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NUMERICAL STUDY OF DETONATION INITIATION BY SPARK DISCHARGE IN A HYDROGEN-OXYGEN HIGH-PRESSURE GAS MIXTURE

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The influence of the initial pressure of the combustible gas mixture on the processes that occur during the initiation of detonation by a spark discharge in a high-pressure hydrogen-oxygen mixture was estimated. A one-dimensional gas-dynamic model in a chemically reacting gas with separation of the vibrational temperature of diatomic molecules from the kinetic temperature of the gas was used for the numerical study. It was simulated that an intensity of the shock wave causing the detonation initiation by a critical regime is below of the detonation wave intensity when the initial gas pressure is 1.013 MPa and the intensity of the shock wave exceeds the detonation wave intensity when the initial gas pressure is 0.304 MPa. It was found out that the process of the detonation initiation falling by a near-critical regime is more longitudinal when the gas pressure is low. Energy deposition history into the spark channel when detonation is initiated at different initial gas pressures was calculated.

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INTRODUCTION

The development of energy-efficient fuel combustion technologies provides competitive advantages of energy equipment. One of the directions for increasing the energy efficiency of power equipment is the transition from deflagration to detonation combustion in the combustible mixture. Environmental friendliness of the equipment is achieved by using hydrogen as a fuel [1]. An increase in the energy efficiency of the combustion cycle in power equipment is provided by an increase in the initial pressure of combustible gas. As a rule, a spark discharge is used to ignite the mixture in the combustor. Depending on the parameters of the spark discharge, either deflagration or detonation combustion of the mixture may occur [2]. Thus, the study of the detonation initiation by a spark discharge in a high-pressure hydrogen-oxygen gas mixture is relevant.

It is necessary to determine the effect of the initial gas pressure on the detonation initiation process to implement a spark-initiated detonation system for power equipment. At the same time, it is necessary to determine the minimum discharge energy at which initiation occurs. Due to the reduction of the energy of the electric discharge, the reduction of the total consumption of electric energy is achieved and the service life of the discharge electrodes is increased caused by the reduction in electric erosion, the mass-dimensional parameters of the system are reduced due to the use of a capacitor of a smaller capacitance, etc.

An experimental study of the detonation initiation in a high-pressure hydrogen-oxygen mixture was carried out in works [3, 4]. According to the results of these studies, a decrease in the critical detonation initiation energy was found with increasing initial gas pressure. In works [5, 6], a numerical study of the influence of the initial pressure of inert gas on the development of a spark discharge was carried out, where the influence of pressure on the efficiency of energy input into the spark discharge was revealed. At the same time, studies of processes that occur during spark initiation of detonation under different pressures of a hydrogen-oxygen gas mixture were not conducted.

The purpose of this work is to find out the influence of the initial pressure of the combustible mixture on the processes that occur during the initiation of detonation by a spark discharge in a high-pressure hydrogen-oxygen gas mixture.

1. A NUMERICAL MODEL OF THE SPARK DETONATION INITIATION

A one-dimensional gas-dynamic model in a chemically reacting gas with separation of the vibrational temperature of diatomic molecules from the kinetic temperature of the gas was used for the numerical study. In this case, the system of gas-dynamic equations are [5, 7]:

$$\frac{\partial \rho}{\partial t}+\frac{1}{r}\frac{\partial (r\rho u)}{\partial r}=0; \qquad (1)$$

$$\frac{\partial \rho u}{\partial t}+\frac{1}{r}\frac{\partial\left[r\left(p+\rho u^2\right)\right]}{\partial r}=\frac{p}{r}; \qquad (2)$$

$$\frac{\partial\left[\rho\varepsilon+\frac{\rho u^2}{2}\right]}{\partial t}+\frac{1}{r}\frac{\partial\left[r\left(u\left(\rho\varepsilon+\frac{\rho u^2}{2}+p\right)+k_T\frac{dT}{dt}\right)\right]}{\partial r}=\sigma E^2-\sum_x \dot{e}_x-W_{em}; \qquad (3)$$

$$\frac{\partial y_i}{\partial t}+\frac{1}{r}\frac{\partial (r u y_i)}{\partial r}=\omega_i,\ \ i=1\ldots 8; \qquad (4)$$

