Modelling of the combustion velocity in UIT-85 on sustainable alternative gas fuel

N M Smolenskaya, N V Korneev

*Togliatti State University, Beloruskaya st. 14, Togliatti, Russian Federation, 445667
bVolga region state university of service, Gagarin st. 4, Togliatti, Russian Federation, 445017

E-mail: *Nata_smolenskaya@mail.ru, bniccyper@mail.ru

Abstract. The flame propagation velocity is one of the determining parameters characterizing the intensity of combustion process in the cylinder of an engine with spark ignition. Strengthening of requirements for toxicity and efficiency of the ICE contributes to gradual transition to sustainable alternative fuels, which include the mixture of natural gas with hydrogen. Currently, studies of conditions and regularities of combustion of this fuel to improve efficiency of its application are carried out in many countries. Therefore, the work is devoted to modeling the average propagation velocities of natural gas flame front laced with hydrogen to 15% by weight of the fuel, and determining the possibility of assessing the heat release characteristics on the average velocities of the flame front propagation in the primary and secondary phases of combustion.

Experimental studies, conducted on a single cylinder universal installation UIT-85, showed the presence of relationship of the heat release characteristics with the parameters of the flame front propagation. Based on the analysis of experimental data, the empirical dependences for determination of average velocities of flame front propagation in the first and main phases of combustion, taking into account the change in various parameters of engine operation with spark ignition, were obtained.

The obtained results allow to determine the characteristics of heat dissipation and to assess the impact of addition of hydrogen to the natural gas combustion process, that is needed to identify ways of improvement of the combustion process efficiency, including when you change the throttling parameters.

1. Introduction

Hydrogen as an additive to natural gas, can significantly improve efficiency and reduce toxicity of exhaust gases of reciprocating ICES. In particular, there is actual necessity for conducting studies when working at low frequencies of the crankshaft rotation, including the throttling modes, which have great influence on the economic and environmental performance of the engine, as the engine is operating in these modes for significant amount of time when driving in the megacity [1].

In this regard, determination of regularities connecting the average velocity of flame propagation and the dissipation characteristics is of high priority. That will allow at the stage of designing of engines, operating on gas fuels, to improve the efficiency of work in these modes.
Accordingly, the purpose of the conducted studies was to develop the computational method for determining dissipation characteristics in engines operating on gas fuels, taking into account the obtained dependences for calculation of the average velocities of the flame front propagation.

2. Experimental technique

Studies of the characteristics of the combustion process and their relationship with parameters of combustion process were conducted on the experimental stand with a single-cylinder installation UIT-85, in which the electric motor maintains the constant velocity, homogeneity of the fuel-air mixture (FAM) was provided by the structure of the heated inlet pipe.

Registration of the combustion front propagation inside the cylinder installation UIT-85 near the spark plugs, was carried out using the ionization sensor installed in the spark plugs adapter. The parameters of the flame front propagation in the combustion chamber and the electrical conductivity in the final phase of combustion were evaluated using the multielectrode ionization sensor, installed in the zone of the combustion chamber, most remote from the spark plug.

In the study the major variable factors were the excess air ratio, varying from 0.8 to the maximum for the extremum dilution (1.3 – 1.7) and composition of gaseous fuels, where the share of natural gas ranged from 85 to 100%, and proportion of hydrogen, from 0 to 15% (by fuel weight). Operation of the installation was carried out at the ignition advance angle, varying from 0 to 30° of the crankshaft position sensor and velocities of 600 and 900 min⁻¹. The experimental procedure included parallel registration by the means of the digital multichannel ADC L-783M, manufactured by the “L-Card” company, of signals from the following sensors: ionization, spark plugs, crankshaft position, and cylinder pressure of the engine, mass air flow, and a gas analyzer, that determines the composition of the mixture by the excess air ratio and toxicity. As a result of experiments the series of oscillograms in each mode of testing was obtained. For each mode, with mathematical analysis the averaged signal indicator pressure signal and the signal from the ionization sensors were obtained, by which the characteristics of heat dissipation and the average velocity of the flame front propagation were obtained.

