Mathematical modeling of detonation wave suppression by cloud of chemically inert solid particles

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1 Problem statement

Lets consider the shock tube, divided into two chambers: high pressure chamber (HPC), at initial moment filled by medium with high parameters of state ($p_1 = 20$ atm, $T_1 = 2000$ K) and low pressure chamber (LPC), $p_0 = 1$ atm, $T_0 = 300$ K, filled by mixture of hydrogen, methane, oxygen and particles distributed in space. After the rupture of the diaphragm, which separates these chambers, begins the process of gas outflow in LPC, in which the contact discontinuity and shock wave (SW) spreads. The latter transforms to detonation wave (DW), suppressing by cold particles. The problem of DW initiation, attenuation and quenching in a mixture of a gas with chemically inert particles has been considered in the frames of nonstationary, one-dimensional, two-velocity and two-temperature model. Chemical reaction in a gas has been described by the detailed system of kinetic equations. Equations for hydrogen oxidation are presented in [1], for methane oxidation the modification of scheme [2] is used.

2 Influence of particles amount on detonation velocity

Parameters of DW in $2H_2 + O_2$ mixtures in motionless filter of SiO_2 particles have been calculated. Fig. 1 shows the calculated value – $\eta = D/D_{CJ}$ versus mass concentration of particles ξ_2; D and D_{CJ} are detonation velocities in gas-particles mixture and Chapman - Jouguet velocity of DW in gas without particles respectively. It is interesting to compare the integral curves of detonation suppression $\eta = \eta(\xi_2)$, obtained for argon and particles. It can be seen that the increase of particles concentration, as well as the growth of the mass concentration of argon leads to decrease of detonation velocity. Particles with diameter d = 1 μm are the most effective for detonation suppression. These results correspond to experimental data, presented in [3]. Relatively big particles (100 μm in diameter) suppress detonation in the same way as it occurs in a mixture with Ar additions. The same figure shows data [4] (mixture of propane with WC). These results correspond to our calculations too. Crossed-markers in the figure correspond to particle mass concentration limits of detonation. For 10 μm and 100 μm particles, these values are 0.33 and 0.88. It corresponds to the critical volume concentration of particles $m_2^* = 2 \cdot 10^{-4}$ and $m_2^* = 2 \cdot 10^{-3}$ respectively. At such conditions classical

DW structure transforms into frozen shock wave (FSW) and subsequent wave of ignition and combustion (WIC).

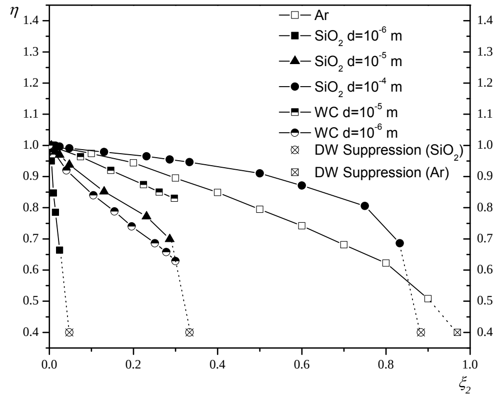

Fig. 1. The dependence of detonation wave velocity deficit on mass concentration of inert components.

Moreover the parameters of DW in $2H_2 + O_2$ mixtures in motile cloud of SiO_2 particles have been calculated. Fig. 2 shows the dependencies of the deficit of the detonation velocity on particle volume concentration for particles with diameter of 10 and 100 μm, designed for motile cloud and motionless filter. It is seen that in the low-volume concentration of the particles these dependences are not very different. The differences begin when the volume concentration approaches to the critical value. Moreover, the smaller the particles, the more different concentration limits. For a 100-micron particles limits differ by 2.5 times and for 10 microns by 5 times. This is explained as follows. Energy weaning from the gas mixture due to gas-particles friction is maximal in the case of DW suppression by motionless particles filter, as in this case, the difference between the velocities of gas and particles is maximal. In the case of motile cloud of particles, this difference will be smaller, and, in addition, will decrease with decreasing the particle diameter. This will reduce the energy weaning from the gas phase and, therefore, the curves of the detonation velocity deficit will be above (Fig. 2) the curves plotted for particle filter. In addition, with decreasing the diameter of the particles the increasing of difference in the concentration limits, obtained for the cloud and particle filter, will occur.

