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NUMERICAL SIMULATION OF SPARK DETONATION INITIATION IN HIGH-PRESSURE HYDROGEN-OXYGEN MIXTURE BY VARIOUS EQUIVALENCE RATIOS

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The influence of equivalence ratio on the detonation initiation by spark discharge in high-pressure hydrogen-oxygen mixture in the critical mode was investigated. A one-dimensional gas-dynamic model in a chemically reacting gas was applied taking into account the influence of the delayed vibrational excitation of diatomic molecules behinds the shock wave on chemical reactions. The two gas mixture compositions were considered where equivalence ratios equaled α = 1 and α = 0.5. The minimal total energy of the spark discharge, causing the detonation initiation, reduces from 5.4 to 1.35 J when the equivalence ratio changes from α = 1 to α = 0.5. It was found out that a reduction in the total energy by decreasing in the equivalence ratio is caused by growth in the detonation sensitivity of the hydrogen-oxygen mixture via an acceleration of the vibrational excitation of diatomic molecules behinds the shock wave.

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INTRODUCTION

National Technical University "Kharkiv Polytechnic Institute" has developed a gas-detonation mortar, in which a mixture of fuel and oxygen is used instead of gunpowder to throw a smoke mine. The peculiarity of the throwing process in such mortars is due to the fact that throwing occurs due to the detonation of a mixture of fuel and oxygen, which is compressed before the initiation of detonation, and the initiation of detonation occurs from a spark discharge. The variation of response time of the fuel and oxidizer valves and the chaotic gas-dynamic process of the fuel-oxygen mixing, leads to a change in the concentration composition of the mixture in shots by similar conditions of combustible charge formation. As a result, the equivalence ratios may be different when mixing fuel with oxygen. Therefore, the influence of the equivalence ratio on the initiation of detonation by a spark discharge in a high-pressure fuel-oxygen mixture should be investigated. The various gas fuels such as hydrogen, propane, butane, etc. can be used in the mortar.

It is known that the equivalence ratio affects the minimum energy at which detonation initiation occurs. This minimum energy is commonly called critical energy. The study of the equivalence ratio influence on the critical energy of detonation initiation is presented in [1, 2]. According to the results of these studies, it was found that the critical energy does not have a minimum value in a stoichiometric combustible mixture, where the equivalence is equal to one. The minimum energy consumption for detonation initiation happens in the case of a slight decrease in the equivalence ratio. But the obtained research results relate to the initiation of detonation in gases at low pressure.

It is known that the initial pressure of the combustible mixture also affects the critical energy of detonation initiation. The results of the study of the influence of pressure on the critical energy are presented in [3 - 6]. However, these studies did not consider the influence of the equivalence ratio on the critical energy. Therefore, the study of the influence of the equivalence ratio on the critical detonation initiation energy in high-pressure combustible gas is relevant.

Spark initiation of detonation can be studied both experimentally and theoretically. In this work, a numerical study of the detonation initiation was carried out using a numerical model developed by K. Korytchenko and others [7 - 9]. The choice of this model is due to the fact that it is verified with the results of experimental studies given in [8].

The aim of this work is to identify the influence of equivalence ratio on the detonation initiation by spark discharge in high-pressure fuel-oxygen mixture in the critical regime.

A NUMERICAL MODEL OF THE SPARK DETONATION INITIATION

A one-dimensional gas-dynamic model in a chemically reacting gas was applied [10 - 12]. Two-temperature model was used to take into account the influence of the delayed vibrational excitation of diatomic molecules behinds the shock wave on chemical reactions. The following system of gas-dynamic equations was used:

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

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

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

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

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

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). Other equations of the numerical model are presented in [5 - 8].

During the investigation the capacitor capacitance was changed to find out 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.

Fixed simulation parameters

Conditions/parameters	Values
the initial gas temperature, K	300
the initial gas pressure, MPa	0.8106
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 two gas mixture compositions were used where equivalence ratios equaled α = 1 and α = 0.5. Thus, following chemical reactions were considered:

$$2H_2+O_2=2H_2O, \quad (6)$$

$$H_2+O_2=H_2O+½O_2. \quad (7)$$

A size of simulation grid was 50 μm. A time step was adaptive.

