INTERACTION OF DETONATION WAVES IN SILANE-AIR MIXTURE WITH CLOUDS OF INERT MICRO- AND NANOPARTICLES

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In the paper physical and mathematical models for the description of the processes of transition, weakening and suppression of detonation in mixtures of silane-air and inert nanoparticles were proposed. On the basis of these models the dependencies of detonation velocity deficit on the size and concentration of inert nanoparticles were found. Two types of detonation flows in gas suspensions of reactive gases and inert nanoparticles were revealed - propagation of weak detonation wave in the gas suspension and destruction of the detonation process. It was determined that the mechanisms of detonation suppression by micro- and nanoparticles are the same and lies in the decay of a detonation wave on frozen shock wave and wave of ignition and combustion. Concentration limits of detonation were calculated. It turned out that in the transition from microparticles to nanoparticles the detonation suppression efficiency does not increase.

Keywords: detonation suppression, silane-air mixture, detailed chemical kinetics, mathematical modeling, gas suspension.

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) [4]. The authors of the papers [5-6] 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 [5-6] 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 silane-air with clouds of inert nanoparticles of SiO_2 are calculated.

Physical and mathematical formulation of the problem. Let's consider a shock tube filled with a gas mixture of silane and air, as well as the cloud of inert 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 (silane and air) 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 [5-6].

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

This model which takes into account the Cunningham correction factor, will be valid only within a specific range of particle sizes. This includes particles we discussed (the sizes from 100 microns to 10 nm). In this range of particle

diameters (from 1 to 100 microns) Cunningham correction factor in the structure of the detonation wave changes its value from 1 (for particles with the diameter ranging from 10 to 100 microns) to 1.2 (for 1 micron particles), in gas suspensions with nanoparticles (for particles with the diameter ranging from 10 to 100 nm) Cunningham correction factor monotonically increases to value $C_c \sim 13$. When the particle size becomes close to the size of the molecules of the surrounding gas, the model has to be unfair, because there is phenomenological approach no longer works.

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 [10]. 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 $\mathrm{Kn} > 10$) [11]: $\tau_T{}^{fm} = \dfrac{\rho_{22} c_{p2} d}{6\alpha p} \sqrt{\dfrac{8\pi\mu T}{R}} \left(\dfrac{\gamma - 1}{\gamma + 1} \right)$, 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 [10], here we use an approximation of the form $\tau_T{}^{tr} = [(\lg \mathrm{Kn} + 2)\tau_T{}^{fm} + (1 - \lg \mathrm{Kn})\tau_T{}^{cont}] / 3$.

It should also be noted that for microparticles with diameters ranging from 1 to 100 μm continuous flow regime is realized, for nanoparticles with diameters ranging from 10 to 100 nm transition regime is realized.

To describe the chemical reactions in the reacting gas mixture we will use the detailed kinetics model [12, 13], taking into account 140 reactions for 25 components. With the help of this model, we previously described the structure of detonation wave in a silane-air mixture [12], the ignition delay times of silane-oxygen and silane-air mixtures [12, 13], the ignition delay times of dual-fuel mixtures of silane-hydrogen [14] and ignition limits of the silane / oxygen and silane / air mixtures [15].

The calculation results. Influence of volume concentration and particle diameter on the DW velocity. Let's consider the processes of propagation, weakening and suppression of DW in a silane-air mixture with inert nanoparticles. Fig. 1 shows the dependences of the detonation velocity deficit ($\eta = \frac{D}{D_{CJ}}$, where D - the detonation velocity in a mixture of gas and particles, D_{CJ} - Chapman-Jouget detonation velocity: $D_{CJ} = 1820$ m/s in silane-air mixture) on the volume concentration of inert particles with diameters ranging from 10 nm to 100 microns.

It is seen in fig. 1 that in the case of DW propagation in particles with the diameter ranging from 10 nm to 10 micron detonation velocity deficit decreases to values $\eta = 0.6$ after which the failure and suppression of DW are occurs. It

should be noted that considered mathematical model is not valid for gas suspensions with particles volume concentration greater than 0.1. So in gas suspension with 100 micron particles in considered range of particles volume concentrations (till value $m_2 = 0.1$) detonation velocity deficit decreases only to value $\eta = 0.85$ and no suppression is observed.