Determination of the experimental data errors was carried out according to GOST R 8.736-2011. The signal amplitude error from the ionization sensors and the signal pressure mostly did not exceed 6% of the time from spark discharge to the occurrence of maximum pressure in the cylinder of the ICE and to an impulse of ion current at ionization sensors – 3%, excess air ratio – 3%; consumption of natural gas and hydrogen – 3%.

3. Results and Discussion

The analysis of the studies of combustion in reciprocating ICEs has shown that the main parameters characterizing the combustion are the velocity of flame propagation in the 1st, 2nd and main phases of combustion, as well as characteristics of heat dissipation. Existing formulas for the flame propagation velocity in turbulent flow, reflecting the process behavior in the best way is the Damkohler – Karlovic model [2], which is often used to calculate combustion in large-scale turbulence. This model is considered to be continuation of Schelkin’s works [2], which, in turn, are often taken as the basis for calculating combustion in small-scale turbulence. In both models, both flow turbulence and laminar combustion rate are considered. Therefore, for modeling the flame front propagation velocity in the combustion chamber of reciprocating ICEs it is necessary to determine the laminar velocity under these conditions, as it is the base to determine the empirical dependences of average velocities of the 1st and main phases of combustion.

From the existing models for calculation of the laminar velocity of the flame front propagation we will choose the model of determining the laminar velocity of flame front propagation for the methane-air mixtures, presented in the Heywood’s work [3]:

\[ U_{L(CH_4)} = U_{0L(CH_4)} \cdot \left( \frac{T_u}{T_0} \right)^{\alpha_{l(CH_4)}} \cdot \left( \frac{P_u}{P_0} \right)^{\beta_{p(CH_4)}} \]  

(1)
where \( U_{\text{L(CH4)}} \) – the normal rate of combustion at \( T_0 = 298 \, K \); \( P_0 = 101325 \, Pa \); \( T_u \) and \( P_u \) – the temperature and pressure for which the calculation is carried out; and the coefficients \( \alpha_{t(CH4)} \) and \( \beta_{p(CH4)} \) – are functions of the mixture composition:

\[
\alpha_{t(CH4)} = 2.18 - 0.8 \cdot (\alpha - 1) \\
\beta_{p(CH4)} = -0.16 + 0.22 \cdot (\alpha - 1)
\]

The current pressure was determined from the indicator diagrams of the pressure and current temperature on the equation of the real gas state at the spark moment.

To determine the normal propagation velocity of the methane-air mixture flame front we will use the data given in [4], which presents the experimental dependence of the normal propagation velocity of the flame front from the volume content of methane in the FAM. As a result of recalibration of the volume content of methane in the mixture to the excess air ratio the graph of the normal propagation velocity of flame front from \( \alpha \) [4] was obtained. Following approximation of this formula, the polynomial describing the dependence of the normal velocity of flame front of methane-air mixture from the air excess factor for \( T_0 = 298 \, K \) and \( P_0 = 1 \, \text{atm} \) was obtained:

\[
U_{\text{L(CH4)}} = -2.7537 \cdot \alpha^4 + 15.612 \cdot \alpha^3 - 32.696 \cdot \alpha^2 + 29.257 \cdot \alpha - 9.0757 
\]

Under the terms of the ongoing research, in ICEs combustion of the natural gas laced with hydrogen to 15% occurs, therefore, it is necessary to determine the laminar propagation velocity of the flame front also for the hydrogen-air mixture. For this we will take the Ujima and Takeno model given in [5]:

\[
U_{L(H2)} = U_{\text{L(CH4)}} \cdot \left( \frac{T'_u}{T_0} \right)^{\alpha_{t(H2)}} \cdot \left( \frac{P_u}{P_0} \right)^{\beta_{p(H2)}} \quad (3)
\]

where \( T_0 = 291 \, K \); \( P_0 = 101325 \, Pa \); \( P_u \) and \( T'_u \) – the pressure and temperature for which the calculation of the normal combustion velocity is conducted, corresponding to the pressure and temperature, defined for the hydrogen-air mixture; \( \alpha_{t(H2)} \), \( \beta_{p(H2)} \) and \( U_{\text{L(CH4)}} \) are determined from the formulas:

\[
\alpha_{t(H2)} = 1.54 + 0.026 \cdot (\alpha - 1) \\
\beta_{p(H2)} = 0.43 + 0.003 \cdot (\alpha - 1)
\]

\[
U_{\text{L(H2)}} = 2.98 - (\alpha - 1.7)^2 + 0.32 \cdot (\alpha - 1.7)^3
\]

where \( \alpha \) – excess air coefficient.

Combustion in the 1st phase is performed to a greater extent in small-scale turbulence, and to develop models of combustion, it is expedient to apply the K.I. Schelkin’s model, where the average velocity of the piston is chosen as the criterion of turbulence, and the influence of the composition of the gas fuel is reflected by the excess air ratio and the proportion of hydrogen in natural gas.

Based on this mathematical analysis, which revealed the contribution of each component in the model, and approximation of the effects of the excess air ratio on changing the flame propagation velocity, with addition of hydrogen, the empirical model was obtained, with the purpose to determine the average propagation velocity of flame front in the 1st phase when operating only on compressed natural gas (CNG) (4) and when operating on CNG with addition of hydrogen up to 15% by weight (5), when the excess air factor \( \alpha \) varies from 0.8 to 1.4:

\[
U_1 = U_{L(CH4)} \cdot \alpha^2 + U_{L(CH4)} \cdot \sqrt{\alpha} \cdot \sqrt{1 + \frac{U_{\text{mps}}}{U_{L(CH4)}}} \quad (4)
\]

\[
U_1 = \left[ U_{L(CH4)} \cdot \alpha^2 + U_{L(CH4)} \cdot \sqrt{\alpha} \cdot \sqrt{1 + \frac{U_{\text{mps}}}{U_{L(CH4)}}} \right] \cdot \left( 1 - \frac{\Delta H}{100} \right)
\]
\[-(4.3 \cdot \alpha^2 - 10.285 \cdot \alpha + 4.6) \cdot \sqrt{\left(U_{\text{mps}} \cdot U_{L(H2)} \cdot \frac{\Delta H}{100}\right)}\]  

where \(U_{\text{mps}}\) – the average velocity of the piston; \(\Delta H\) – share of the addition of hydrogen by mass in fuel, %. 

The check of adequacy of the obtained models for calculation of the propagation velocity of flame in the 1st phase of combustion for UIT-85 when operating on CNG and CNG with the share of hydrogen of 5, 10 and 15%, (4 and 5) is shown in Fig. 1, when the crankshaft rotation velocity \(n = 900\) min\(^{-1}\), compression ratio \(\varepsilon = 7\) and the ignition advance angle = 13° of the crankshaft position sensor. In average, divergence of the calculated values with the experimental ones is less than 2.5%, for \(\alpha\) close to stoichiometric, 0.1 m/s, and the maximum discrepancy does not exceed 8%, amounting to 0.35 m/s for \(\alpha = 0.8\). From this it follows that by using the calculation formula accurately you can determine the average velocities of flame propagation in the 1st phase, changing the parameters of engine velocity, mixture composition and additives of hydrogen in TBC. This indicates high degree of convergence of results of calculation performed by empirical models with experimental results for the studied operating modes.

![Figure 1](image)

**Figure 1** – Comparison of experimental results with the model for average propagation velocity of flame front in the 1st phase of combustion in UIT-85, operating on CNG and CNG with the share of hydrogen of 5, 10 and 15%.