SIMULATION RESULTS

It was found out that the detonation initiation occurs in the chemical reaction by the equation (6) when the capacitor capacitance is C ≥ 12 nF. The failure of detonation happens by the equivalence ratio of α = 1 when C ≤ 11 nF. When the equivalence ratio was reduced to α = 0.5, the detonation initiation occurs by C ≥ 3 nF and the failure of detonation happens by C ≤ 2 nF. As a result, the minimal total energy of the spark discharge, causing the detonation initiation, reduces from 5.4 to 1.35 J when the equivalence ratio changes from α = 1 to α = 0.5. Thus, the critical regimes of the detonation initiation were considered. The conclusion about the detonation initiation or its failure was based on the consideration of the pressure history in the spark discharge. The result of the pressure history simulation for considered cases are given in Figs. 1 - 4. Numbers of the pressure profile in these figures correspond to the following time: 1 – 0.2 μs; 2 – 0.5 μs; 3 – 1 μs; 4 – 2 μs; 5 – 3 μs. It is observed that the pressure profile in the shock wave is practically the same at time of 2 and 3 μs in these figures. It allows us to assume that the detonation initiation takes place in Figs. 1, 3. When the failure of detonation happens it is observed the gradual pressure decrease in the pressure wave during the spark channel expansion in Figs. 2, 4.

Comparison of the pressure profiles at the detonation waves in Figs. 1, 3 at time of 2 and 3 μs shows that the maximum of the pressure reduces from 20 to 17.5 MPa when equivalence ratio fails from α = 1 to α = 0.5.

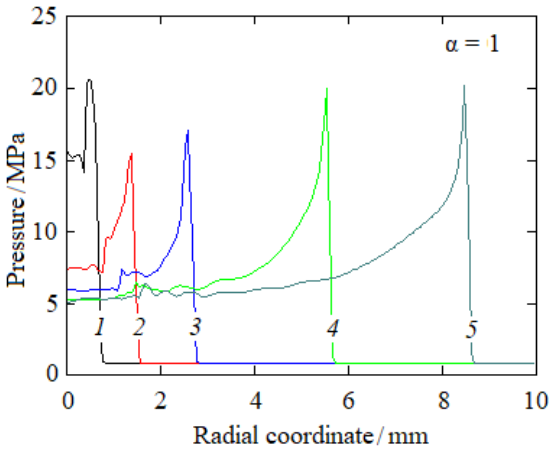

Fig. 1. Pressure history in the spark discharge by the detonation initiation when equivalence ratio is α = 1

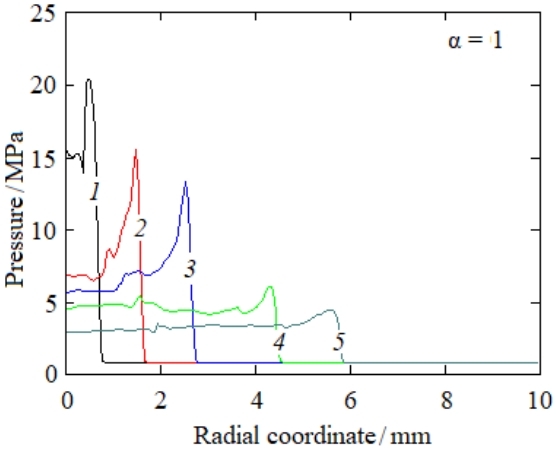

Fig. 2. Pressure history in the spark discharge by the failure of detonation when equivalence ratio is α = 1

It is observed a stable pressure profile of the detonation waves at time of 2 and 3 μs in Figs. 1, 3. Evaluating the location of a front of the detonation wave at these time points, velocities of the detonation wave were calculated.

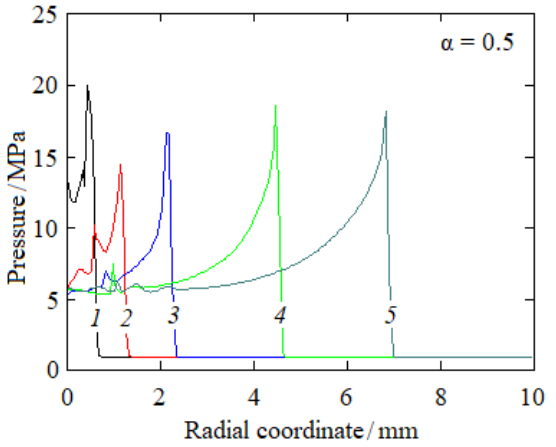

Fig. 3. Pressure history in the spark discharge by the detonation initiation when equivalence ratio is α = 0.5

When the equivalence ratio is α = 1, the detonation velocity is about 2900 m/s. The detonation velocity reduces to 2300 m/s by α = 0.5.