Thus, in gas suspensions with particles with diameters ranging from 10 nm to 10 microns the two flow regimes exist: 1. stationary propagation of attenuated DW at velocities D lower than D_{CJ} (DW velocity deficit ranging from 0.6 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 [1-2, 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.

Besides that, it is seen, that the efficiency of DW suppression in silane-air mixture in the transition from 100 nm to 10 nm particles does not increase, dependences goes at each other.

In our earlier paper [6], and also in [7], the existence of two types of detonation flows in gas suspensions of reacting gases and inert particles were

shown – frozen flow (at particle diameters of more than 100 μm) and equilibrium flow (at particle diameters less than 1 μm) with a continuous transition between them. It turned out that when the diameter of the particles is less than 1 μm at a constant volume concentration of the particles the detonation velocity remains practically unchanged. The same thing is observed in Fig. 1 at particle diameters of 10 nm, 100 nm, 1 μm - all the dependencies far from the concentration limit goes practically to each other.

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 – $m_2^* = 4 \cdot 10^{-2}$.

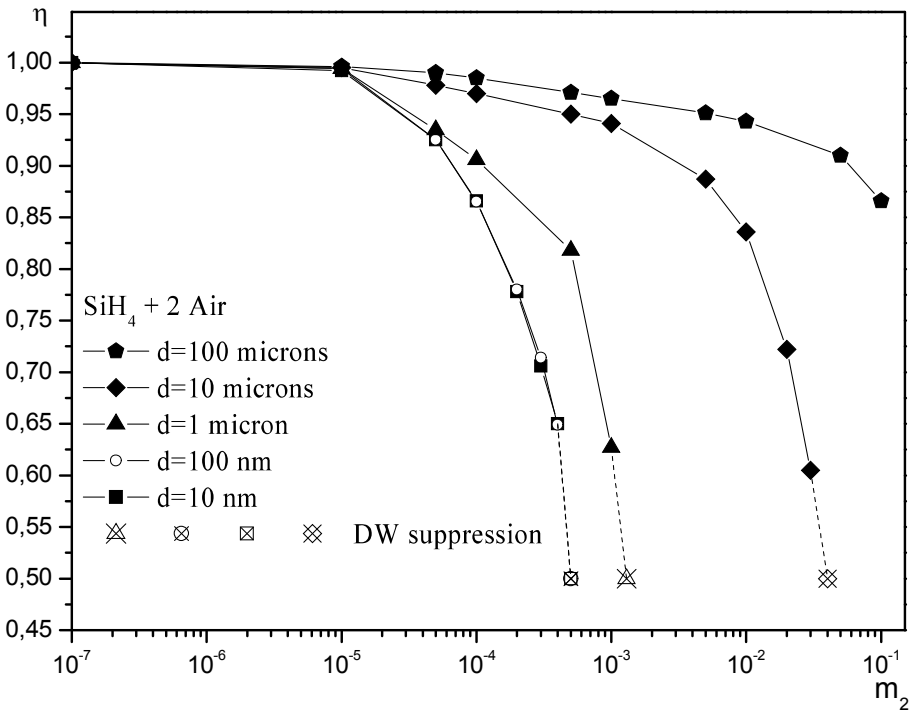

Fig. 1. The dependencies of DW velocity deficit in the stoichiometric silane-air mixture on the inert particles volume concentration.

Conclusions.

The physical and mathematical model describing the processes of propagation, attenuation and suppression of the detonation process in the mixtures of silane and air 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 attenuated DW at velocities less than Chapman-Jouget velocity; 2. the DW suppression. Furthermore, it is determined that the mechanisms of detonation suppression by micro- and nanoparticles are quite similar.

Concentration limits of detonation were calculated. It turned out that in the transition from microparticles to nanoparticles the detonation suppression efficiency does not increase.

