HEAT AND MASS TRANSFER IN COMBUSTION PROCESSES

DETERMINATION OF THE PARAMETERS OF SELF-IGNITION OF GASEOUS MIXTURES IN ADIABATIC COMPRESSION

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A study has been made of the distinctive features of self-ignition and combustion of fuel-air mixtures containing methane, hydrogen, and ethylene in adiabatic compression.

Keywords: *rapid-compression facility, adiabatic compression, self-ignition, combustion, induction time, methane, hydrogen, ethylene.*

Introduction. The necessity of minimizing the discharge of harmful substances into the atmosphere and reducing the consumption of energy resources calls for investigations aimed at changing traditional approaches to the burning of organic fuels, optimizing working processes in combustion chambers, updating the design of engines, and introducing new kinds of fuels. In recent years, the task of ensuring savings in fuel resources through the utilization of secondary raw materials and production by-products has been set. Thus, mixtures of special gases (methane, hydrogen, ethylene, and others) are formed in a number of technological processes based on hydrocarbon splitting. The possibility of utilizing them subsequently in the gas engines of cogeneration facilities for production of electric and thermal energy will make it possible to optimize the local energy consumption of an enterprise, which will ensure a reduction in the manufacturing cost of products.

Gas engines are traditionally designed to operate with natural gas. Change in the composition of the fuel can have a substantial effect on both its detonation properties and the operation of the entire propulsion system, namely, the degree of compression and regime of ignition of the mixture in the combustion chamber. In this connection, when mixtures of special gases are utilized as fuels it is desirable to investigate beforehand their motor properties under conditions as close to actual ones as possible. Such thermodynamic conditions are easily modeled using rapid (adiabatic)-compression facilities that are capable of generating high pressures and temperatures of a medium for a period of longer than 10 msec with the total monitoring of its running parameters during the steps of compression and combustion of the mixture [1–4]. Owing to the short duration of the compression process, the heat-removal time decreases and the basic volume of the investigated gas turns out to be heat-insulated, since its cooling due to the heat loss is confined to a thin layer of the gas along the combustion-chamber walls. Limited heat removal ensures that the temperature, pressure, and concentration of the medium in the central region of the compressed mixture are spatially uniform.

In this work, we have studied the distinctive features of self-ignition and combustion of fuel-air mixtures with different percentages of methane, hydrogen, and ethylene in the ranges of pressures and temperatures that are characteristic of operating parameters in the chambers of gasoline and diesel internal-combustion engines and of power-generating (gas-piston) units.

Experimental Facility, Calculation of the Temperature, and Composition of the Investigated Mixtures. A diagram of the rapid-adiabatic-compression facility is shown in Fig. 1; its basic specifications are as follows:

Maximum degree of compression   51
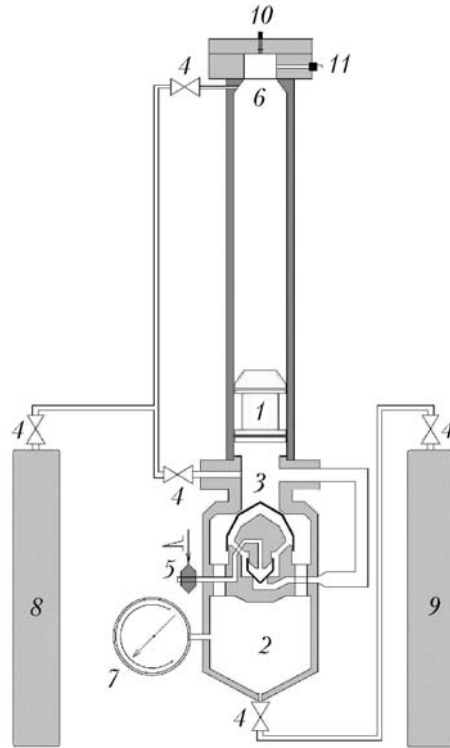Compression time   30–50 msec

Fig. 1. Diagram of the rapid-compression facility: 1) piston; 2) high-pressure chamber; 3) control valves; 4) gate; 5) electromagnetic valve; 6) combustion chamber; 7) manometer; 8) cylinder with the investigated gas; 9) cylinder with a propelling gas; 10) piezoelectric pressure sensor; 11) light guide.

