NUMERICAL SIMULATION OF THE ENERGY DISTRIBUTION INTO THE SPARK AT THE DIRECT DETONATION INITIATION

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A numerical model of the direct initiation of the detonation in gases exposed to the action of the spark discharge taking into consideration the retarded vibrational excitation of molecules behind the shock wave front has been developed. The calculations showed that the critical time of the energy input into the spark discharge is equal to the separation time of the shock wave from the current – conductive channel of the spark. The model allows for the prediction of the availability or unavailability of a direct initiation depending on the parameters of electrical discharge circuit.

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1. INTRODUCTION

Spark discharge is a simple sourse of direct detonation initiation in gases. However, the efficiency of total energy consumption for spark discharge initiation is very low. Low efficiency of spark discharge in the generation of shock wave was experimentally revealed by Ya. Zel'dovich et al. in 1956 [1]. Experimental confirmation for low efficiency of spark in the direct detonation initiation was obtained by R. Knystautas and J. Lee in 1975 [2]. In accordance with [3], the parameters of electrical circuit have influence on the total energy of detonation initiation. However, the methods which allow increasing efficiency of detonation initiation haven't been determined yet. To improve the efficiency of spark detonation initiation in gases, it is necessary to identify the interrelation between the parameters of the electrical circuit and the processes occurring in the spark channel. A lot of works have been analyzed, in which only the processes or only some part of the processes occuring at the spark detonation initiation were studied. Next, the mechanisms which determine basic interrelationships between the processes were identified. As a result, a model for the spark detonation initiation which allows predicting the presence or absence of initiation depending on the parameters of electrical discharge circuit was created. The developed model allows revealing the area, form, quantity and time at which the spark discharge energy is released or absorbed. The results of these studies are presented in the paper.

2. BASIC PROCESSES OCCURRING IN THE SPARK AT THE DETONATION INITIATION

Direct detonation initiation in gases is performed under the influence of the shock wave. In the spark discharge, the shock wave is formed after formation of highly-ionized conductive channel. In high-current spark discharges, the main energy release also occurs after formation of the channel. Therefore, detonation can be studied from the process of channel extension. Heating of the spark channel occurs under the action of current flowing through this channel. Therefore, the energy input into the conductive channel is determined by the parameters of electrical discharge circuit (e.g, *RLC*-circuit). The energy input leads to the temperature and pressure growth in the spark channel. This is accompanied by channel expansion as a result of mass transfer processes (gas dynamics processes) and heat transfer processes. In the high-temperature area, the heat transfer is most intensively provided due by radiation and electronic thermal conductivity. The increase of high-temperature area is accompanied by dissociation and ionization processes. Some part of the spark energy is emitted irreversibly from the discharge area. Due to supersonic expansion of the conductive channel, the gas mass travels outside the conductive channel. This expansion leads to the formation of a shock wave. Formation of the shock wave is followed by nonequilibrium chemical reactions accompanied by the release and absorption of chemical energy. The process of excitation of molecules behind the shock front influences the reaction rate. Detonation initiation

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occurs at the sufficient intensity of the shock wave. The area in which the main processes occur at the spark detonation initiation in gases is shown on Fig.1.

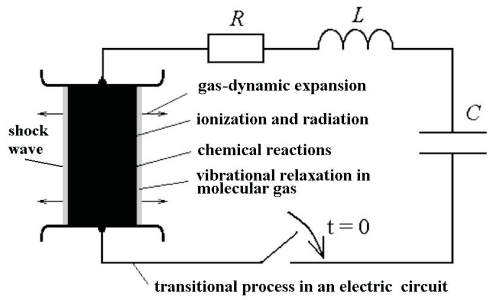

Fig.1. *Processes which determine expansion of the spark channel in reactive gases*

3. NUMERICAL MODEL OF THE SPARK DETONATION INITIATION

Slow vibrational excitation of molecules behind the shock front was not taken into account in the spark detonation initiation model which was developed earlier [4]. The earlier model results allowed correct description of energy transformation processes which occur in the spark discharge and discharge circuit. However, in accordance with simulation results, the initiation of detonation occurred at the discharge energy being several times smaller than the experimental data. To obtain results which are similar to the experimental results, the effect of vibrational temperature on the chemical reaction rate was taken into account. As a result, the following basic equations for detonation initiation model were obtained:

$$\frac{\partial \vec{a}}{\partial t} + \frac{1}{r}\frac{\partial r\vec{b}}{\partial r} = \frac{1}{r}\vec{f}, \qquad (1)$$