$$\frac{\partial y_x e_x}{\partial t} + \frac{1}{r}\frac{\partial (r u y_x e_x)}{\partial r} = y_x \dot{e}_x + e_x \omega_x, \ \ x = 1{,}2, \qquad (5)$$

where ρ is gas density; u is velocity, p is pressure, ε is the specific internal energy of the gas, k_T is thermal conductivity, E is electric field strength, σ is the electrical conductivity of the gas, W_{em} is radiative loss, r is the radial coordinate, t is time, T is gas temperature, y_i is the molar concentration of the i-th component (H_2, O_2, H_2O, H, O, OH, H_2O_2, HO_2), ω_i is the rate of change in concentration of the i-th component of the mixture caused chemical reactions, ω_x is source term for the vibrational energy, e_x is the vibrational energy of molecular oxygen and hydrogen (H_2, O_2).

A local thermal equilibrium model was applied to evaluate the electrical conductivity of gas in the region where the gas temperature exceeds 8000 K. Sahaionization equation was used for the calculation insingly ionized gas (hydrogen) and doubly-ionized oxygen. Other details of the numerical model are presented in [5].

During the investigation the capacitor capacitance was changed under the conditions of a change in the initial gas pressure to study the minimum total energy of the discharge leading to the detonation initiation (a critical regime). Other simulation conditions did not change. The specified conditions are given in Table 1.

Table 1

Fixed simulation parameters

Conditions/parameters	Values
the gas mixture composition	$2H_2$+ O_2
initial gas temperature, K	300
the length of the spark gap, mm	3.5
the circuit inductance, µH	2
the circuit resistance, Ω	0.1
the capacitor charging voltage, kV	30
the energy used to form a conductive channel, mJ	14
the initial energy input radius, mm	0.05

The study of the detonation initiation in a stoichiometric hydrogen-oxygen gas mixture at room temperature was conducted. The initial pressure of the gas mixture was 0.304, 0.5067, 0.8106, and 1.013 MPa. A size of simulation grid was 50 µm. A time step was adaptive.

2. SIMULATION RESULTS

As a result of the calculation (equations (1)-(5)), the minimum capacitor capacitance was determined, depending on the initial gas pressure, at which detonation is initiated. The values of the calculated capacitance and the corresponding total discharge energy are presented in Table 2.

We observe from Table 2 that in the case of an increase in the initial gas pressure, there is a decrease in the total energy of the discharge to initiate detonation. We also have that the increase in the total energy of the discharge is not directly proportional to the decrease in pressure. At the same time, with increasing pressure, the difference in the change in the total energy of the discharge decreases. For example, an increase in pressure from 0.304 to 0.5067 MPa, that is, by a factor of 1.67, leads to a decrease in the total energy of the discharge from 75.15 to 12.6 J, that is, by a factor of 5.9. At the same time, an increase in pressure from 0.5067 to 1.013 MPa, i.e. 2 times, leads to a decrease in the total energy of the discharge from 12.6 to 4.05 J, i.e. 3.1 times. The revealed trend qualitatively coincides with the results of experimental studies of works [8, 9], according to the results of which a sharp decrease in the critical energy of detonation initiation was observed when the initial gas pressure is up to 0.5 MPa, and a slow decrease in the critical energy happens at higher gas pressure.

Table 2

Results of calculation of detonation initiation conditions at different initial gas pressures

The absolute pressure of the mixture, MPa	Capacitor capacitance, nF	Minimum total detonation initiation energy, J
0.304	$166 < C < 167$	$74.7 < Q_{total} < 75.15$
0.5067	$27 < C < 28$	$12.15 < Q_{total} < 12.6$
0.8106	$11 < C < 12$	$4.95 < Q_{total} < 5.4$
1.013	$8 < C < 9$	$3.6 < Q_{total} < 4.05$

Let us consider the process of initiation of detonation at different initial gas pressures in more detail. We will carry out the process comparison for the minimum total detonation initiation energy. The pressure distribution in a spark discharge, when the detonation initiation takes place, at the initial gas pressure of 1.013 and 0.3039 MPa are presented in Figs. 1, 2.