Volume of the combustion chamber	$4.9 \cdot 10^{-2}$ dm^3
Maximum initial volume	2.5 dm^3
Diameter of the combustion chamber	50 mm
Diameter of the piston	75 mm
Height of the combustion chamber	25 mm
Maximum stroke of the piston	556 mm

The process of compression is carried out by piston 1 activated by a compressed propelling gas (air or helium). The pulsed character of compression is achieved by rapid pressure feed from a high-pressure chamber to the volume under the piston using the system of control valves 3. Change in the pressure in the chamber in the compression step with a time resolution of 10^{-5} sec is recorded using the PCB Piezotronics piezoelectric sensor 10 connected to one channel of a digital oscilloscope; the startup of the oscilloscope is locked in step with the arrival of a master pulse at the opening of an electromagnetic valve 5. The signal from the photomultiplier connected to the internal volume of the combustion chamber 6 using light guide 11 is simultaneously recorded on the oscilloscope's channel. This enables us to record the dynamics of glow in the combustion chamber and, consequently, to determine the instant of ignition of the mixture. Synchronous recording of signals from the pressure sensor and the photomultiplier makes it possible to accurately determine the delay of ignition of the investigated composition under specified thermodynamic conditions. The difference in the cross-sectional areas of the piston and the high-pressure chamber and the pulsed character of compression make it possible to obtain a final pressure that is 10–15 times higher than the propelling-gas pressure. The atmospheric initial pressure is set in the combustion chamber 2 and in the volume under the piston.

We carry out methodological experiments on compression of air and hydrogen with the aim of determining the operating characteristics of the facility and its operating regimes. Figure 2 compares the ideal adiabat of the process under study and the adiabat allowing for the temperature dependence of the heat capacity of the gas to the experimental values obtained in compression of air and hydrogen. Unlike the data for air, the maximum pressure in the
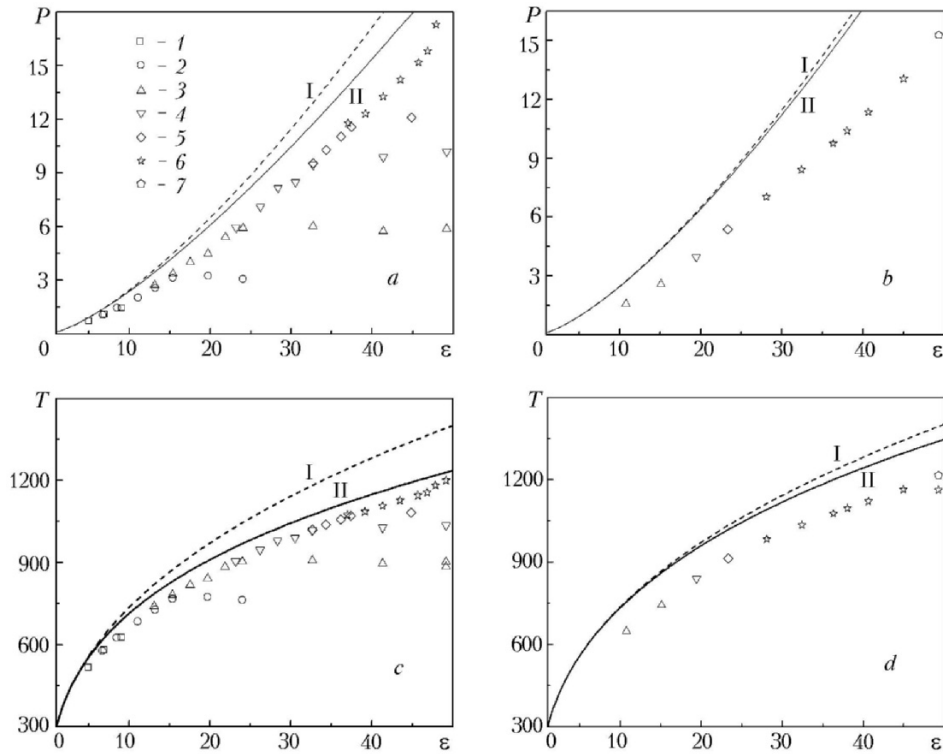
Fig. 2. Maximum pressure of air (a) and hydrogen (b) and temperature of air (c) and hydrogen (d) in the chamber vs. degree of compression at different air pressures in the high-pressure chamber: I and II) theoretical adiabat without allowance for the temperature dependence of the heat capacity and with allowance for it respectively; experimental dots at pressures in the high-pressure chamber of: 1) 0.53, 2) 0.69, 3) 0.88, 4) 1.08, 5) 1.16, 6) 1.27, and 1.39 MPa. P, MPa; T, K.