Where the column vectors are equal to:

$$\vec{a} = \begin{pmatrix} \rho \\ \rho u \\ \rho\varepsilon + \rho u^2/2 \\ y_i \\ y_x e_x \end{pmatrix},$$

$$\vec{b} = \begin{pmatrix} \rho u \\ p + \rho u^2 \\ u(\rho\varepsilon + \rho u^2/2 + p) + k_T dT/dr \\ u y_i \\ u y_x e_x \end{pmatrix},$$

$$\vec{f} = \begin{pmatrix} 0 \\ p \\ r(\sigma E^2 - \sum_x \frac{de_x}{dt} - Q_{em}) \\ r\dot{\omega}_i \\ r[y_x \frac{de_x}{dt} + e_x \dot{\omega}_x] \end{pmatrix}, \qquad (2)$$

where ρ is gas density, u is velocity, p is pressure, ε is internal energy per the mass unit (without taking into account the vibrational energy of the components H_2, O_2); k_T is heat conductivity coefficient; E is the electric field intensity in the column of the discharge channel; σ is plasma conductivity in the channel; Q_{em} is discharge energy loss for radiation; r is radius coordinate; T is gas temperature (translational and rotational); y_i is molar concentration of the i-th component (H_2, O_2, O_2O, H, O, OH, H_2O_2, HO_2); $\dot{\omega}_i$ is velocity of changing of the i-th component in mixture due to chemical reactions; $\dot{\omega}_x$ is velocity of charging the x-th mode due to chemical reactions; e_x is vibrational energy for 1 *mole* of the x-th mode (H_2,O_2); de_x/dt is velocity of changing specific vibrational energy of the x-th mode (H_2, O_2) as result vibrational and translational relaxation. It is assumed in the model that local thermodynamic equilibrium is set in the conductive channel. The processes occurring outside the conductive channel was calculated in accordance with non-equilibrium chemical kinetics of hydrogen combustion [5]. In reactions which don't involve the x-th mode, the rate constants of chemical reactions depend on the translational and rotational temperature T. In chemical reactions involving the x-th mode, the reaction rate depends on the effective temperature T_{ef} as follows:

$$k_k(T_{ef,x}) = A_k T_{ef}^{nk} exp[-\frac{E_{ak}}{kT_{ef,x}}], T_{ef,x} = T^s T_{v,x}^{1-s}, \qquad (3)$$

where $k_k(T_{ef,x})$ is the constant of the k-th reaction rate involving the x-th mode depending on the effective temperature; $T_{ef,x}$ is the effective temperature of the x-th mode; A_k, n_k, E_{ak} are the coefficients in generalized Arrhenius formula; s is the parameter of model; T is translational and rotational temperature; $T_{v,x}$ is rotational temperature of the x-th mode. The connection between the electrical processes in the discharge circuit and the processes which occur in the conductive channel of the spark was provided by the equations:

$$L\frac{di}{dt} + [R_c + R_{spark}(t)]i + \frac{1}{C}\int_0^t i dt = U_0, \qquad (4)$$

$$R_{spark} = l_{sp}(\int_0^{r_{sp}} 2\pi r\sigma dr)^{-1}, E = \frac{R_k}{i} l_k,$$

where C is electrical capacity of capacitor; R_c is active resistance of the discharge circuit; L is inductivity of the discharge circuit; U_0 is initial voltage of capacitor charge; l_{sp} is length of discharge gap (channel)); r_{sp} is radius of conductive channel; i is discharge current. See [4, 6] for more detailed information about the model.

4. RESULTS OF NUMERICAL SIMULATION

Testing of the model was carried out in accordance with the experimental results obtained by V. Kamenskihs and J. Lee [7]. The conditions of numerical study are presented in Table. The developed model allows understanding the reasons of detonation failure. Below there are the results of calculation in accordance with the simulation variant No.1 (Fig.2,a-d). In the variant N. 1, there was no detonation initiation.