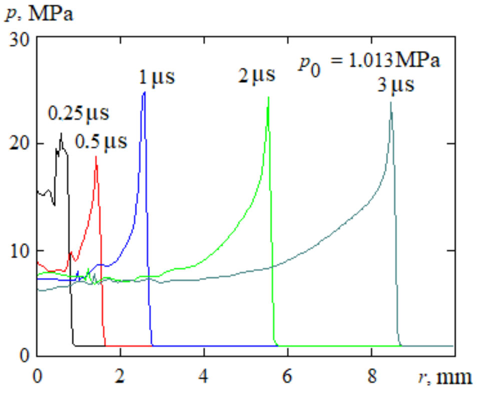

Fig. 1. Pressure distribution along the radial coordinate at different time under the conditions of initiation of detonation at an initial pressure of 1.013 MPa

We observe that the maximum pressure in the shock wave practically does not change at 1, 2, and 3 µs. This indicates the propagation of the detonation wave in the mixture. The increase in pressure in the shock wave relative to the initial pressure occurs 23...25 times. Based on the results of research in [8], under the conditions of an initial gas pressure of 1.013 MPa, a 21-fold increase in pressure in the detonation wave was calculated. That is, the results coincide with a deviation of 10...20 %, which confirms the reliability of the calculations.

Based on the comparison of pressure distributions at different initial gas pressures (see Figs. 1, 2), we have a difference in the shock wave, which leads to the initiation of detonation, in relation to the parameters of the detonation wave. In particular, at a lower initial pressure (p_0 = 0.3039 MPa), the maximum pressure in the shock wave exceeds the maximum pressure of the detonation wave for a time of 0.25 and 0.5 μs. Thus, the maximum pressure in the shock wave for a time of 0.25 μs equals more than 12 MPa, for a time of 0.5 μs this pressure equals more than 9 MPa (see Fig. 1). The maximum pressure in the detonation wave at an initial pressure of 0.3039 is equal to 7.5...8 MPa. In contrast to this pressure ratio, at the initial pressure p_0 = 1.013 MPa, the maximum pressure in the shock wave for the time of 0.25 and 0.5 μs is less than the maximum pressure of the detonation wave. Thus, the maximum pressure in the shock wave for a time of 0.25 μs equals more than 20 MPa, for a time of 0.5 μs this pressure equals more than 19 MPa (see Fig. 2). The maximum pressure in the detonation wave at an initial pressure of 1.013 is 24...25 MPa.

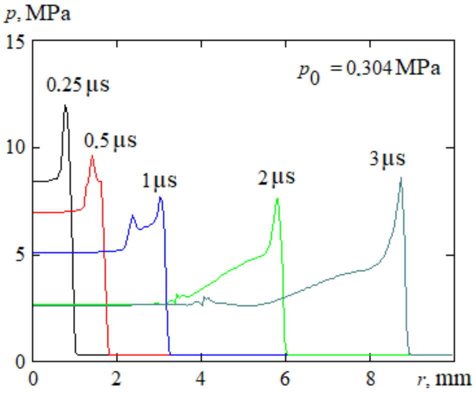

Fig. 2. Pressure distribution along the radial coordinate at different time under the conditions of initiation of detonation at an initial pressure of 0.304 MPa

It should be taken into account that the detonation wave is a shock-wave complex consisting of a shock wave, behind the front of which chemical reactions occur with a certain delay [10]. The thermodynamic state of the gas corresponds to the parameters of the detonation wave in the area of the chemical reactions. The delay in the chemical reactions behind the shock wave front is caused by the delay in the vibrational excitation of molecules, which reduces the rate of chemical reactions. Based on the evaluation of the delay, it is possible to determine the area of the achievement of the thermodynamic parameters of the gas corresponding to the Chapman-Jouguet condition. To determine the delay, we will use the results of the calculation of the change in the vibrational temperature of the gas. The results of calculating the distribution of kinetic and vibrational gas temperature at a time of 3 μs are presented in Fig. 3.

