Physical and Mathematical Modeling of Interaction of Detonation Waves in Mixtures of Hydrogen, Methane, Silane and Oxidizer with Clouds of Inert Micro- and Nanoparticles

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1   Introduction

The addition of inert particles in the reactive gas mixture is one of methods of modification and control of combustion and detonation in such mixtures. For example, the addition of chemically inert microparticles reduces the velocity of detonation [1-3], change the length of the chemical reaction zone of the detonation wave (DW) [3]. The authors of the papers [4-6] have been defined the concentration limits of detonation in a mixture of hydrogen-oxygen, methane-oxygen and methane-hydrogen-oxygen while suppressing DW by clouds of inert microparticles. Furthermore, in [4-6] it has been shown that the most effective in detonation suppressing the smaller diameter particles. In [7-8], it was shown that the addition of inert microparticles destroys the cell structure of the DW in some model mixture. In [9] the detonation cell size in a stoichiometric silane-air mixture with the microparticles of Al_2O_3 are calculated and revealed that the increasing of the mass fraction of particles in the mixture leads to increasing the detonation cell size.

Thus, the processes of interaction of DW with clouds of inert microparticles studied in detail. In this paper the interaction of DW in mixture of hydrogen-oxygen and methane-oxygen with clouds of inert nanoparticles of SiO_2 are calculated.

2   Physical and mathematical formulation of the problem

Let's consider a shock tube filled with a gas mixture of hydrogen, methane, silane and oxygen, as well as the cloud of inert micro- and nanoparticles of SiO_2 located in the low pressure chamber (LPC) at a certain distance from the membrane separating the high and low pressure chambers. Conditions in LPC: pressure equal to 1 atm, temperature of gas mixture equal to 300K. After the rupture of the diaphragm in the LPC the DW is initiated, which prior to the interaction with the cloud enters the Chapman-Jouget regime. Mathematical model of the mechanics of the reacting gas mixtures and inert particles represents the

system of equations of the dynamics of the gas mixture and solid particles and has the form shown in our previous studies [4-6, 10].

For very small particles when the particle size becomes comparable with the mean free path of the gas molecules, the expression of the drag force should be complemented with the Cunningham correction

factor: $C_c = 1 + \dfrac{2\lambda}{d}\left[1.257 + 0.4e^{-\frac{1.1d}{2\lambda}}\right]$, where d - the particle diameter, $\lambda = \dfrac{k_b T}{\sqrt{2}\pi d_g^2 p}$ - mean free path of

gas molecules, $p, T,$ - pressure and temperature of gas, k_B - Boltzmann constant, d_g - the diameter of the surrounding gas molecules. Drag force has following form:

$$f = \frac{3\mathrm{m}_2 \rho_{11}}{4\mathrm{d}}\frac{C_D}{C_c}|u_1 - u_2|(u_1 - u_2),$$

where C_D - drag coefficient, m_2 - particles volume concentration, ρ_{11} - gas mixture true density, u_1, u_2 - gas mixture and particles velocity, respectively.

The characteristic times of thermal relaxation for the nanoparticles are determined by the change in the mode of the particles flow from the continuum to free-molecular [11]. In the continuum flow mode (at $\mathrm{Kn} < 0.01$) characteristic time of thermal relaxation describes by the following dependence $\tau_T^{cont} = d^2 \rho_{22} c_{v2} / 6\lambda_1 \mathrm{Nu}$. For free-molecular flow regime (at $\mathrm{Kn} > 10$) [12]:

$\tau_T^{fm} = \dfrac{\rho_{22} c_{p2} d}{6\alpha p}\sqrt{\dfrac{8\pi\mu T}{R}}\left(\dfrac{\gamma-1}{\gamma+1}\right)$, where $Kn = \dfrac{\lambda}{d}$ - Knudsen number. Here ρ_{22}, c_{p2} - the true density and

heat capacity of the particles, μ - molar mass of ambient gas, α - the accommodation rate. In the range of Knudsen numbers $0.01 \div 10$ there is a transitional flow regime [11], here we use an approximation of the form $\tau_T^{tr} = [(\lg\mathrm{Kn}+2)\tau_T^{fm} + (1-\lg\mathrm{Kn})\tau_T^{cont}]/3$.

To describe the chemical reactions in the reacting gas mixture we will use the detailed kinetics models: for the hydrogen-oxygen mixture - model [6, 13, 14], taking into account 38 reactions for 8 component; for methane-oxygen mixture - model [4, 15], taking into account the 92 reaction for 15 components, for silane-air mixture - model [10, 16].

