Detonation initiation assisted with pre-excitation of the reactive medium by non-equilibrium plasma

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1 Introduction

Recently the several approaches were proposed to use the non-equilibrium plasma to initiate detonation in pulsed detonation engines, operating on conventional but the weakly sensitive to detonation hydrocarbon fuels. In [1] the nanosecond discharge in the form of fast ionization wave was used to initiate detonation in the stoichiometric propane-oxygen mixture at pressures below atmospheric (0.2 – 0.6 atm) and energy depositions of the order of 0.1 - 10 J depending on the fraction of the nitrogen in the mixture (from 12% to 60%). Authors of [2] used pulsed corona discharge to ignite the ethylene- and propane-air mixtures (atmospheric pressure) at several points inside the shock tube and thus accelerate the deflagration-to-detonation transition due to more rapid pressure increase inside the ignition section. The energy deposition by plasma was about 0.6 J and only deflagration-to-detonation with the run-up distance about 1 m was observed. Both techniques [1, 2] used the plasma to directly ignite the reactive mixture, which required extremely high over-voltages and relatively high energy input. The required parameters of the electrical discharges could be achieved only with the specially designed complex techniques and infrastructure.

The compromise between the energy cost of the detonation initiation and complexity of the installation could be achieved by combining the classical method of detonation initiation [3], e.g. shock wave from the spark, and increase of the chemical activity of the reactive medium in local inhomogeneities [4]. Such local pre-excitation of the medium can be intentionally achieved with the non-equilibrium plasma. The usefulness of this approach was demonstrated experimentally in [5], where the pulsed corona chemically excited the propane-oxygen-nitrogen mixture at atmospheric pressure, while the conventional spark was used for ignition/detonation initiation. This technique allowed to initiate detonation in stoichiometric propane/butane-oxygen mixture diluted with up to 50% of nitrogen with overall energy deposition (pulsed corona and spark) 0.5 J and at short distance (less than 0.2 m).

The main argument for application of the non-equilibrium plasma in detonation initiation is related with the observation, that such plasma can produce chemically active species which broaden the ignition limits and reduce the ignition delays [1] thus stimulating the detonation initiation. But the detonation formation is a non-stationary process of coupling between the leading shock wave and ignition front. Therefore even for the qualitative judgement about the result of the coupling not only the chemical but gas dynamical processes and their mutual influence should be taken into account.

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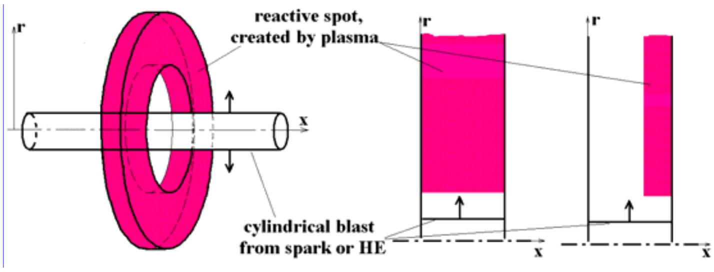
In the present work the theoretical investigation of the detonation initiation process by a shock wave, propagating in reactive gas, preliminary excited by the non-equilibrium plasma is carried out. It is based on computational fluid dynamics simulations of the detonation initiation with detailed account for the increased chemical activity of the reactive gas by localized (in space) plasma pre-excitation.

2 Problem description

As it was shown in [5], the preliminary chemical activation of the reactive mixture by non-equilibrium plasma could significantly reduce the critical conditions for the detonation initiation by sparks. Bearing this in mind, we consider a model problem of detonation initiation by the shock waves, produced by sparks or high explosives, in the reactive medium, where the plasma have already created some inhomogeneities in chemical properties – reactive spots, i.e. pre-excited the medium.

The 2D cylindrically symmetric situation is considered (see Figure 1). The detonation in the stoichiometric propane-oxygen mixture diluted with 45% of nitrogen at atmospheric conditions (298K, 1 atm) is initiated by a shock wave from cylindrical high-pressure region with temperature 3000K and pressure P_e varied to adjust the energy E_e, deposited in to the blast wave; its radius r_e = 0.5 mm.

The region exposed by plasma is placed on the distance L from the center of the high-pressure region. Two cases are analyzed separately. The first one examines the situation, when this region is assumed as infinite along the axis of symmetry and the problem can be treated as 1D effectively (though the 2D simulation is conducted). The second one examines the situation, when the region with increased chemical activity is finite in axial direction and its width is equal to 1 mm. The length of this region in the radial direction is equal to 10 mm.