From the above results, we have a slight delay in the vibrational excitation of molecules behind the shock wave front, which is equal to 0.1…0.3 mm by a linear scale. But if we consider this delay on the pressure curve (see Fig. 1), we observe that the pressure rise is by a factor of 21 after this interval. Therefore, it is possible to assert that the calculation results of this work match the results of work [8].

We observe that when the energy of the spark discharge does not exceed the critical value, the intensity of the shock wave decreases during the development of the spark discharge. Thus, the profiles of pressure distribution in the spark discharge whena fall of detonation initiation happens at the initial gas pressure of 1.013 and 0.3039 MPa are provided in Figs. 4, 5.

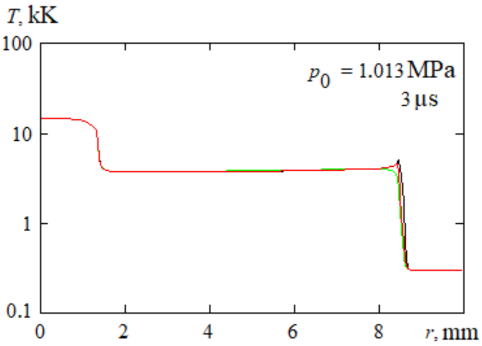

Fig. 3. Temperature distribution along the radial coordinate at different times by the detonation initiation at an initial pressure of 1.013 MPa: black color is the kinetic gas temperature; red color is the vibrational temperature of molecular oxygen; green color is the vibrational temperature of molecular hydrogen

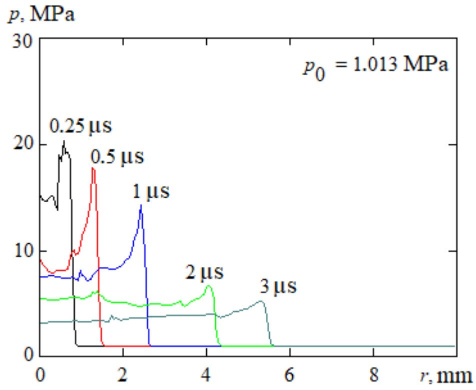

Fig. 4. Pressure distribution along the radial coordinate at different times at an initial pressure of 1.013 MPa when detonation initiation falls

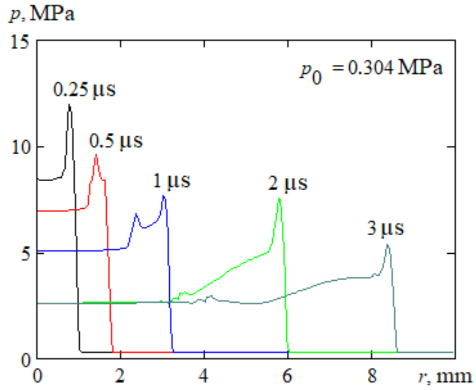

Fig. 5. Pressure distribution along the radial coordinate at different times at an initial pressure of 0.3039 MPa when detonation initiation falls

In both calculation variants, for different initial pressures of the gas, we observe a decrease in the intensity of the shock wave during the spark expansion. But at a lower initial pressure, the process of reducing the intensity is more extended in time. Longer attenuation of the wave with a decrease in pressure is caused by prolonged input of energy from the capacitor discharge. This is caused by an increase in the total energy of the discharge, at which the initiation of detonation is achieved, in case of a decrease in the initial pressure of the gas. Prolonged energy release of the spark discharge increases the chemical energy released behind the shock wave. As a result, we observe a slower attenuation of the shock wave in the event of a decrease in the initial pressure of the gas mixture.

The extended action of the shock wave, which initiates detonation, under the conditions of a decrease in the initial gas pressure, is caused by the expansion of the chemical reaction zone due to the increase in the delay in the vibrational excitation of molecules behind the front of the detonation wave. In particular, Figs. 6 and 7 show the change in the concentration of reactive components during the passage of a detonation wave through a gas mixture at different initial gas pressure. The distribution is presented for a time of 3 μs from the start of detonation initiation. The arrow shows the current position of the shock wave front. The width of the chemical reaction zone is highlighted by dotted lines.