Table 1: Simulation parameters

Initial simulation data	Simulation variant N1	Simulation variantN2
Active resistance, Ohm	0.1	0.1
Inductivity of discharge circuit, μH	0.9	0.9
Capacity, μF	2	2
Initial voltage of capacitor charge, kV	14	15
Length of discharge gap, mm	3.5	3.5
Detonation mixture	$H_2 + 0.5O_2$	$H_2 + 0.5O_2$
Initial thermodynamic parameters of mixture	Normal conditions	Normal conditions

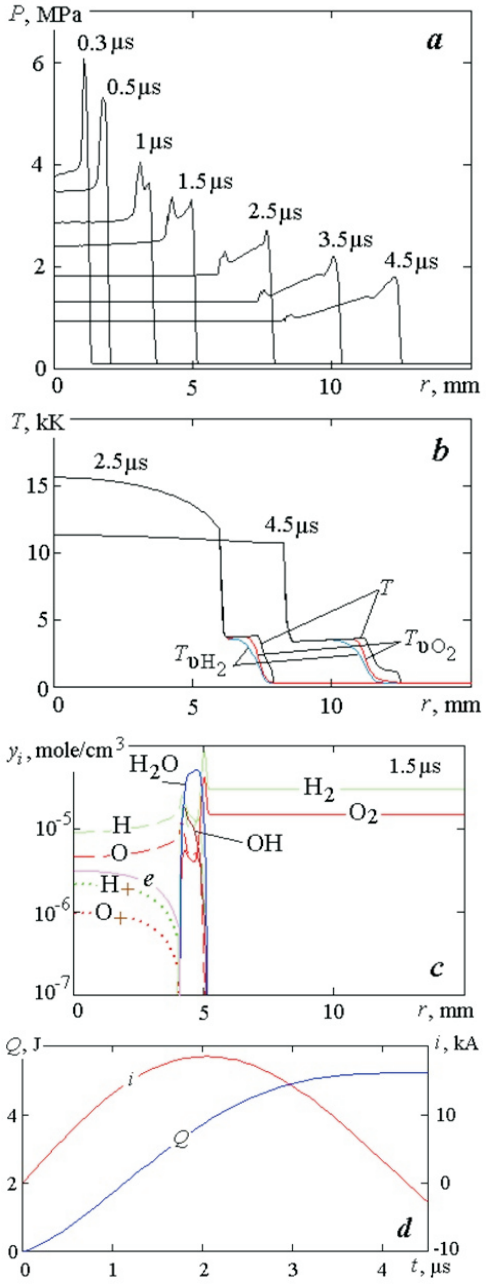

Fig.2. *The fields of pressure* (a)*, temperature* (b)*, concentration distribution at the time interval of* $1,5\,\mu s$ (c) *and energy* Q *input into the spark channel* (d) *in simulation variant N. 1*

This result corresponds to the experimental data of [7]. The failure of detonation initiation is explained as follows. The pressure distribution (Fig.2,a) shows that the parameters of the shock wave generated in the spark at the time interval up to $1\,\mu s$ are sufficient for detonation initiation. However, in this time interval there are almost no conditions for hydrogen combustion. Thus, the distribution of component concentration for the time of $1.5\,\mu s$ (Fig.2,c) and the pressure distribution up to this time show that the hydrogen combustion (emission of the chemical energy) occurs between the spark channel and the shock wave front. In the time interval up to $1\,\mu s$, the wave front coincides with the spark channel where $10000\,K$ gas temperature is reached. The area between the shock front and the conductive channel is expanded after $1\,\mu s$. Hydrogen combustion occurs in this area. However, the intensity of the shock wave at the time when the wave starts going away from the conductive channel was insufficient. As the intensity of the shock wave is reduced, the rate of vibrational relaxation is slowed down. Therefore, the increase in the distance between the shock wave front and the combustion front in the process of discharge initiation is observed (Fig.2,b). The energy input into the spark channel is slowed down as the energy approaches the first half-period of the discharge (Fig.2,d). Thus, the intensity of the shock wave decreases. This indicates the failure of direct detonation initiation.

The results of calculation of the simulation variant N. 2 are presented on Fig.3,a-d. In variant N. 2, the detonation is initiated. This corresponds to the experimental data of [7]. By the time of the shock wave separation from the conductive channel, which corresponds to the time of $1\,\mu s$, the jump in the pressure of the wave front reaches about $3.9\,MPa$ (see Fig.3,a). It should be noted that slow vibrational relaxation during simulation allows separation of the shock wave front from the detonation front. The width of the area where vibrational relaxation occurs is about $1\,mm$ (see Fig.3,b). The width of this area corresponds to the distance between the shock wave front and the detonation wave front. Comparison of the simulation results in accordance with two calculation options shows that the critical time of detonation initiation in relation to the spark discharge is equal to the time of shock wave separation from the spark channel. In the process of spark discharge development, the spark channel resistance is reduced by several orders of magnitude (see Fig.3,c).