Примечание [KIA1]: Add Case 1, Case 2 in Figure 1

Figure 1. Schematic representation of the direct initiation of detonation by blast wave after preliminary plasma action. Two-dimensional cylindrical symmetry.

Detonation initiation process is described by 2D axis-symmetric system of Euler equations with chemical reactions source terms. The numerical solution of the Euler equations was obtained with the computational software CFD++® of Metacomp, Inc. At the side boundaries of the computational domain the symmetry plane boundary conditions were set. The size of the computational domain was chosen to be 1.5 mm in axial direction, 10 mm in radial direction, the mesh spacing $5\cdot10^{-4}$ mm.

The combustion of the propane and oxygen in the main mixture is described by one-step reaction

$$C_3H_8 + O_2 = CO_2 + H_2O,$$
$$w = K\cdot[C_3H_8]\cdot[O_2],\ K = k\cdot\exp(-E_a/RT)\ \mathrm{cm^3/(mol\cdot s)},\ k = 3.5\cdot10^{14}\ \mathrm{cm^3/(mol\cdot s)},\ E_a = 190\ \mathrm{kJ/mol},$$

which is consistent with experimental correlation on ignition delay time in propane.

The action of the non-equilibrium plasma on reactive medium results in the generation of the active particles (atoms, radicals). It results in shorter ignition delay time behind incident shock wave compared with the main mixture. To describe this plasma-induced effect the new values of the rate constant k' and activation energy E_a' of the reaction were introduced. The special procedure for calculation of the k' and E_a' was developed with the aid of Chemical Workbench® software suite of Kintech Lab, Ltd. It included simulation of the non-equilibrium plasma of the pulse discharge to calculate the mixture composition after the plasma action; simulation of the ignition delay time of the mixture with the modified composition at elevated conditions similar to that behind blast wave; calculation of the k' and E_a' on the basis of the known k and E_a. For example, at the discharge energy input 136 J/g the new effective values are $k' = 10^{12}$ cm^3/(mol·s), E_a'= 76 kJ/mol, the reaction rate after plasma action increases in 3 – 20 times for the temperatures from 1300 K up to 2000 K.

3 Results

Homogeneous medium. It is well known that there is a critical value E_e^* of the energy deposited into the blast wave below which no detonation initiation is observed. For the mixture and conditions under consideration the parametric simulations were conducted, which gave $E_e^* \approx 3.2$ J/cm.

Medium with the reactive spots created by non-equilibrium plasma. Let us consider the case when the blast energy is equal to 0.4 J/cm and no detonation initiation in homogeneous medium is observed.

Results of the simulations in the inhomogeneous medium when the plasma created extended region along the symmetry axis, L = 1 mm, (Figure 1, middle picture) are presented on the Figure 2. The problem is effectively 1D and the pressure and temperature distributions are given along the line with x = 0. It is seen that after several oscillations of the leading front (pressure oscillated between 70 atm and 120 atm), the shock wave and ignition front decouple each other and detonation fails. This means, that even under the plasma action the 1D case under consideration is under-critical.

Additional set of the simulations allowed to estimate a critical value of the direct initiation energy in that case E_{e1d}^* = 1 J/cm (compare with E_e^* = 3.2 J/cm, i.e. three times less).

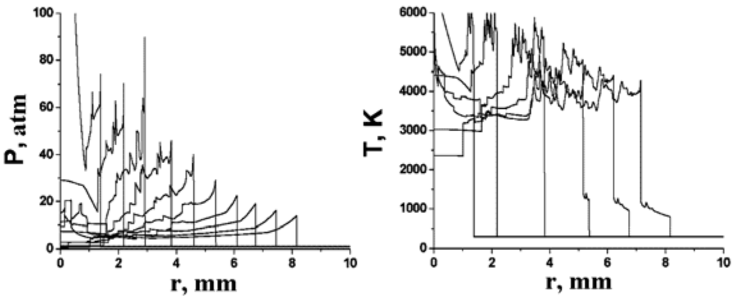


Figure 2. Pressure and temperature profiles in the process of the direct detonation initiation in the medium with extended (along symmetry axis) region of the plasma action. E_e = 0.4 J/cm, L = 1 mm.

Results of the simulation, when the plasma created the region, localized in axial direction and on the distance L = 1 mm from the axis (Figure 1, right picture), are presented on the Figure 3. It is seen that just after the interaction of the overdriven detonation wave from blast with the local inhomogeneity (reactive spot created by plasma) the flow structure becomes two-dimensional: the transversal disturbances are formed, amplified and become transversal detonation waves. The origin of these waves is the disturbance of the subsonic (with respect to leading shock) reaction zone and in consequence of the leading shock of the detonation front. At the position, where the 1D model (Figure 2) fails, the multidimensional detonation still propagates.

