Modelling the average velocity of propagation of the flame front in a gasoline engine with hydrogen additives

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Abstract. The paper presents models for calculating the average velocity of propagation of the flame front, obtained from the results of experimental studies. Experimental studies were carried out on a single-cylinder gasoline engine UIT-85 with hydrogen additives up to 6% of the mass of fuel. The article shows the influence of hydrogen addition on the average velocity propagation of the flame front in the main combustion phase. The dependences of the turbulent propagation velocity of the flame front in the second combustion phase on the composition of the mixture and operating modes. The article shows the influence of the normal combustion rate on the average flame propagation velocity in the third combustion phase.

1. Introduction
The use of alternative fuels reduces toxicity without changing the design in SI Engines. Hydrogen is considered as an alternative fuel and hydrogen is intended as a substitute for fuel from petroleum products. The main reason for this is that when hydrogen is burned water is formed and there are no pollutants such as CO, CO$_2$, C$_n$H$_m$ or solid particles. The combustion characteristics of hydrogen provide a high combustion rate and minimum ignition energy, this allows us to expand the limits of effective depletion of the mixture. Also interest in hydrogen is that hydrogen can be obtained by electrolysis of water [1,2].

For the analysis of the influence on the efficiency and toxicity of the SI Engines work process of design and operational factors and also chemical composition of fuel, it is necessary to know the mechanism of flame propagation in the combustion chamber [3, 4]. Most often in the studies the surface mechanism of the propagation of the flame front [5, 6, 7]. When a uniformly mixed mixture is burned in a turbulent flow, the fresh mixture is separated from the combustion products by a thin curved flame front. In the combustion chamber of a piston engine with an external mixture formation, the same mechanism takes place. The application of this mechanism makes it possible to identify the main combustion characteristics that determine the propagation of a flame in the combustion chamber.

The most appropriate characteristics are:

– the velocity of turbulent flame propagation, as an integral indicator of the rate of chemical reactions and gas-dynamic and thermal conditions;
– the normal flame propagation velocity, as an integral measure of the rate of chemical reactions.

Knowledge of these characteristics will allow us to assess the dynamics of combustion, which determines the toxicity and efficiency of the work process. Therefore, the aim of the work is an experimental study of the influence of the composition of the mixture, the compression ratio, the ignition timing and the rotation frequency on the average propagation velocity of the flame front in various combustion phases.
2. Experimental technique

Experimental studies were carried out on a single-cylinder UIT-85 unit. Geometric parameters of the engine: the cylinder capacity is 0.652 liters, the cylinder diameter is 85 mm, the piston stroke is 115 mm, the compression ratio is 5.9 and 7. The electric motor keeps the revolutions constant: 600±6, 900±9 min⁻¹. The uniformity of the fuel-air mixture is provided by heating the intake manifold.

Registration of the movement of the flame front inside the UIT-85 cylinder (Figure 1a) was carried out by ionization sensors. Ionization sensors are installed in a special adapter (Figure 1b). In the adapter, the ionization sensors are arranged as follows: proximity (ionization sensor 3) is located at a distance 77 mm away from the spark plug; distant (ionization sensor 5) is located at a distance 91.3 mm away from the spark plug; central (ionization sensor 4) is installed in a 4 mm hole at a distance of 9.75 mm from the plane of the combustion chamber. This location of the ionization sensors makes it possible to evaluate the propagation parameters of the flame front in the main combustion phase and in the sensor location area at different levels of turbulence [8].

![Diagram of the combustion chamber of the UIT-85](image.png)

**Figure 1.** Diagram of the combustion chamber of the UIT-85 (a), where 1 – spark plug; 2 – pressure sensor Kistler, 3 – proximity ionization sensor; 4 – central ionization sensor; 5 – distant ionization sensor; (b) general view of the adapter with ionization sensors

The proximity ionization sensor was used to determine the average propagation velocity of the flame front in the main phase, that is from spark plug to ionization sensor 3. The central ionization sensor was used to estimate changes in the propagation velocity of the flame front in the third combustion phase. We assume that the volume formed by the cavity of the hole where the sensor is mounted will ensure that there is no effect of large-scale turbulent pulsations on combustion in the zone of the sensor. This corresponds to the combustion conditions characteristic of the third combustion phase. The turbulent propagation velocity of the flame front in the installation zone of the ionization sensors was determined from the time of the signal between the near and far ionization sensor. It can be considered as the corresponding average velocity of propagation of the flame front in the second phase of combustion.