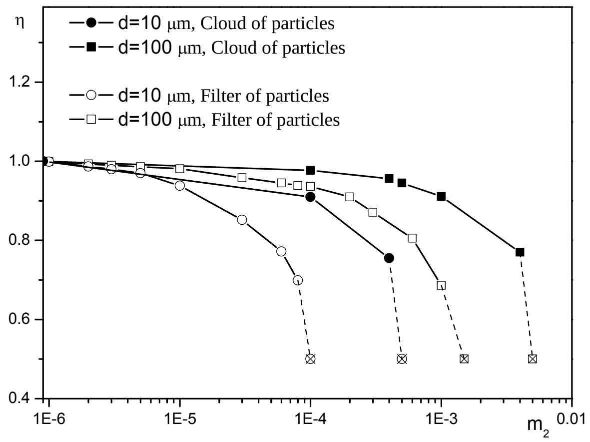

Fig. 2. The dependence of detonation wave velocity deficit on volume concentration of inert particles. Comparison of the data obtained for filter and for cloud of particles.

3 Determination of critical length of inert particle filter and cloud

In addition to determine the concentration limits of detonation (for the mass concentration of particles) it is an important task to determine the length of the particle filter and cloud, which quenches the DW. This length will be called as critical - L_*. Clouds and filters with subcritical length does not quench the DW. If the particle cloud length is less than critical reinitiation of DW behind the cloud occurs. The calculations with filter of 100 μm particles shows, that critical length of this filter is equal to 30 cm. Thus shown the two possible regimes of flow, realized after wave complex consisting of FSW and WIC leaving the filter: reinitiation of detonation, when $L < L_*$ and quenching detonation, when $L \geq L_*$. The calculations of detonation suppression by motile cloud of particles have shown that these two regimes are exist in this case. In addition, in the case of motile particles in a cloud of 30 cm length quenching detonation does not occur, but the cloud of 40 cm length leads to quenching detonation.

4 The suppression of detonation in methane-oxygen and methane-hydrogen-oxygen mixture by cloud of inert particles.

Next, we describe similar calculations of detonation suppression in methane-oxygen mixtures with cloud of inert particles. Fig. 3 shows the dependence of the detonation velocity deficit on the volume concentration of inert particles for particle diameter of 10 microns and 100 microns. It can be seen that the increasing of volume concentration of the particles leads to decreasing of deficit of the detonation velocity. In addition, at a constant volume concentration of particles and decreasing of diameter we also have a decreasing of detonation velocity deficit. Thus, the effect of concentration and diameter of particles on the detonation velocity deficit in the methane-oxygen mixture is similar to the effect on the deficit of the detonation velocity in the hydrogen-oxygen mixture.
Also, it is interesting to compare the dependence for the hydrogen-oxygen and methane-oxygen mixtures. These dependencies are shown in Fig. 3. As seen from the fig. the dependences for methane-oxygen mixture are always right to dependencies for hydrogen-oxygen mixture at the same particle diameter. This is caused by the strong influence of gas-particles friction, as mentioned above. In addition, in Fig. 3 crossed markers denote to the limits of detonation. In methane-oxygen mixture, these limits for 10 micron and 100 micron particles equal to $m_2^* = 2 \cdot 10^{-3}$ and $m_2^* = 3 \cdot 10^{-2}$, respectively.

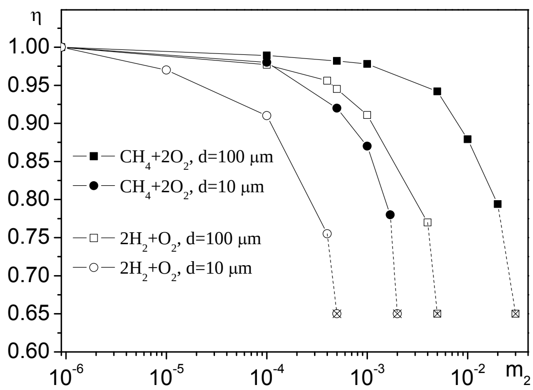

Fig. 3. The dependence of the detonation velocity deficit in the mixtures of methane-oxygen and hydrogen-oxygen on the volume concentration of particles.