The main phase of combustion \((U_{1+2})\) involves the 1st and 2nd phase of combustion [6,7,8] in which combustion mainly takes place under the influence of large-scale turbulence, therefore, to develop empirical models of the propagation of the flame front in the main phase, the Damkohler – Karlovic model has been chosen [2,6,9]. In this model, the average propagation velocity of the flame front in the 1st phase of combustion was adopted as the laminar velocity, and the activating effect of hydrogen on the combustion process is considered. Such parameters of the engine as the filling ratio, which determines the throttling conditions, compression ratio and the ignition timing, calculated using the ratio of the volume at the time of supplying sparks to the operating volume, were also considered in
the model. In the result the empirical relationship for calculating the average propagation velocity of
the flame front in the main phase of combustion for CNG and CNG with addition of hydrogen up to
15% by weight of the fuel (6) was obtained:

\[ U_{1+2} = 1.3 \cdot \sqrt{U_1} \cdot \sqrt{U_{\text{mps}}} \cdot \sqrt{\eta_v} \cdot e^{\left(\frac{\varepsilon \cdot V_h}{V_v}\right)} + \sqrt{2 \cdot U_{\text{mps}} \cdot U_1 \cdot \frac{U_1^2}{1.3} \left(1 - e^{\left(\frac{U_{\text{mps}}}{U_1}\right)}\right)} \] (6)

where \( \eta_v \) – the filling ratio; \( \varepsilon \) – compression ratio; \( \frac{V_\theta}{V_h} \) – the ratio of the volume at the time of
supplying sparks to the operating volume.

The convergence of the obtained model with the experimental data is presented in Fig. 2. for UIT-
85 with operating mode \( n = 900 \text{ min}^{-1} \), ignition advance angle = 13° of the crankshaft position sensor,
at operating with CNG and CNG with addition of hydrogen of 5, 10 and 15% of the fuel weight.

The average discrepancy of the calculated values with the experimental ones is about 1%, for \( \alpha \)
close to stoichiometric 0.15 m/s, the maximum discrepancy does not exceed 5%, amounting to 0.5 m/s
for \( \alpha = 0.8 \). From this it follows that by using the calculation formula accurately you can determine
the average velocities of flame propagation in the main phase by changing the engine velocity, mixture
composition and fraction of hydrogen in the gas composite fuel.

\[ \begin{align*}
U_{1+2} & = 1.3 \cdot \sqrt{U_1} \cdot \sqrt{U_{\text{mps}}} \cdot \sqrt{\eta_v} \cdot e^{\left(\frac{\varepsilon \cdot V_h}{V_v}\right)} + \sqrt{2 \cdot U_{\text{mps}} \cdot U_1 \cdot \frac{U_1^2}{1.3} \left(1 - e^{\left(\frac{U_{\text{mps}}}{U_1}\right)}\right)} \\
\end{align*} \] (6)

Figure 2 – Comparison of experimental results with the model ones for average propagation velocity
of the flame front in the main combustion phase in UIT-85, operating on CNG and CNG with the
share of hydrogen of 5, 10 and 15%.

To determine the energy parameters of the engine it is necessary to know the characteristics of heat
dissipation. In Russia, the most common is the heat dissipation characteristics, proposed by I. I. Wiebe
[10,11]:

\[ \begin{align*}
\end{align*} \]
where \( \chi_z \) — the share of active burned mixture; \( \varphi_z \) — duration of the combustion process; \( \varphi \) — the current angle from beginning of the combustion process; \( m \) — the indicator of the combustion behavior.

One of the drawbacks of the model of I.I. Wiebe in relation to calculation of the heat release characteristics, is the lack of relation between parameters \( m \) and \( \varphi_z \) with the characteristics of flame front propagation in the conditions of ICE, especially when operating on alternative gaseous fuels consisting of natural gas and hydrogen up to 15%.

The mathematical analysis provided us the possibility to determine the indicator of the combustion process behavior \( m \) and the duration of combustion \( \varphi_z \), included in the dissipation model (7), depending on the average propagation velocity of flame in the 1st and main phases of combustion, which are presented in models (5) and (6).