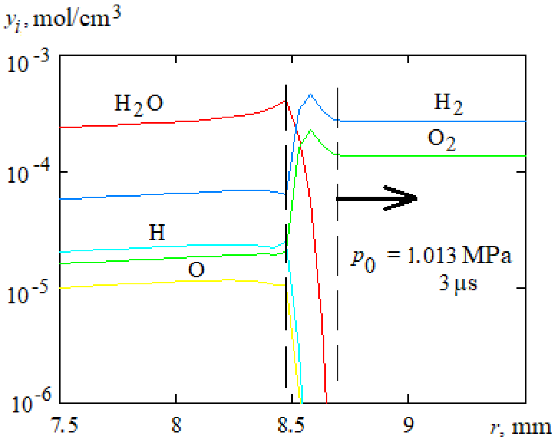

Fig. 6. Distribution of molar concentration of components along the front of the detonation wave at an initial gas pressure of 1.013 MPa

As a result of comparing the width of the chemical reaction zone during the propagation of the detonation wave in gas at different initial pressures (see Figs. 6 and 7), we observe an increase in the width of this zone in case of a decrease in the pressure of the gas charge. The approximate width of the chemical reaction zone, which includes the region of delay in the vibrational excitation of molecules, is equal to 0.2 mm at a pressure of 1.013 MPa (see Fig. 6) and 0.3 mm at a pressure of 0.304 MPa (see Fig. 7).

The slower rate of the chemical reaction behind the shock wave front in the case of a decrease in the initial pressure of the charge requires a prolonged action of the shock wave, which ensures the initiation of detonation.

Let's compare the energy input into the spark discharge over time at different initial gas pressures when detonation is initiated. The results of the discharge energy input calculation are presented in Fig. 8.

We observe that the input of energy at the initial stage of spark discharge development is practically the same at different initial gas pressures. Also, the growth of energy is practically linear in the section up to the critical time of detonation initiation. In particular, we observe a linear increase in energy up to a time of 0.25 μs under conditions of an initial pressure of 1.013 MPa and up to a time of 1 μs under conditions of an initial pressure of 0.304 MPa.

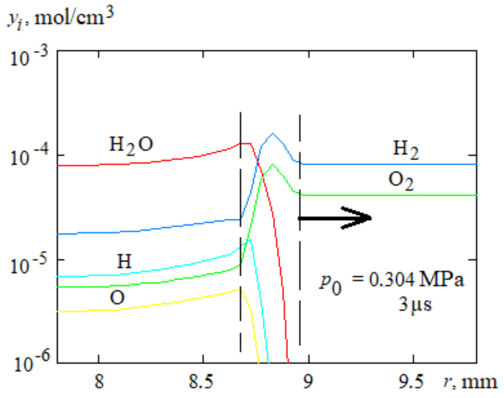

Fig. 7. Distribution of molar concentration of components along the front of the detonation wave at an initial gas pressure of 0.304 MPa

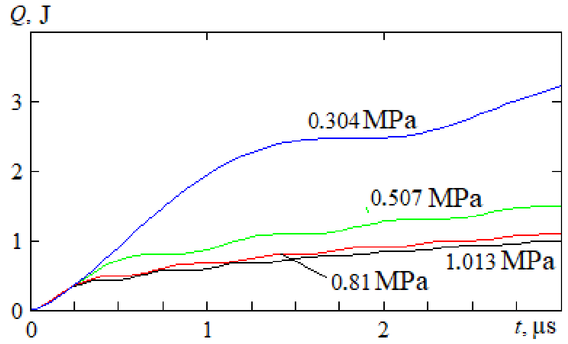

Fig. 8. Energy deposition history into the spark channel when detonation is initiated at different initial gas pressures

The deposition of energy into the spark channel is caused by the heat release which depends on the discharge current. Therefore, let's compare the currents that lead to the initiation of detonation at different initial gas pressures. The calculated currents are shown in Fig. 9.