The parameters by which the combustion process was evaluated:
- the average velocity of flame front propagation in the main phase of combustion (first and second phases):
  \[ U_{1+2} = \frac{77}{t_3}, \]  \hspace{1cm} (1)
  where \( t_3 \) – the time from a spark discharge to the appearance of a signal on the proximity sensor of ionization;
- the average velocity of flame front propagation in the second phase of combustion (between the proximity and distant ionization sensor):
  \[ U_2 = \frac{14.27}{t_5 - t_3}, \]  \hspace{1cm} (2)
where $t_5$ – the time from a spark discharge to the appearance of a signal at the distant ionization sensor;
$t_3$ – the time from a spark discharge to the appearance of a signal on the proximity sensor of ionization;
$U_3$ – the average velocity of flame front propagation in the third phase of combustion (between the proximity and central ionization sensor):

$$U_3 = \frac{11}{t_4 - t_3},$$

where $t_3$ – the time from a spark discharge to the appearance of a signal on the proximity sensor of ionization; $t_4$ – the time from a spark discharge to the appearance of a signal on the central ionization sensor.

The investigations were carried out at the following ignition timing angles 9, 13, 16, 21, 23, 29 BTDC for each of the rotation frequencies and for each compression ratio.

The experiment was based on parallel recording of signals by a multichannel analog digital converter PCI-1712L-AE. Signals were recorded from the following sensors: ionization, induction spark sensor, optical sensor for the position of the crankshaft, with precision 0.27 degree steps of the rotation angle, pressure sensor Kistler, installed in the adapter with a spark plug, mass flow sensor Bosch. Gasoline and hydrogen were fed separately into the intake manifold for the carburetor, the mass flow rate of gas was determined from the calibrated duty ratio of the injectors. The toxicity and the coefficient of excess air ($\alpha$) were determined from the gas analyzer and the lambda sensor LSU 4.9.

3. Results and Discussion

The Figure 2 shows the results of experimental studies of the average propagation velocity of the flame front in the main combustion phase. The following symbols are used in the Figure 2 and Figure 3: the compression ratio 5.9 and 7; the rotation frequency of 600 and 900 min$^{-1}$; 16, 21, 25 BTDC; 0, 3, 5 fraction of added hydrogen as a percentage of the mass of fuel. It can be seen from the Figure 2 that the addition of hydrogen increases the average velocity of propagation of the flame front in the main combustion phase. The nature of the effect of the addition of hydrogen depends on the change in the rotational speed. The influence of the compression ratio is compensated by an increase in the ignition timing, which increases the heat evolution in the second combustion phase.
The influence of hydrogen addition in the gasoline-air mixture on the average propagation velocity of the flame front in the main combustion phase

The figure shows the effect of the addition of hydrogen to the gasoline-air mixture on the turbulent propagation velocity of the flame front in the second combustion phase. It can be seen from the figure that an increase in the average velocity of propagation of the flame front in the second phase of combustion occurs for all the investigated compositions of the mixture and the operating conditions of the engine. With an increase in the fraction of hydrogen, the dependence of the average velocity of propagation of the flame front in the second phase of combustion on the excess air coefficient. Because with an increase in the normal combustion rate, the flame front tends to become thinner and its propagation speed increasingly depends on the rate of involvement of the fresh mixture, which is determined by the turbulence of the flow. It can be seen from the Figure 3a, that the addition of 3 and 5% of hydrogen leads to approximately the same increase in the propagation velocity of the flame front between the ionization sensors.

The Figure 3b shows the effect of the addition of hydrogen to the benzene-air mixture on the propagation velocity of the flame front in the cavity of the central sensor hole. Where smaller turbulent pulsations and the absence of vortex motion are characteristic fuel-air mixture, which allows us to represent the motion of the flame front in a given section, as combustion in the case of small-scale turbulence. It can be seen from the Figure 3b that the addition of hydrogen in the rich mixture range from $\alpha = 0.7$ to $\alpha = 0.85$ practically does not affect the combustion rate and starting from $\alpha = 0.9$ and poorer the effect of the hydrogen additive becomes noticeable, and when the mixture is depleted its influence increases.
Combustion in the main phase determines the performance indicators and is largely responsible for the toxicity of the engine. As shown by experimental studies (Figure 2), the addition of hydrogen leads to an increase in the average propagation velocity of the flame front in the main phase.

The obtained effect is ensured by the following:

- explained from the standpoint of the chain mechanism of combustion reactions of hydrocarbon mixtures in which the reaction of one hydrogen atom leads to the formation of three hydrogen atoms [6, 9]. Therefore, the chemical kinetics of combustion of hydrocarbon fuels is improved, since hydrogen is the active center of combustion.