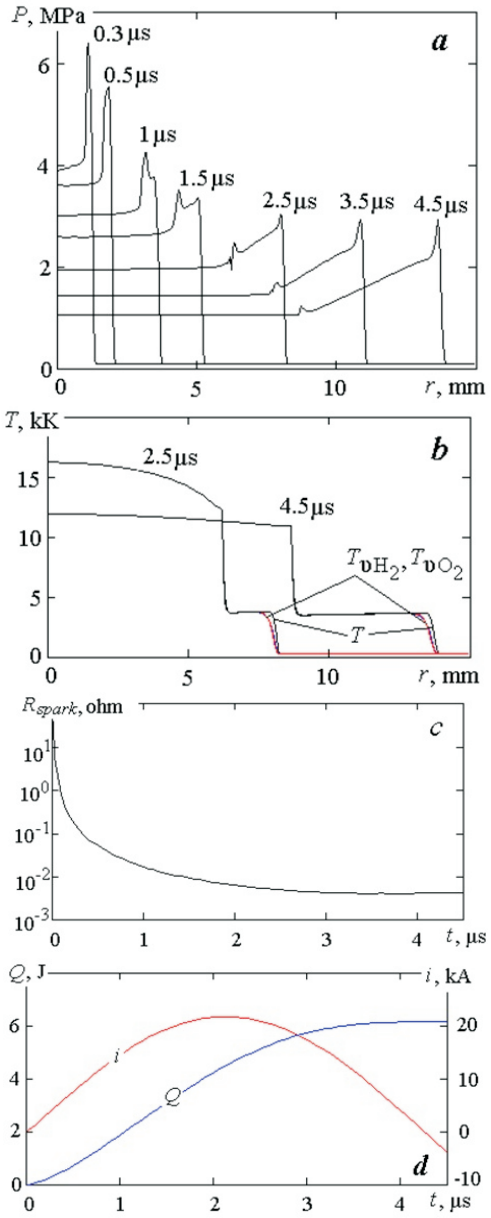

Fig.3. *The fields of pressure (a), temperature (b), change of resistance spar k(c) and input energy Q in the spark channel (d) in simulation variant N. 2*

Therefore, the usage of average resistance of spark in [7] at the calculation of effective energy input into the spark channel allow only approximate estimation of the energy value. If we assume that in the simulation variant N. 2 the effective energy corresponds to the detonation initiation energy (see Fig.3,d) introduced during $1-2\,\mu s$, this energy should be reduced to the unit length of the gap and will be $5-14\,J/cm$. In the simulation variant, the total energy was $225\,J$. The effective energy of detonation initiation wasn't more than $4.5\,J$.

Energy absorption and emission was studied in various processes. The combustion energy starts exceeding the energy introduced into the spark in $3.5\,\mu s$ (see Fig.4). The transition occurs at the energy of about $6\,J$. The main part of the discharge energy in the process of detonation initiation is absorbed by the dissociation process. It is followed by the energy consumption for the ionization process. Some part of the discharge energy is irrecoverably spent for radiation.