The obtained empirical models are represented by the formulas (8) and (9):

\[
m = \frac{180 \cdot U_{\text{mps}}}{S} \ln \left( \frac{S_1 \cdot U_{\text{mps}}}{U_1} \right) - \ln \left( \frac{180 \cdot \left( S_1 \cdot U_{\text{mps}} + S_{1+2} \cdot U_{\text{mps}} \right)}{S \cdot \left( U_1 + U_{1+2} \right)} \right) + 1
\]

\[
\varphi_z = \frac{\pi}{S} \left( \frac{S_{1+2} \cdot U_{\text{mps}}}{U_{1+2}} + \frac{2 \cdot S_1 \cdot U_{\text{mps}}}{U_1} \right)
\]

where \( S \) — the piston stroke length, mm; \( S_1 \) and \( S_{1+2} \) — distance of the flame moving in the 1st and main phases of combustion, respectively, mm.

The convergence of the obtained models is shown in the following ranges of operation:

- velocity range from 600 to 900 min\(^{-1}\);
- ignition advance angle from 8 to 30° of the crankshaft position sensor;
- actual air excess factor from 0.8 to 1.3.

The obtained models in relation to determination of the parameters of the heat release characteristics and velocities of flame propagation have a high convergence with experimental data in the specified range.

4. Conclusion
1. In the result of modelling of the flame propagation velocity in the UIT-85 the empirical models of average velocities of the flame front propagation in the 1st and the main phases of combustion for natural gas with the ratio of hydrogen up to 15\% by weight were obtained.
2. The dependence of the heat release characteristics from the velocities of flame front propagation in the 1st and the main phases of combustion, which is presented in the form of empirical models for determination of \( m \) and \( \varphi_z \), was identified.
3. The calculation method for determination of the dissipation characteristics in a low frequency range of rotation of the crankshaft, including the modes of throttling, will allow at the design stage to evaluate the influence of the composition of alternative gaseous fuels on parameters of economic and environmental performance of the engine.
References

[1] Smolenskaya N.M., Smolenskii V.V, Bobrovskij I., Research of polytropic exponent changing for influence evaluation of actual mixture composition on hydrocarbons concentration decreasing on deep throttling operation, IOP Conf. Series: Earth and Environmental Science 50 (2017) 012016 doi:10.1088/1755-1315/50/1/012016.

[2] Warnatz J., Maas U., Dibble R.W., Combustion. Physical and Chemical Fundamentals, Modeling and Simulation, Experiments, Pollutant Formation, 4th Edition, ISBN-13 978-3-540-25992-3 4th ed. Springer Berlin Heidelberg New York, 2006 - 378 p.

[3] Heywood J.B., Internal Combustion Engine Fundamentals, McGraw-Hill, – New York : McGraw-Hill, 1988. – 931 p.

[4] Law C.K. Combustion physics, Cambridge: Cambridge university press, 2006. – 722 p.

[5] Verhelst S. A study of the combustion in hydrogen-fuelled internal combustion engines, PhD thesis, Gent: Gent University, 2005. – 278 p.

[6] Smolenskaya N.M. Improving the efficiency of spark ignition engines through the use of composite gas fuels, dissertation of the candidate of technical sciences, Moscow: MAMI University, 2015. – 165 p.

[7] Shaikin A.P., Galiev I.R., On the effect of temperature and the width of the turbulent combustion zone on the ionization detector readings, Technical Physics, 61(8) (2016) 1206-1208. Information on https://www.scopus.com/inward/record.uri?eid=2-s2.0-84981489611&partnerID=40&md5=2a171a70052f225423d5f1082d29a746 DOI: 10.1134/S1063784216080247.

[8] Shaikin A.P., Galiev I.R., Relationship of flame propagation speed for methane-hydrogen fuel of a Internal Combustion Engine with parameters of ion current and hydrogen concentration, Russian Aeronautics (iz VUZ). 2016. V.59(2). P.249-253 DOI: 10.3103/S106879981602015X

[9] Hitrin L.N., Physics of Combustion and Explosion, MGU, Moscow, 1957.p.337 – 411

[10] Vibe I. I. The new operating cycle of the engine. Combustion rate and duty cycle of the motion engines, Sverdlovsk, Mashgiz, 1962. - 271 p.

[11] Kavtaradze, R.Z. Theory of piston engines. Special chapters, Moscow, MSTU. Bauman. 712 p.