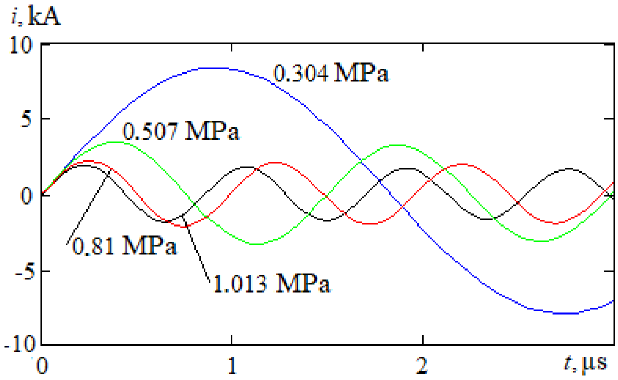

Fig. 9. Discharge currents when detonation is initiated at different initial gas pressures

According to the calculation results, we observe that the discharge currents in the initial time (from 0 to 0.2 μs) practically coincide. This explains the coincidence in energy input during this time interval (see Fig. 8). A time comparison of the discharge currents and energy input into the spark channel explains that the curves of step-by-step energy input into the discharge are caused by a current oscillation during the discharge.

The increase in the period of current oscillation during which detonation is initiated, in the case of a decrease in the pressure of the gas, is caused by an increase in the minimum value of the capacitance by which detonation is initiated. This is due to the non-variable inductance of the discharge circuit. Neglecting the attenuation of the current, the oscillation period in the LC-circuit is determined by the equation

$$T = 2\pi\sqrt{LC}. \tag{6}$$

From equation (6), we have that the growth of the period under conditions of growth of capacitance is caused by the constant inductance of the discharge circuit.

We also observe an increase in the current amplitude when the initial pressure of the gas decreases. Neglecting current damping, the current amplitude in the LC-circuit is given by equation

$$i_{max} = U_0\sqrt{\frac{C}{L}}. \tag{7}$$

From equation (7), we have that in the case of an increase in capacitance, at constant values of the capacitor charging voltage and inductance, the current amplitude increases.

From the discharge current (Fig. 9), we observe that the amplitudes of the first and subsequent periods of oscillations decrease gradually. However, the difference between the energy input during the first half-cycle of the discharge and the subsequent half-cycles is significant (see Fig. 8). In the paper [11], where the development of a spark discharge in oxygen was studied, it was found that this was caused by a significant excess of the resistance of the spark channel in the first half-cycle of the discharge in relation to the resistance of the spark channel in the subsequent periods of the discharge. To confirm this effect, a calculation of the change in resistance over time in a hydrogen-oxygen mixture was carried out. The results of the calculation of the change in the resistance of the spark channel at different initial gas pressures are presented in Fig. 10.

The results of these studies show that under the conditions of initiation of detonation, the resistance of the spark channel in the first half-cycle of the discharge exceeds this resistance in the subsequent periods of the discharge, regardless of the initial gas pressure.

Taking into account the influence of the resistance of the spark channel on the deposition of energy into the discharge, a comparison of the resistance history under conditions of initiation and the absence of initiation of detonation was made. The results of such a comparison for a discharge in a gas by a pressure of 1.013 MPa and a capacitor capacitance of 8 and 9 nF are presented in Fig. 11.

From the above results, we have that the spark resistance in the considered calculation cases have minor deviations, which can be explained by differences in discharge capacitance. Thus, the occurrence of a detonation wave does not lead to a significant effect on the resistance of the spark channel.

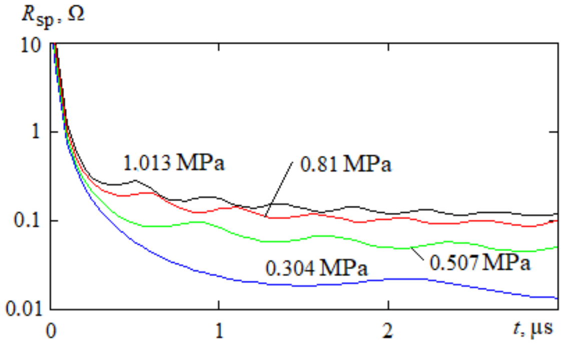

Fig. 10. Time history of the spark channel resistance when the detonation initiation is successful at different initial gas pressures