Further evolution proceeds in essentially two-dimensional manner with propagation and leading shock wave and ignition front decoupling, propagation of the transversal waves, their collisions and re-initiation of the detonation. Thus, this case is supercritical – the detonation is initiated as a multi-front wave.

Additional set of the parametric simulations allowed to estimate a critical value of the direct initiation energy E_{e2sd}^* = 0.3 J/cm (L = 0.5 mm), E_{e2d}^* = 0.4 J/cm (L = 3.5 mm), which is considerably less then E_{e1d}^* and E_e^*. If $L > r^*$ then the $E_{e2d}^* = E_{e1d}^* = E_e^*$ and r^* is the distance, where the leading shock and ignition front decouple in the case of homogeneous medium.

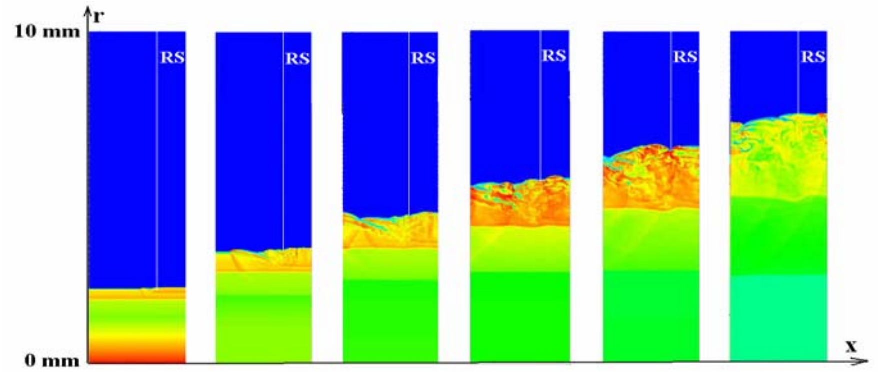


Figure 3. 2D temperature plots, demonstrating the successful direct detonation initiation in the medium with finite (along symmetry axis) region of the plasma action. E_e = 0.4 J/cm, L = 1 mm, RS – reactive spot.

4 Conclusions

As it was demonstrated in [5], the pre-excitation of the reactive medium by non-equilibrium plasma could be a cost-effective way to stimulate and accelerate the detonation initiation by conventional techniques. The present theoretical work focuses on the role of the stimulating effect of the non-equilibrium plasma in detonation initiation process. As example the shock wave initiation of gaseous detonation in the presence of the reactive spots (after plasma action) is considered.

It was shown, that pre-excitation of the reactive medium by plasma can actually result in appreciable reduction of the critical energy of the detonation initiation by the shock waves – order of magnitude, when the inhomogeneities are local in the direction, transversal to propagation of the blast wave. In that case the extension of the limits of detonation initiation is due to plasma activation of the reactive mixture. This results in disturbance of the reaction zone of the propagating overdriven detonation (blast wave) and subsequent transition to multi-headed detonation front structure.

The results obtained show that usually used qualitative explanations of the plasma effect on detonation formation process, based on chemical kinetics analysis, are not sufficient because other agents – shock waves – are not allowed for. The present simulations (2D vs. 1D) show, that the gas dynamic waves could be important part of the detonation formation process and only their interaction with the chemical processes can correctly describe the detonation formation assisted with non-equilibrium plasma.

This work was partially supported by RFBR grant 08-07-13557-ofi_c.

References

[1] E.N.Kukaev, D.L.Tsyganov, V.P.Zhukov, S.M.Starikovskaia, A.Yu.Starikovskii (2004). AIAA Paper 2004-0870.

[2] Wang F., Jiang C., Kuthi A., Gundersen M., Brophy C., Sinibaldi J., Lee L. (2004). AIAA Paper 2004-0834.

[3] J.H.S. Lee (1977). Annual Review of Physical Chemistry, Vol. 28, pp. 75 – 104.

[4] A.A. Borisov (1974), Acta Astron, Vol. 1, pp. 909–20.

[5] A.A. Borisov, A.F. Galkin, V.K. Zhivotov, S.A. Zaitsev, G.M. Konovalov, S.V. Korobtsev, M.F. Krotov, D.D. Medvedev, B.V. Potapkin, R.V. Smirnov (2007). High Energy Chemistry, Vol. 41, No 5.