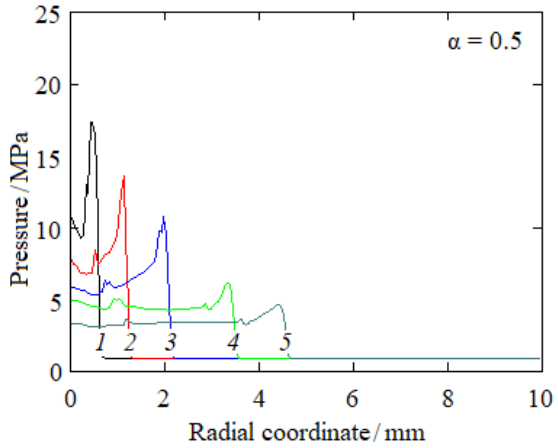

Fig. 4. Pressure history in the spark discharge by the failure of detonation when equivalence ratio is α = 0.5

An evolution of the temperature distributions along the radial coordinate in the spark discharge by α = 1 and α = 0.5 is presented in Figs. 5, 6.

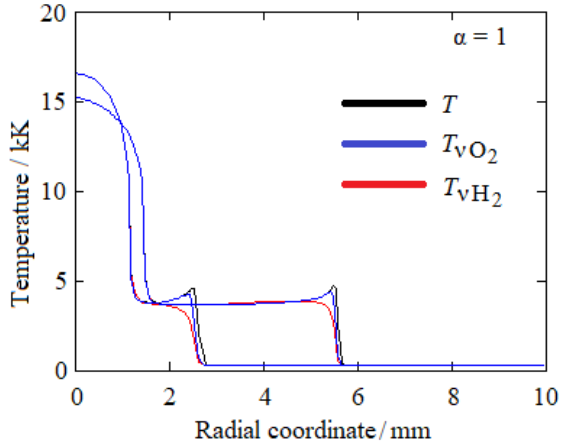

Fig. 5. Distribution of temperatures along the radial coordinate in the spark discharge at time of 1 and 2 μs when equivalence ratio is α = 1

Comparison of the distribution of vibrational temperatures in Fig. 5 shows that the vibrational excitation of the hydrogen is delayed comparing with the vibrational excitation of the oxygen when the equivalence ratio is α = 1. In contrast in Fig. 6, the vibrational excitation of the hydrogen precedes the vibrational excitation of the oxygen when the equivalence ratio is α = 0.5. It allows us to assume that a reduction in the total energy by decreasing in the equivalence ratio is caused by growth in the detonation sensitivity of the hydrogen-oxygen mixture via an acceleration of the vibrational excitation of diatomic molecules behinds the shock wave.

Comparison of the concentration distribution in the combustion region presented in Figs. 7, 8 shows that a concentration of molecular hydrogen exceeds a concentration of molecular oxygen when α = 1 in Fig. 7 in contrast to these values of the concentrations by α = 0.5 in Fig. 8.

Distributions of charged particle concentration along the radial coordinate in the spark discharge for α = 1 and α = 0.5 are given in Figs. 9, 10.

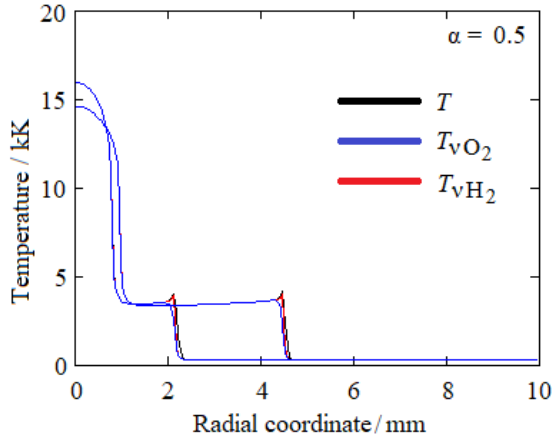

Fig. 6. Distribution of temperatures along the radial coordinate in the spark discharge at time of 1 and 2 μs when equivalence ratio is α = 0.5

Distributions of molar concentration of species along the radial coordinate in the spark discharge by α = 1 and α = 0.5 is presented in Figs. 7, 8.