3   The calculation results. Influence of volume concentration and particle diameter on the DW velocity

First of all, let's consider the processes of propagation, weakening and suppression of DW in a hydrogen-oxygen mixture with inert nanoparticles. Fig. 1 shows the dependences of the detonation velocity deficit

($\eta = \dfrac{D}{D_{CJ}}$, where D - the detonation velocity in a mixture of gas and particles, D_{CJ} - Chapman-Jouget

detonation velocity: $D_{CJ} = 2750$ m/s in hydrogen-oxygen mixture and $D_{CJ} = 2440$ m/s in methane-oxygen mixture) on the volume concentration of inert particles with diameters ranging from 10 nm to 100 microns. The data for micro particles are taken from [5]. It is seen in fig. 1 that in the case of DW propagation in particles with the diameter ranging from 10 nm to 1 micron detonation velocity deficit decreases to values $\eta = 0.45$ while for the micro particles with the diameters ranging from 10 microns to 100 microns this parameter decreases only to values $\eta = 0.75$ after which the failure and suppression of DW are occurs. Thus, for all considered sizes of the particles, the two flow regimes exist: 1. stationary propagation of weakened DW at velocities D lower than D_{CJ} (in the micro particles with a DW velocity deficit ranging from 0.75 to 1, in the nanoparticles with a DW velocity deficit ranging from 0.45 to 1); 2.

the suppression of DW. Possible types of detonation flows in gas suspensions of reactive gases and inert micro particles, as well as the scenario of DW suppression by micro particles described in detail in [1, 5-6], in which the suppression means splitting of DW to frozen shock wave (SW) and front of ignition and combustion. In the case of DW suppression by nanoparticles it is also seen the decay of the DW to frozen SW and front of ignition and combustion. I.e. the mechanisms of detonation suppression by micro- and nanoparticles are the same.

Furthermore, it should be noted that in hydrogen-oxygen mixture the concentration limits of detonation, i.e. minimum volume concentration of inert particles suppressing the DW, are close for the particles with diameters of 10 nm, 100 nm, 1 micron, 10 micron. For 10 nm and 100 nm particles the critical (minimum) volume concentration of particles $- m_2^* = 6 \cdot 10^{-4}$, for 1 micron $- m_2^* = 4 \cdot 10^{-4}$, for 10 microns $- m_2^* = 5 \cdot 10^{-4}$. Thus it is seen that the tendency of increasing of detonation suppression efficiency with decreasing of the inert particles size in the transition from micro- to nanoparticles is violated.
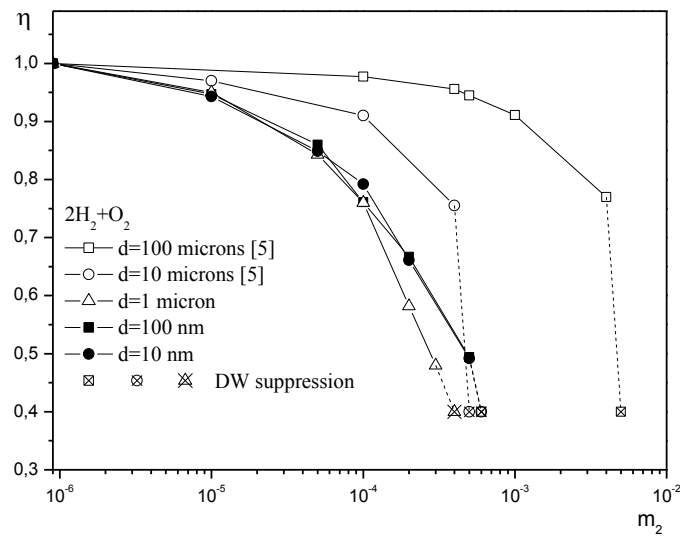

Figure 1. The dependencies of DW velocity deficit in the stoichiometric hydrogen-oxygen mixture on the inert particles volume concentration. Comparison of the effectiveness of DW weakening and suppression by micro- and nanoparticles.

Fig. 2 shows the dependence of detonation velocity deficit in methane-oxygen mixture on volume concentration of inert particle with diameters ranging from 10 nm to 100 microns. The data for micro particles are taken from [4]. It is seen that the all above-described flow regimes in the hydrogen-oxygen mixture are valid for the methane-oxygen mixture. However, for gas suspension with 1 micron particles, the decreasing of the DW velocity deficit is observed only till the value $\eta = 0.8$, after which the failure and suppression of DW are occurs. In addition, violation of the tendency of increasing the efficiency of DW suppression is observed in the methane-oxygen mixture. Critical volume concentrations of inert particles are follow: for 10 nm $- m_2^* = 1.5 \cdot 10^{-3}$, for 100 nm $- m_2^* = 1.3 \cdot 10^{-3}$, for 1 micron $- m_2^* = 2 \cdot 10^{-4}$, for 10 microns $- m_2^* = 2 \cdot 10^{-3}$.