Thus, it is interesting to see how the concentration limits and dependence of the detonation velocity deficit changes with dilution methane-oxygen mixture by hydrogen. Presumably, these relations should shift to the left to the dependencies for hydrogen-oxygen mixture. Fig. 4 shows the dependencies of detonation velocity deficit on volume concentration of particles for mixtures of methane-hydrogen-oxygen and methane-oxygen. It is seen that when we dilute the mixture by hydrogen the dependencies shift further to the right. This can be explained as follows. Diluting the mixture by hydrogen, we, on the one hand, increased energy weaning due to friction, but on the other hand, increased heat release in chemical reactions zone. But, as it turned out, the heat release is increased by an amount greater than the energy weaning by friction. However, the difference in the values of these parameters increased slightly as dependence is not strongly shifted to the right.

In addition, in Fig. 4 crossed markers denote to the limit of detonation. In methane-hydrogen-oxygen mixture, these limits for 10 micron and 100 micron particles equal to $m_2^* = 3\cdot 10^{-3}$ and $m_2^* = 4\cdot 10^{-2}$, respectively. Thus, it is evident that the concentration limits of detonation in a mixture of methane-hydrogen-oxygen changed slightly compared to the limits in a mixture of methane-oxygen.

Fig. 3 and 4 shows that the critical volume concentrations that suppress the DW, the largest in the mixture of methane-hydrogen-oxygen and the lowest in the hydrogen-oxygen mixture.

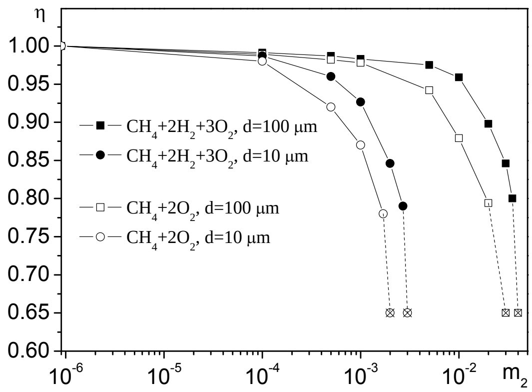

Fig. 4. The dependence of the detonation velocity deficit in the mixtures of methane-oxygen and methane-hydrogen-oxygen on the volume concentration of particles.

5 Conclusions

The physical and mathematical models of attenuation and suppression of detonation in mixtures of hydrogen and methane with an oxidant by injecting a cloud of inert particles in a two-speed, two-temperature approximation of mechanics of heterogeneous media, based on the detailed kinetics, was suggested.

The effect of volume concentration and particle diameter on the DW velocity was investigated. The concentration (in mass and volume concentration of particles) limits of detonation was found. It was shown that the critical volume concentrations that suppress DW, the largest in the mixture of methane-hydrogen-oxygen and the lowest in the hydrogen-oxygen mixture. Comparison the results of calculations of detonation suppression by filter and by cloud of particles revealed that the dependences of detonation velocity on the volume concentration of the particles are close at low concentrations and different at concentrations close to critical.

The geometric limits of detonation, i.e. the minimum length of the filter and cloud of particles, which leads to quenching detonation, was determined. Comparison of simulation results showed that the geometric limits of detonation in the cases of suppression of DW by filter or by cloud of particles differ slightly.

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References

[1] Bedarev I.A., Fedorov A.V. (2006). Comparative Analysis of three Mathematical Models of Hydrogen Ignition. Combustion, Explosion and Shock Waves 1: 26.

[2] Westbrook C.K., Urtiew P.A. (1983). Use of chemical kinetics to predict critical parameters of gaseous detonation. Combustion, Explosion and Shock Waves 6: 65.

[3] Wolanski, P., Liu J.C., Kaufman C.W., Nicholls J.A. and Sichel M. (1988). The Effect of Inert Particles on Methan-Air Detonations. Archivum Combustionis 8: 15.

[4] Borisov A. A., Gel'fand B. E., Gubin S. A. and Kogarko S. M. (1975). Effect of inert solid particles on detonation of a combastible gas mixture**.** Combustion, Explosion and Shock Waves 11: 909.