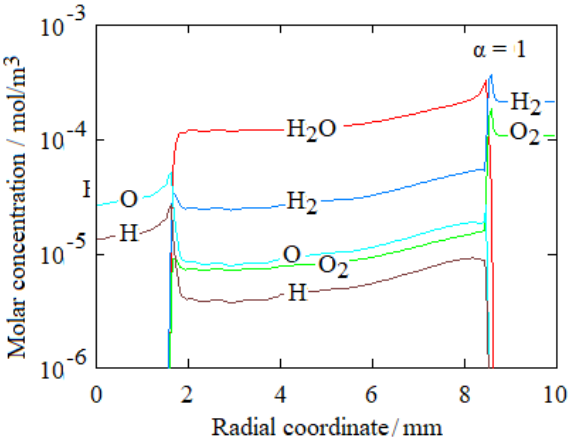

Fig. 7. Distribution of molar concentration of species along the radial coordinate in the spark discharge at time of 3 μs when equivalence ratio is α = 1

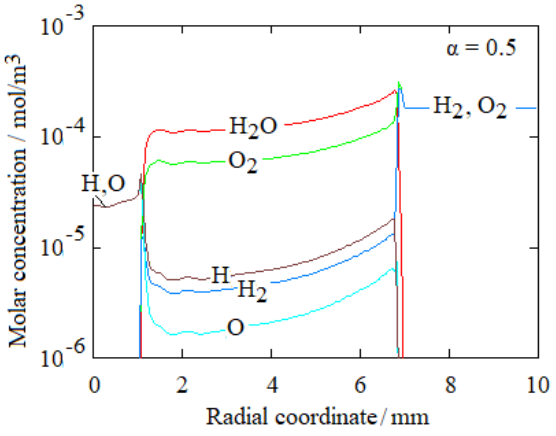

Fig. 8. Distribution of molar concentration of species along the radial coordinate in the spark discharge at time of 3 μs when equivalence ratio is α = 0.5

It is observed that the concentration of the hydrogen ions exceeds the concentration of the oxygen ions as by α = 1 as by α = 0.5. It can be explained by values of the ionization energy where the first ionization energy of hydrogen is 13.5984 eV that is slightly lower than the first ionization energy of oxygen (13.6181 eV).

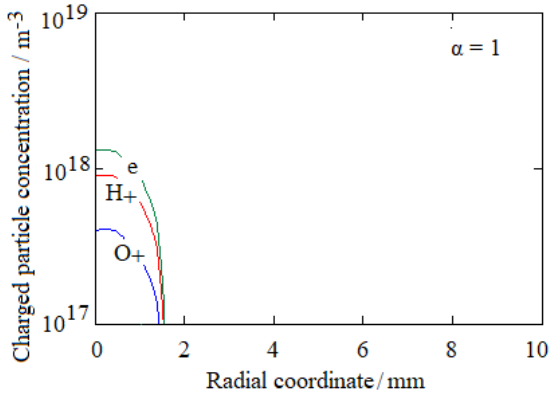

Fig. 9. Distribution of charged particle concentration along the radial coordinate in the spark discharge at time of 3 μs when equivalence ratio is α = 1

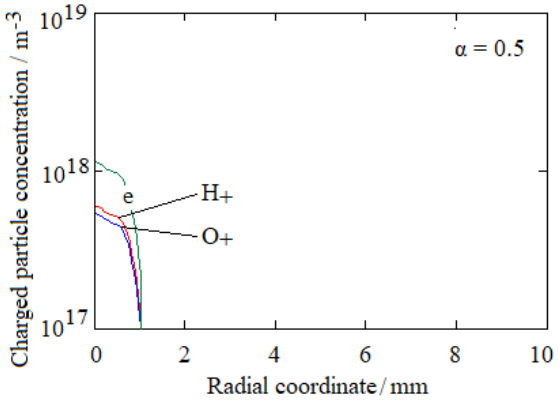

Fig. 10. Distribution of charged particle concentration along the radial coordinate in the spark discharge at time of 3 μs when equivalence ratio is α = 0.5

Histories of the energy deposition in the spark discharge and the spark resistance by various equivalence ratios are given in Figs. 11, 12.