measuring volume in compression of hydrogen significantly differs from the corresponding theoretical values. This disagreement is primarily a consequence of the high thermal conductivity of hydrogen, which leads to a considerable increase in the level of heat loss to the walls of the facility, and of the large coefficient of its diffusion and the ensuing loss of the compressible gas through the piston's compression rings.

From the presented plots, it is clear that the initial pressure of the propelling gas in the measuring volume must be increased to ensure the highest possible parameters of compression. If the pressure level is insufficient, the piston has no time to reach the point of its maximum travel, the so-called top dead center, and stops in a certain intermediate cross section of the tube. The maximum pressure in the chamber is stabilized and is nearly independent of the initial position of the piston (degree of compression of the mixture) at the same pressure of the propelling gas in the high-pressure chamber (Fig. 2a).

The compressed-mixture temperature is determined from the signals of the pressure sensor. For this purpose the assumption of the adiabatic character of the process at the center of the combustion chamber is used. As has been indicated above, the heat loss through the chamber walls in the compression step and after the piston has stopped are localized mainly in the thin boundary layer along the surface, whereas the flow core remains heat-insulated. Therefore, although the process itself is not adiabatic, we can use the equations of adiabatic compression for the central region of the internal volume. Then the temperature can be determined from the equation

$$\int_{T_0}^{T_{a.c}} \frac{1}{(\gamma(T) - 1)\,T}\,dT = \ln \varepsilon \,. \tag{1}$$
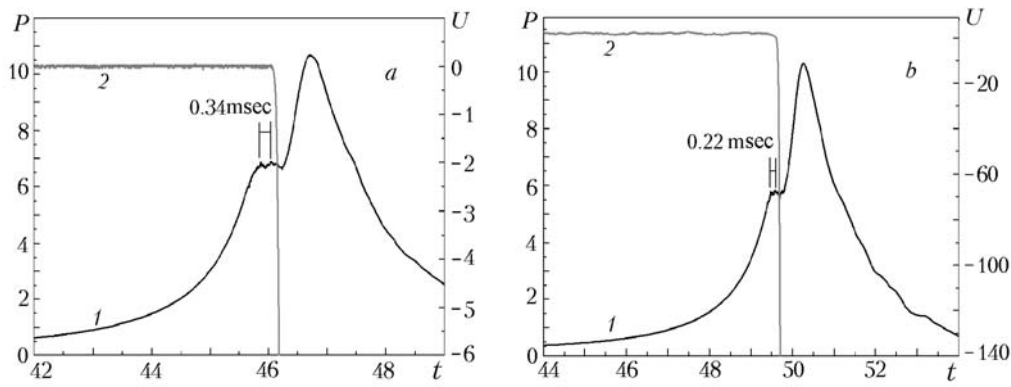
Fig. 3. Change in the pressure in the combustion chamber (1) and the signal from the photomultiplier (2) for a degree of compression of 25.8 for lean mixtures No. 1 (a) and No. 2 (b). P, MPa; U, V; t, msec.

