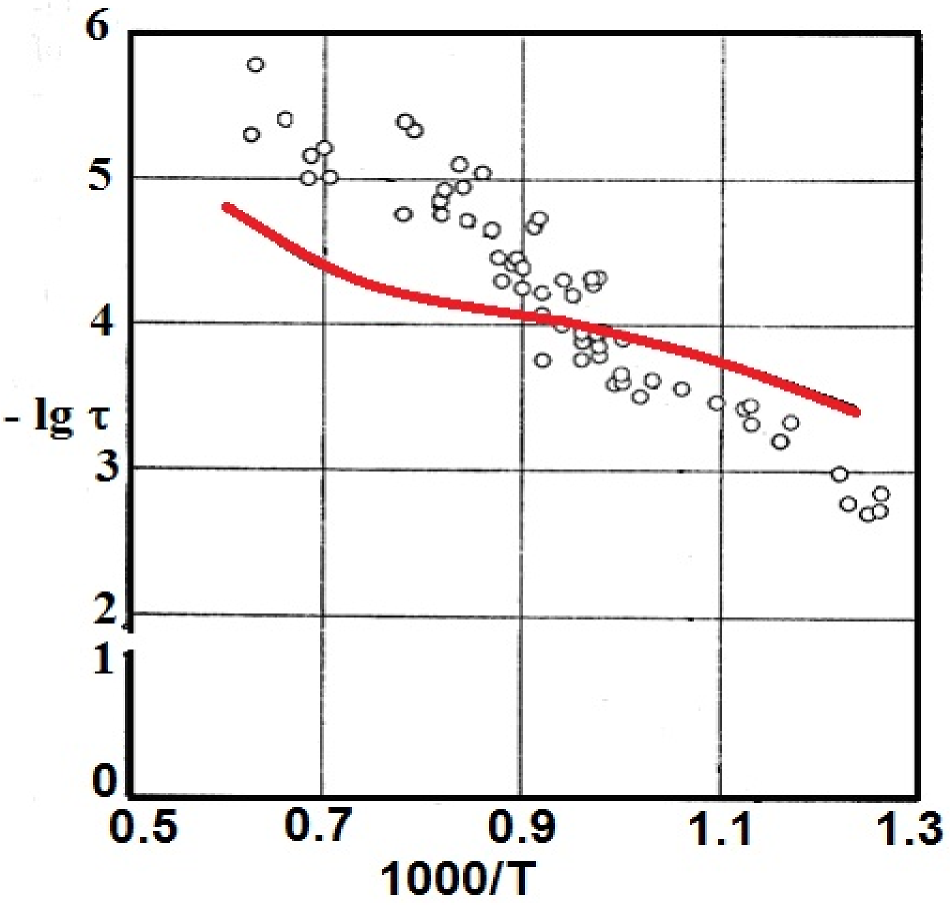

Figure 5 : Comparison of experimental data [19] on the periods of a delay (points) for the mix $H_2 + O_2$ (1:1, 1 atm) and calculated delay periods by equation (11) (a continuous curve) for $[H]_0=0$, $In_0=0$, $O_2 = 750.10^{19} / (2\ T_0)$ cm^{-3}, other parameters are specified in the text.

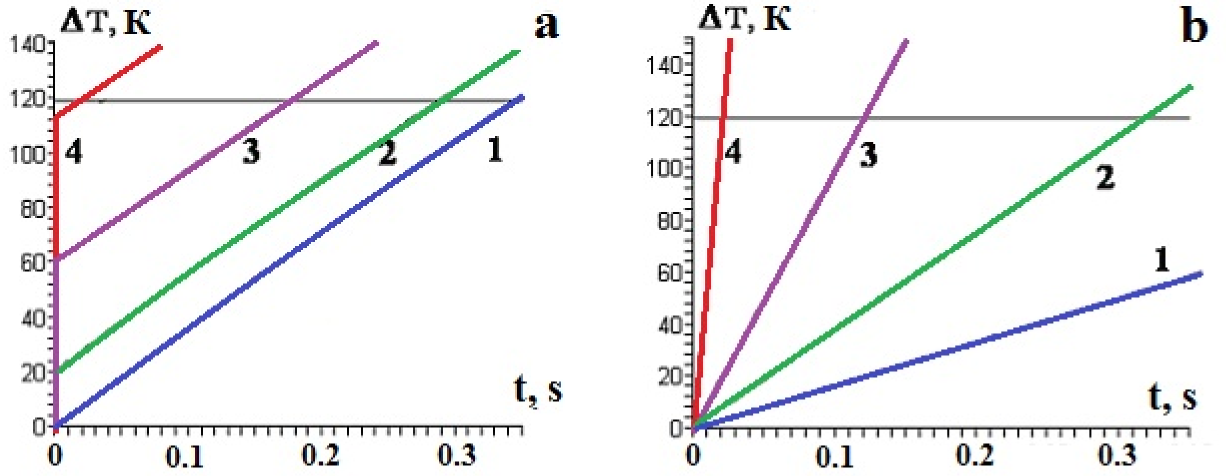

Figure 6 : The calculated values of the delay period from crossing of the graphics of the equation (9) and a straight line of $\frac{RTo^2}{E} \cong 120$

a) for various values $[H]_0$ at given concentration of additive of In=2%, 1 – $[H]_0 =0$, 2 – $[H]_0 =10^{17}$ cm^3, 3 – $[H]_0 =3.101^{7}$ cm^3, 4 - $[H]_0 =7.10^{17}$ cm^3;

b) For various In values at a given value $[H]_0 =10^{14}$ cm^3 and concentration of additive 4 –In=0.5, 3 –In=1%, 2 In=2%, 1 - In=4%.