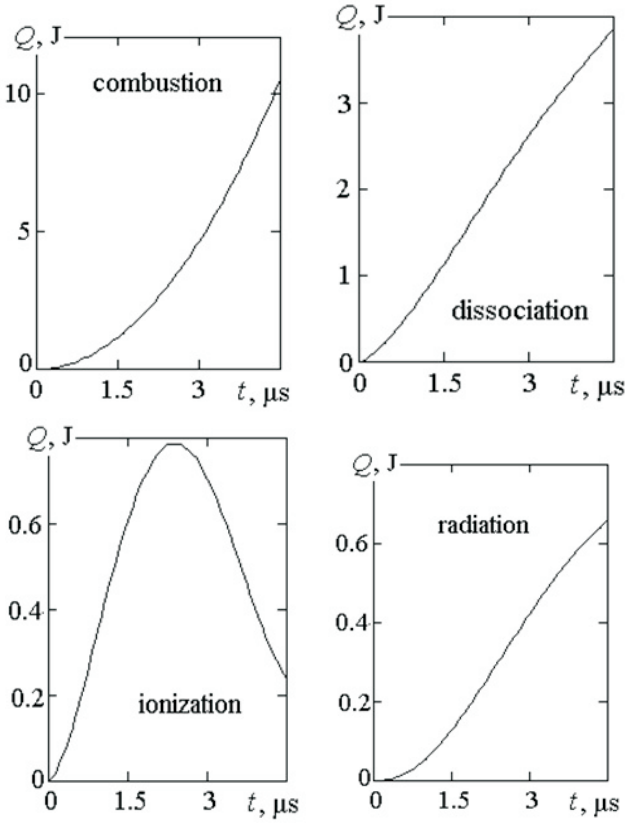

Fig.4. *Changes of energy released or absorbed by different processes in time in simulation variant N. 2*

Thus, the numerical investigations allowed specifying the area, form, quantity, and time at which the spark discharge energy is released or absorbed. The developed model will be used to increase the efficiency of the electro discharge method for detonation initiation.

References

1. Ya.B. Zel'dovich, C.M. Kogarko, N.N. Simonov. Experimental investigation of spherical detonation // *Soviet Journal of Technical physics.* 1956, v.26 (8), p.1744-1756.

2. R. Knystautas, JHS. Lee. On the effective energy for direct initiation of gaseous detonations // *Combustion and flame.* 1976, v.27, p.221-230.

3. V. Levin, et al. Initiation of gas detonation by means of electrical discharge // *Proc. Of International Symposium on Combustion and Atmospheric Pollution..* 2003, p.290-293.

4. K.V. Korytchenko, E.V. Poklonskiy, P. Krivosheyev. Model of the spark discharge initiation of detonation in a mixture of hydrogen with oxygen // *Russian Journal on Physical Chemistry.* B. 2014, v.8(5), p.692-700.

5. E.L. Petersen, R.K. Hanson. Reduced kinetics mechanisms for ram accelerator combustion // *Journal of Propulsion and power.* 1999, v.15(4), p.591-601.

6. K.V. Korytchenko, E.V. Poklonskiy, D.V. Vinnikov, D.V. Kudin. Numerical simulation of gasdynamic stage of spark discharge in oxygen // *Problems of Atomic Science and Technology.* 2013, N4(86), p.155-161.

7. V. Kamenskihs, JHS. Lee. Measurement of critical energy for direct initiation of spherical detonations in stoichiometric high-pressure H2-O2 mixture *Proc. 22nd ICDERS.* 2009, p.157-159.

ЧИСЛЕННОЕ МОДЕЛИРОВАНИЕ РАСПРЕДЕЛЕНИЯ ЭНЕРГИИ В ИСКРОВОМ РАЗРЯДЕ ПРИ ПРЯМОМ ИНИЦИИРОВАНИИ ДЕТОНАЦИИ

К. В. Корытченко, В. И. Голота, Д. В. Кудин, А. В. Сакун

Разработана численная модель прямого инициирования детонации в газах искровым разрядом, учитывающая замедленное колебательное возбуждение молекул за фронтом ударной волны. Рассчитано, что критическое время введения энергии в искровой разряд равняется времени отрыва ударной волны от токопроводящего канала искры. Модель позволяет предсказать наличие или отсутствие прямого инициирования в зависимости от параметров электрической разрядной цепи.

ЧИСЕЛЬНЕ МОДЕЛЮВАННЯ РОЗПОДІЛУ ЕНЕРГІЇ В ІСКРОВОМУ РОЗРЯДІ ПІД ЧАС ПРЯМОГО ІНІЦІЮВАННЯ ДЕТОНАЦІЇ

К. В. Коритченко, В. І. Голота, Д. В. Кудін, О. В. Сакун

Розроблена чисельна модель прямого ініціювання детонації в газах іскровим розрядом, яка враховує уповільнене коливальне збудження молекул за фронтом ударної хвилі. Розраховано, що критичний час введення енергії в іскровий розряд дорівнює часу відриву ударної хвилі від струмопровідного каналу іскри. Модель дозволяє передбачити наявність або відсутність прямого ініціювання залежно від параметрів електричного розрядного кола.