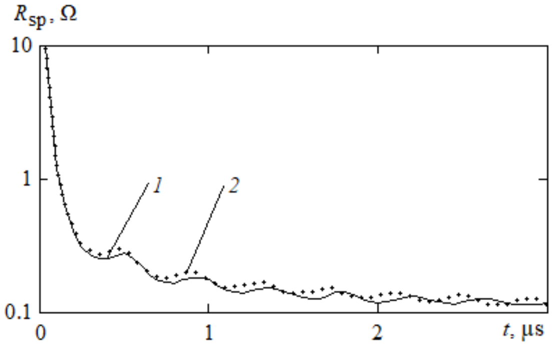

Fig. 11. Comparison of a time-variation of the resistance 1 of the spark channel when the detonation initiation occurs (solid curve) with resistance 2 when the detonation initiation falls (dotted curve)

The appearance of a detonation wave leads to an increase in the gas-dynamic flow. This is reflected in the change in the kinetic energy of the gas. Thus, a comparison of the kinetic energy in cases of occurrence and absence of detonation initiation allows us to approximately determine the critical time of detonation initiation. The results of the calculation of the change in the kinetic energy of the gas flow for the capacitor discharge with a capacity of 8 and 9 nF in a gas by a pressure of 1.013 MPa are presented in Fig. 12.

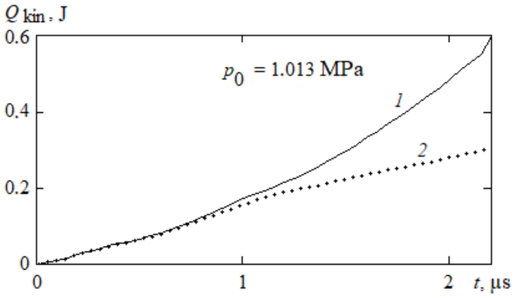

Fig. 12. Time history of the kinetic energy of the gas flow in a spark discharge with the capacitor capacitances of 9 nF (1 – solid line) and 8 nF (2 – dotted line) by an initial gas pressure of 1.013 MPa

From the obtained results, we observe that the growth of the difference between the kinetic energies in the considered calculation options is observed after 0.7...0.8 μs. With a capacitance of 8 nF, detonation does not occur, and with a capacitance of 9 nF, detonation occurs. This time corresponds to the critical time of detonation initiation. Thus, the results of such studies can be used to approximately determine the critical time of detonation initiation. At the same time, specifying the critical time requires additional calculations with interruption of the discharge current.

CONCLUSIONS

The influence of the initial pressure of the combustible gas mixture on the processes that occur during the initiation of detonation by a spark discharge in a high-pressure hydrogen-oxygen mixture was estimated. The minimum capacitor capacitance was determined, depending on the initial gas pressure, at which detonation is initiated. For example, an increase in pressure from 0.304 to 0.5067 MPa, that is, by a factor of 1.67, leads to a decrease in the total energy of the discharge from 75.15 to 12.6 J, that is, by a factor of 5.9. It was found out that a comparison of the kinetic energy in cases of occurrence and absence of detonation initiation allows us to approximately determine the critical time of detonation initiation.

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ЧИСЕЛЬНЕ ДОСЛІДЖЕННЯ ІНІЦІЮВАННЯ ДЕТОНАЦІЇ ІСКРОВИМ РОЗРЯДОМ У ВОДНЕВО-КИСНЕВІЙ ГАЗОВІЙ СУМІШІ ВИСОКОГО ТИСКУ

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Оцінено вплив початкового тиску горючої газової суміші на процеси, що відбуваються під час ініціювання детонації іскровим розрядом у воднево-кисневій суміші високого тиску. Для чисельного дослідження використано одновимірну газодинамічну модель у хімічно реагуючому газі з відокремленням коливальної температури двоатомних молекул від кінетичної температури газу. Виявлено, що інтенсивність ударної хвилі, що викликає ініціювання детонації у критичному режимі, є нижчою за інтенсивність хвилі детонації при початковому тиску газу 1,013 МПа, а інтенсивність ударної хвилі перевищує інтенсивність хвилі детонації при початковому тиску газу 0,304 МПа. Встановлено, що процес ініціювання детонації у критичному режимі є більш поздовжнім за низького тиску газу. Розраховано часову залежність вкладення енергії в іскровий канал при ініціюванні детонації за різного початкового тиску газу.