Due to the heat loss, the actual temperature of the mixture will always be lower than that calculated from Eq. (1). Based on the assumptions made, we can compute the value of the actual temperature from the measured pressure using the following equation:

$$\int_{T_0}^{T_c} \frac{\gamma(T)}{(\gamma(T)-1)\,T}\,dT = \ln\left(\frac{P_c}{P_0}\right). \tag{2}$$

The calculated values of the temperature in the combustion chamber after the compression of air and hydrogen respectively are shown as dots in Fig. 2c and d. The dependences of the adiabatic temperature on the degree of compression, which have been calculated using Eq. (1), are marked by the curves. It is seen that the actual gas temperature differs from its ideal value. The difference in the temperatures is the largest in compression of hydrogen. As in the case of pressure, this is primarily due to the high thermal conductivity of hydrogen.

In the work, we investigate three fuel mixtures differing in the composition of fuel. As a basic mixture we consider that of air and a methane-hydrogen fraction formed during the technological process of polyethylene production: $0.34H_2 + 0.62CH_4 + 0.04C_2H_4$ (mixture No. 1). Furthermore, to study the action of enrichment of the methane-hydrogen fraction with hydrogen or ethylene on ignition regimes and on the possibility of the high-frequency instability developing in combustion we also investigate air mixtures with the fuel of the following composition: $0.44H_2 + 0.52CH_4 + 0.04C_2H_4$ (+10% H_2, mixture No. 2) and $0.34H_2 + 0.58Ch_4 + 0.08C_2H_4$ (+4% C_2H_4, mixture No. 3).

Self-ignition is studied for both the stoichiometric ratio of the fuel and the oxidant $\phi = 1$ and the excess of the oxidant $\phi = 0.75$. The experiments are carried out for degrees of compression of the mixture of 15–25, which corresponds to the ranges of temperatures 720–910 K and pressures 2.8–6.8 MPa that are much higher than the maximum parameters realized in the combustion chambers of spark-ignition gas engines.

Ignition of Mixtures of Special Gases in Rapid Compression. Figure 3 shows the dynamics of change in the pressure and the proper glow of mixtures No. 1 and No. 2 in the chamber in their compression and ignition for $\phi = 0.75$ and a degree of compression of 25.8.