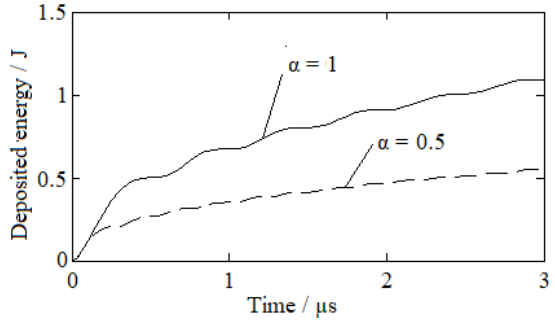

Fig. 11. History of the energy deposition in the spark discharge by various equivalence ratios

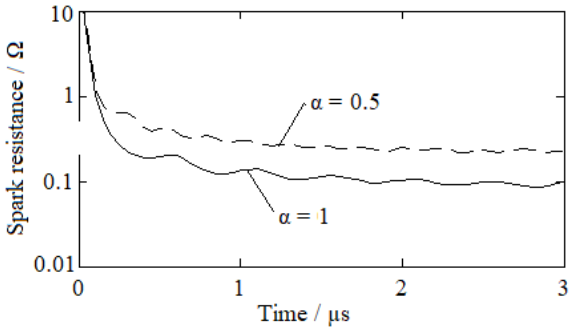

Fig. 12. History of the spark resistance by various equivalence ratios

Although the minimal total energy leading to detonation initiation when α = 1 exceeds this energy when α = 0.5 by a factor of 4, the deposited energy when α = 1 exceeds deposited energy when α = 0.5 by a factor of 2. It is caused by reducing in the spark resistance with growth of the total energy of the discharge.

CONCLUSIONS

The influence of equivalence ratio on the detonation initiation by spark discharge in high-pressure hydrogen-oxygen mixture in the critical mode was investigated. It was found out that the vibrational excitation of the hydrogen is delayed comparing with the vibrational excitation of the oxygen when the equivalence ratio is α = 1. In contrast, the vibrational excitation of the hydrogen precedes the vibrational excitation of the oxygen when the equivalence ratio is α = 0.5. The reduction in the total energy by decreasing in the equivalence ratio is caused by growth in the detonation sensitivity of the hydrogen-oxygen mixture via an acceleration of the vibrational excitation of diatomic molecules behinds the shock wave.

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ЧИСЛОВЕ МОДЕЛЮВАННЯ ІНІЦІЮВАННЯ ДЕТОНАЦІЇ ІСКРОВИМ РОЗРЯДОМ У СУМІШІ ВОДНЮ ТА КИСНЮ ВИСОКОГО ТИСКУ ЗА РІЗНОГО ФАКТОРА ЕКВІВАЛЕНТНОСТІ

Б.Г. Любарський, С.Ю. Кривошеєв, В.І. Галиця, О.В. Єресько, О.В. Сакун, Д.Б. Любарський

Досліджено вплив фактора еквівалентності на ініціювання детонації іскровим розрядом у водневокисневій суміші високого тиску в критичному режимі. Застосовано одновимірну газодинамічну модель у хімічно реагуючому газі з урахуванням впливу уповільненого коливального збудження двоатомних молекул за ударною хвилею на хімічні реакції. Розглянуто два склади газових сумішей, де фактор еквівалентності дорівнювали $\alpha = 1$ та $\alpha = 0{,}5$. Мінімальна повна енергія іскрового розряду, що викликає ініціювання детонації, зменшується з 5,4 до 1,35 Дж при зміні фактора еквівалентності з $\alpha = 1$ на $\alpha = 0{,}5$. Виявлено, що зменшення повної енергії при зменшенні фактора еквівалентності зумовлене зростанням детонаційної чутливості воднево-кисневої суміші через прискорення коливального збудження двоатомних молекул за ударною хвилею.