- as shown in [6, 9, 10], in the zone of the combustion reaction the excess air factor $\alpha_{ZR}$ differs from $\alpha_P$ ahead of the flame front. This is a consequence of the difference in molecular diffusion coefficients of fuel and oxygen. For most hydrocarbon-air mixtures, including gasoline-air, $\alpha_{ZR} > \alpha_P$, and for hydrogen-air and methane-air mixtures $\alpha_{ZR} < \alpha_P$. Consequently, when hydrogen is added to the depleted gasoline-air mixture, a relative increase in hydrogen occurs in the fuel-air mixture, which leads to an increase in both the normal and turbulent rates of propagation of the flame front as compared to the depleted gasoline-air mixture of the same composition. The increase in the combustion rate makes it possible to carry out the combustion process in less time and in a smaller volume near the top dead center.

From the results obtained, it can be seen that the main effect is the addition of hydrogen on the duration of the third combustion phase. This phase is very important when working on poor mixtures, as it affects the toxicity of unburned hydrocarbons. Until now, her research has been neglected. Many researchers have shown that the combustion process with small-scale turbulence is significantly influenced by the normal combustion rate, taking into account the turbulent diffusion of the molecules of the mixture. Therefore, we present known calculation models for determining the normal propagation velocity of the tribal front at a temperature and pressure corresponding to the instant of the appearance of the signal on the central ionization sensor.
From the existing models for calculating the laminar velocity of the flame front propagation we will choose the model of determining the laminar velocity of the flame front propagation for the mixtures of gasoline, presented in the Heywood’s work [9]:

\[ U_L = U_{0L} \left( \frac{T_u}{T_0} \right)^{\alpha L}, \left( \frac{P_u}{P_0} \right)^{\beta P}, \]

Where \( U_{0L} \) – the normal rate of combustion gasoline at \( T_0 = 298 \) K and \( P_0 = 0.1 \) MPa:
\[ U_{0L} = 30.5 - 54.9 \cdot (\phi - 1.21)^2, \text{ sm/s;} \]
\[ T_u, P_u \] – the temperature and pressure for which the calculation is carried out;
\[ \alpha_L, \beta_P \] – power-law coefficients of the function, depending on the coefficient of excess air:
\[ \alpha_L = 2.18 - 0.8 \cdot (\phi - 1), \]
\[ \beta_P = -0.16 + 0.22 \cdot (\phi - 1). \]

According to the conditions of the conducted researches, combustion of gasoline with hydrogen additive up to 6%. Let us determine the laminar propagation velocity of the flame front for a hydrogen-air mixture. For this we adopt the model Iijima and Takeno, presented in the work [2, 6].

The current pressure is determined from the pressure indicator diagram, and the current temperature by the equation of state of the real gas, taking into account the compressibility.

As a result of the mathematical analysis, models for calculating the propagation velocity of the flame front in the third phase of combustion:
- when working on gasoline:
\[ U_3 = \left( \frac{V_p}{V_a} \right) \cdot \left( \frac{U_{mps} - U_L}{U_{mps}} + U_{mps} \right) \left( 1.9 \cdot \alpha^2 - 3.1 \cdot \alpha + 0.6 \right); \]
- when working on gasoline with hydrogen additives:
\[ U_3 = \left( \frac{V_p}{V_a} \right) \cdot \left( U_{mps} \cdot (1 - \Delta H) + U_{LH}, \Delta H) + U_{mps} \cdot \left( 1 + \alpha \cdot (\varepsilon + 1) \cdot \left( \frac{H_f}{H_f - 1} - 1 \right) \right) \right) \left( 1.9 \cdot \alpha^2 - 3.1 \cdot \alpha + 0.6 + 2 \cdot \Delta H \right); \]

where \( V_p \) – the chamber volume at the time of the spark, L; \( V_a \) – the total cylinder capacity, L; \( U_{mps} \) – the average piston speed, m/s; \( U_L \) – the normal velocity of flame propagation of isooctane in the third phase of combustion, m/s; \( \Delta H \) – the fraction of hydrogen additive by mass of fuel; \( U_{LH}, \Delta H \) – the normal velocity of distribution of a flame of hydrogen in the third phase of combustion, m/s; \( \alpha \) – the coefficient of excess air; \( \varepsilon \) – the compression ratio;
\[ H_f = \frac{0.145 \cdot (1 - \Delta H) + \Delta H}{(1 - \Delta H) + l_{gasoline} \cdot \alpha \cdot (1 - \Delta H) + l_{H_2} \cdot \Delta H \cdot \alpha + \Delta H} \]

the total mass fraction of hydrogen in the fuel-air mixture; \( H_f = \frac{0.145}{1 + l_{gasoline} \cdot \alpha} \)

the theoretically necessary amount of air in kg for complete combustion of 1 kg of gasoline and hydrogen, respectively.