During the motion of the piston, the chamber pressure grows smoothly due to the compression of the mixture. At the end of the compression, the maximum pressure is attained in the chamber; for these experiments, it is 5.7–6.2 MPa; the chamber temperature calculated from Eq. (2) corresponds to the range 870–885 K. Self-ignition of the compressed mixtures occurs with a delay at the top dead center on attainment certain conditions. The instant of ignition corresponds to a sharp change in the photomultiplier signal, which has been produced by the chemiluminescence from the volume of the reactive mixture, and to the additional growth in the pressure in combustion. The ignition delay is defined as the time interval between the instant at which the maximum compression pressure is attained, with the piston at the top dead center, and the appearance of glow in the chamber. Its duration is dependent on both the composition of the fuel mixture and the thermodynamic conditions in the combustion chamber. Under the same thermo-
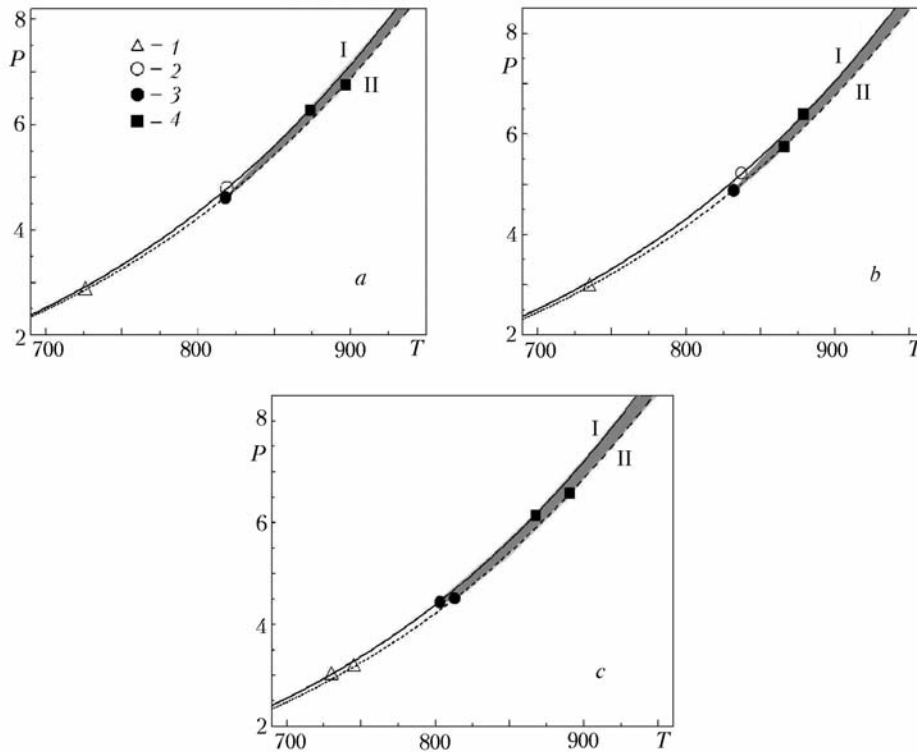
Fig. 4. Thermodynamic conditions realized in compression of mixtures No. 1 (a), No. 2 (b), and No. 3 (c): I and II, adiabats with allowance for the temperature dependence of the heat capacity at $\phi = 1$ and $\phi = 0.75$ respectively; 1 and 3) $\varepsilon = 15.04$ and 2 and 4) 21.33 (1 and 2, without self-ignition; 3 and 4, self-ignition). P, MPa; T, K.

dynamic conditions, the ignition delay in enriched mixtures No. 2 and No. 3 is shorter that the delay in basic mixture No. 1, which is explained by the higher concentration of active gases (hydrogen and ethylene).

In the studied range of conditions, the self-ignition of the mixtures in the chamber is accompanied by a smooth growth in the pressure without sharp pulsations and jump. This points to a stable combustion. Despite the presence of large amounts of chemically active hydrogen and ethylene, no detonation effects are observed in compression of the mixtures in the studied range of temperatures and pressures. Since the piston is not fixed at the top dead center in this facility, the ignition time exerts a substantial influence on the level of maximum pressure in the chamber, since the pressure of the compressed mixture has time to decrease before combustion because of the backward motion of the piston. Therefore, the pressures in the combustion chamber are maximum (10–11 MPa) in chemically more active mixtures No. 2 and No. 3 at $\phi = 1$ and $\phi = 0.75$ and in mixture No. 1 at $\phi = 0.75$ with a small ignition delay. For basic mixture No. 1 at $\phi = 1$ and the same degree of compression, the pressure in the chamber does not exceed 5.5 MPa, which is due to the reduction in the pressure and the temperature of the mixture by the instant of its self-ignition because of the backward motion of the piston.

In the experiments, we have established the regions of thermodynamic conditions under which self-ignition of fuel mixtures occurs. Theoretical values of the medium's parameters in adiabatic compression with allowance for the temperature dependence of the heat capacity of the gas are shown as curves in Fig. 4, whereas the experimental values corresponding to different degrees of compression are shown as dots. The coincidence of the dots and the curves is explained by the fact that the medium's temperature is computed from the measurements of the maximum pressure using the adiabatic-compression equation. The dots and regions of thermodynamic states for which the self-ignition of fuel mixtures is observed are colored gray. It is seen that the investigated compositions do not ignite for $\varepsilon = 15$, and only lean mixtures ($\phi = 0.75$) and stoichiometric mixture No. 3 ignite for $\varepsilon = 21$. These results are consistent with the regularities obtained in experiments with shock tubes [5, 6]. In these works, it has been shown that in air mixtures of ethylene, methane, and hydrogen, the ignition delays increase with decrease in the medium's