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REFERENCES

1. **Fedorov A.V., Fomin P.A., Fomin V.M., Tropin D.A., Chen J.-R.** Mathematical Analysis of Detonation Suppression by Inert Particles. Kao Tech Publishing, Kaohsiung, Taiwan. 2012. 143 p. ISBN 978-986-88423-0-4.

2. **Fedorov A.V., Fomin P.A., Fomin V.M., Tropin D.A., Chen J.-R.** Physical - mathematical modeling of detonation suppression by clouds of fine particles: monograph / Institute of Theoretical and Applied Mechanics SB RAS; NSUACE (Sibstrin). -Novosibirsk: NSUACE (Sibstrin). 2011. 156 p. [Fiziko - matematicheskoe modelirovanie podavlenija detonacii oblakami melkih chastic : monografija / In - t teoret. i prikl. mehaniki SO RAN; NGASU (Sibstrin). Novosibirsk: NGASU (Sibstrin). 2011. 156 s.]
3. **Fomin P.A., Chen J.R.** Effect of Chemically Inert Particles on Parameters and Suppression of Detonation in Gases // Combustion, Explosion, and Shock Waves. – 2009. – V. 45, # 3. – P. 303–313.
4. **Borisov A.A., Gel'fand B.E., Gubin S.A., Kogarko S.M.** Effect of inert solid particles on detonation of a combustible gas mixture // Combustion, Explosion and Shock Waves. – 1975. – V. 11, # 6. – P. 774-778.
5. **Tropin D.A., Fedorov A.V.** Physicomathematical modeling of detonation suppression by inert particles in methane-oxygen and methane-hydrogen oxygen mixtures // Combustion, Explosion and Shock Waves. – 2014. – V. 50, # 5. – P. 542-546.
6. **Fedorov A.V., Tropin D.A.** Modeling of detonation wave propagation through a cloud of particles in a two-velocity two-temperature formulation // Combustion, Explosion and Shock Waves. – 2013. – V. 49, # 2. – P. 178-187.

7. **Papalexandris M.V.** Numerical simulation of detonations in mixtures of gases and solid particles // J. Fluid Mechanics. – 2004. – V. 507. – P. 95–142.
8. **Shafiee H., Djavareshkian M.H.** CFD Simulation of Particles Effects on Characteristics of Detonation // International Journal of Computer Theory and Engineering. – 2014. – V. 6, # 6. – P. 466-471.
9. **Fedorov A.V., Fomin P.A., Tropin D.A., Chen J.R.** Modeling of explosion hazards and its mitigation in the silane-air mixtures // Proceedings of the universities. Building. [Modelirovanie opasnosti vzryva i smjagchenie ego posledstvij v silano-vozdushnyh smesjah // Izvestija vuzov. Stroitel'stvo.]. – 2014. # 9-10. – P. 108-125.
10. **Sundaram D.S., Yang V., Zarko V.E.** Combustion of nano aluminum particles (Review) // Combustion, Explosion and Shock Waves. – 2015. – V. 51, # 2. – P. 173-196.
11. **Filippov A.V., Rosner D.E.** Energy transfer between an aerosol particle and gas at high temperature ratios in the Knudsen transition regime // International Journal of Heat and Mass Transfer. – 2000. – V. 43, # 1. – P. 127-138.
12. **Tropin D.A., Fedorov A.V.** Physicomathematical modeling of ignition and combustion of silane in transient and reflected shock waves // Combustion, Explosion and Shock Waves. – 2015. – V. 51, # 4. – P. 431-438.

13. **Tropin D.A., Fedorov A.V.** Physical and mathematical modeling of ignition, combustion and detonation of silane-hydrogen-air mixtures // Journal of Loss Prevention in the Process Industries. – 2017. DOI: 10.1016/j.jlp.2017.02.029
14. **Tropin D.A., Fedorov A.V.** Ignition of a two-fuel hydrogen–silane mixture in air // Combustion, Explosion, and Shock Waves. – 2017. – V. 53, # 1. – P. 1–7.
15. **Tropin D.A., Fedorov A.V.** Calculation of flammability limits of silane-oxygen and silane-air mixtures // Combustion, Explosion and Shock Waves. – 2016. – V. 52, # 1. – P. 40-44.