Analysis of the results of studies of the features of the propagation of the flame front with the addition of hydrogen in the fuel-air mixture made it possible to establish the mathematical dependences of the average rates of propagation of the flame front in the second and main phases of combustion on the propagation velocity of the flame front in the third phase and the operating conditions of the engine.
Analysis of the experimental results showed that the flame in the main combustion phase propagates along the turbulent mechanism. Therefore, for the basic model for calculating the average propagation velocity of the flame front in the main combustion phase, the formula Karlowetz (7) [11]:

$$U_r = U_l \cdot \left(1 + \frac{2u'}{U_l} \cdot \frac{1 - \frac{U_l}{u'} \cdot \left(1 - e^{-\frac{u'}{U_l}}\right)}{}\right), \quad (7)$$

where $U_r$ – the turbulent velocity of flame front propagation, $U_l$ – the laminar flame propagation velocity, $u'$ – the flow turbulence.

In it instead of the laminar velocity of propagation of the flame front, the average velocity of propagation of the flame front in the third phase of combustion (5) and (6), where combustion proceeds under the influence of small-scale turbulence, which is close in nature to laminar combustion [2, 5, 7, 12]. The velocity of turbulent pulsations was expressed in terms of the average piston speed, because the turbulence of the flow is proportional to the number of revolutions [5]:

$$U_{mp_s} = S \cdot \frac{n}{30},$$

where $S$ – the piston stroke, $n$ – the engine speed.

A model for calculating the average propagation velocity of the flame front in the main combustion phase:

$$U_{1+2} = U_{mp_s} \left(\frac{V_\theta}{V_a}\right)^{0.325} + U_3 \cdot \left(1 + \frac{2 \cdot U_{mp_s}}{U_3} \cdot \left(1 - e^{-\frac{U_{mp_s}}{U_3}}\right) - 2 \cdot \left(1 - e^{-\frac{U_{mp_s}}{U_3}}\right)\right) \quad (8)$$

A model is obtained that takes into account the influence of the physico-chemical properties of the mixture and the effect of the regime parameters of the engine on the propagation velocity of the flame front in the second combustion phase:

$$U_2 = U_{mp_s} \left[(\alpha - 1) \cdot 10 \cdot \left(\frac{H_c}{H_f} - 1\right) + \left(\frac{V_\theta}{V_a}\right)^{0.525}\right] + U_3 \cdot \left(1 + \frac{2 \cdot U_{mp_s}}{U_3} \cdot \left(1 - e^{-\frac{U_{mp_s}}{U_3}}\right) - 2 \cdot \left(1 - e^{-\frac{U_{mp_s}}{U_3}}\right)\right) \quad (9)$$

The obtained models have good convergence (the discrepancy with the experimental results does not exceed 5%) in the following ranges of operation of a single-cylinder unit UIT-85:

- the rotation frequency $n = 600, n = 900$ min$^{-1}$;
- the ignition timing from 9 to 29 BTDC;
- the coefficient of excess air from 0.7 to 1.5.

The obtained mathematical models for determining the average propagation velocities of the flame front in different combustion phases make it possible to determine the influence of the parameters of the operation of the gasoline engine and the effect of hydrogen on the rate of heat generation. This is necessary for the design of gasoline engines with improved environmental performance due to the addition of hydrogen. It is known that the concentration of NOx in exhaust gases is largely determined by the temperature of the combustion products and the rate of lowering of the temperature upon expansion, CH are determined by the area of the layer frozen at the wall at the appropriate temperature and pressure, which are determined by the average propagation speed of the flame front in the second and third phases of combustion.

4. Conclusion
1. As a result of simulation of the combustion process in UIT-85, empirical models of average velocities of flame front propagation in the second, third and main phases of combustion for the conditions of a single-cylinder gasoline plant with a hydrogen content of up to 6% by mass of fuel.
2. The addition of hydrogen increases the rate of propagation of the turbulent flame front of the gasoline-air mixture in the second phase of combustion due to an increase in the normal combustion rate and high diffusion activity of hydrogen, this increases the burning area and the dynamics of heat generation.

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