If we compare the effectiveness of DW suppression in mixtures of hydrogen-oxygen and methane-oxygen, it is seen that the micro particles with the diameter ranging from 10 microns to 100 microns, and from 10 nm to 100 nm effectively suppress the detonation in hydrogen-oxygen mixture, whereas the 1 micron particle effectively suppress the detonation in methane-oxygen mixture.
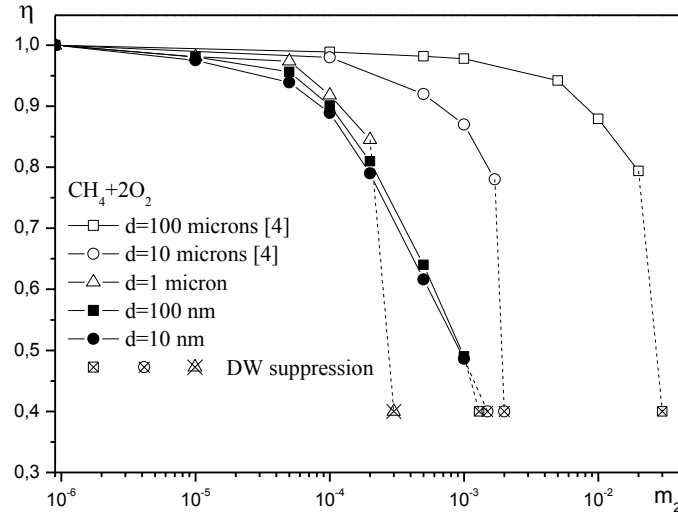
Figure 2. The dependencies of DW velocity deficit in the stoichiometric methane-oxygen mixture on the inert particles volume concentration. Comparison of the effectiveness of DW weakening and suppression by micro- and nanoparticles.

Fig. 3 shows the dependence of the detonation velocity deficit in silane-air mixture on volume concentration of inert particle diameters with diameters ranging from 10 nm to 100 microns. It is seen that the all above-described flow regimes in the hydrogen-oxygen and methane-oxygen mixtures are valid for the silane-air mixture. However, the efficiency of DW suppression in silane-air mixture by inert particles is much less than in hydrogen-oxygen and methane-oxygen mixtures. The detonation wave velocity deficit decreases much slower at the increasing of particles concentration in silane-air mixture compared with hydrogen-oxygen and methane-oxygen mixture. In addition, violation of the tendency of increasing the efficiency of DW suppression at the decreasing of diameter of nanoparticles is observed in the silane-air mixture too. Critical volume concentrations of inert particles suppressing the DW in silane-air mixture are follow: for 10 nm $- m_2^* = 5 \cdot 10^{-4}$, for 100 nm $- m_2^* = 5 \cdot 10^{-4}$, for 1 micron $- m_2^* = 1.5 \cdot 10^{-3}$, for 10 microns $- m_2^* = 4 \cdot 10^{-2}$. Besides that, in mixtures with nanoparticles detonation limits (critical volume concentrations of inert particles which suppress the detonation) in silane-air and hydrogen-oxygen mixtures approximately the same.
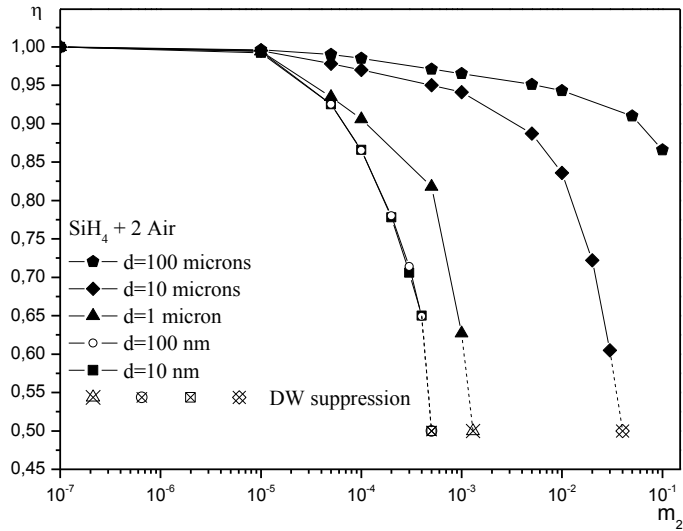
Figure 3. The dependencies of DW velocity deficit in the stoichiometric silane-air mixture on the inert particles volume concentration. Comparison of the effectiveness of DW weakening and suppression by micro- and nanoparticles.

4   Conclusions

The physical and mathematical models describing the processes of propagation, attenuation and suppression of the detonation process in the mixtures of hydrogen, methane, silane and oxidizer by inert micro- and nanoparticles were proposed. Based on these models the dependencies of detonation velocity deficit on the size and concentration of inert micro- and nanoparticles were found.

It was revealed that the same types of detonation flows exists in the mixture of gas and nanoparticles, as in gas suspensions with micro particles: 1. stationary propagation of weakened detonation wave at velocities less than Chapman-Jouget velocity; 2. the detonation wave suppression. In addition, it is determined that the mechanism of detonation suppression by micro- and nanoparticles are quite similar and consists in the splitting of detonation wave into frozen shock wave and ignition and combustion wave.

The concentration limits of detonation were calculated. It was shown that the detonation limits in these mixtures are similar for particles with diameters ranging from 10 nm to 1 micron. It was determined that the tendency of increasing of detonation suppression efficiency at inert particles size decreasing during the transition from micro- to nanoparticles is violated. It was revealed that in the gas suspensions with nanoparticles the concentration limits of detonation in hydrogen-oxygen and silane-air mixture is approximately the same.

Acknowledgements

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