temperature; in lean mixtures, the induction time is shorter that that in stoichiometric ones. Disagreement with this regularity has been found for ethylene-air mixtures in the region of low temperatures: Ignition delays for stoichiometric compositions were shorter than those for lean mixtures. This fact explains the ignition of ethylene-enriched stoichiometric mixture No. 3 for $\varepsilon = 21$ (Fig. 4c), whereas the remaining studied stoichiometric compositions did not ignite for this degree of compression.

Conclusions. The methodological experiments on compression of air and hydrogen have demonstrated the possibility of using the developed facility for modeling of the compression step of internal-combustion engines and gas-piston units in the case of cold start.

During the investigations, we have established the distinctive features of self-ignition of stoichiometric ($\phi = 1$) and lean ($\phi = 0.75$) air mixtures of hydrogen, methane, and ethylene in compression up to pressures of 2.8–6.8 MPa and temperatures of 720–910 K. It has been shown that self-ignition of the above compositions is possible only for a degree of compression above 21 (average effective pressure of the medium 4.5–5.0 MPa and temperature 800–830 K.) A stable and smooth combustion without detonation effects and sharp pressure pulsations is observed.

Increase in the concentration of hydrogen or ethylene as part of the fuel substantially decreases the self-ignition delay and has no effect on the character of combustion in the investigated range of conditions. In turn the decrease in the induction time causes the level of maximum pressure developed in the combustion chamber to increase, which can have a positive effect on the operating efficiency of power-generating facilities.

The experiments have demonstrated the possibility of utilizing air mixtures of hydrogen, methane, and ethylene as a fuel for gas-piston power-generating units. This work was carried out within the framework of the State Program of Applied Research "Vodorod" under the assignment "Vodorod 14."

NOTATION

P, pressure, Pa; T, temperature, K; t, time, sec; U, voltage, V; γ, adiabatic exponent; ε, degree of compression; ϕ, stoichiometric coefficient. Subscripts: a.c, state after adiabatic compression; c, state after compression; 0, initial state.

REFERENCES

1. M. T. Donovan, X. He, B. T. Zigler, T. R. Palmer, M. S. Wooldridge, and A. Atreya, Demonstration of a free-piston rapid compression facility for the study of high-temperature combustion phenomena, *Combust. Flame*, **137**, 351–365 (2004).
2. S. M. Gallagher, H. J. Curran, J. Würmel, and J. M. Simmie, The oxidation of propane at elevated pressures in a rapid compression machine. An experimental and modeling study, *Proc. Third Joint Meeting of the U.S. Sections of the Combustion Institute*, Chicago, IL, USA, March 2003.
3. C. K. Westbrook, W. J. Pitz, J. E. Boercker, H. J. Curran, J. F. Griffiths, C. Mohamed, and M. Ribaucour, Detailed chemical kinetic reaction mechanisms for autoignition of isomers of heptane under rapid compression, *Proc. Combust. Inst.*, **29**, 1311–1318 (2002).
4. P. Beeley, J. F. Griffiths, and P. Gray, Rapid compression studies on spontaneous ignition of isopropyl nitrate. Pt. II: Rapid sampling, intermediate stages and reaction mechanisms, *Combust. Flame*, **39**, 269–281 (1980).
5. V. V. Martynenko, O. G. Penyazkov, K. A. Ragotner, and S. P. Shabunya, High-temperature ignition of hydrogen and air at high pressures downstream of the reflected shock, *Inzh.-Fiz. Zh.*, **77**, No. 4, 100–107 (2004).
6. O. G. Penyazkov, K. L. Sevrouk, V. Tangirala, and N. Joshi, High-pressure ethylene oxidation behind reflected shock waves, *Proc. Combust. Inst.*, 2009, doi:10.1016/j.proci.2008.06.194.