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To cite this article: A V Fedorov and D A Tropin 2017 J. Phys.: Conf. Ser. 894 012099

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Mathematical description of ignition, combustion and propagation of detonation in reacting gas mixtures in the presence of micro- and nanoparticles

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Abstract. The physical and mathematical models for the description of the processes of ignition, combustion and propagation of detonation in mixtures of hydrogen-oxygen, methane-oxygen and silane-air in the presence of inert micro- and nanoparticles were proposed. On the basis of these models the dependencies of detonation velocity deficit vs the size and concentration of inert micro- and nanoparticles were found. Two modes of detonation flows in gas suspensions of reactive gases and inert nanoparticles were revealed: - propagation of weak detonation wave in the gas suspension, - destruction of the detonation process. It was determined that the mechanisms of detonation suppression by micro- and nanoparticles are closed and lies in the splitting of a detonation wave to frozen shock wave and ignition and combustion wave. Concentration limits of detonation were calculated. It turned out that in the transition from microparticles to nanoparticles the detonation suppression efficiency does not increase.

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) [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. The detonation cell size in a stoichiometric silane-air mixture with the microparticles are calculated in [9]. It is revealed that the increasing of the mass fraction of particles in the mixture leads to increasing the detonation cell size.

Thus, the processes of ignition, combustion, propagation and interaction of DW with clouds of inert microparticles was studied in details. In this paper the interaction of DW in mixture of hydrogen-oxygen, methane-oxygen and silane-air with clouds of inert micro- and nanoparticles are calculated.

2. Physical and mathematical formulation of the problem
Let's consider a shock tube filled with a gas mixture of hydrogen-oxygen or methane-oxygen or silane-air, 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 diaphragm, 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 [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: $C_c = 1 + \frac{2\lambda}{d} \left[ 1.257 + 0.4e^{\frac{1.4d}{2\lambda}} \right]$, where $d$ - the particle diameter, $\lambda = \frac{k_B T}{\sqrt{2\pi m_{\text{gas}}}}$ - mean free path of gas molecules, $p, T$ - pressure and temperature of gas, $k_B$ - Boltzmann constant, $d_{\text{bc}}$ - the diameter of the surrounding gas molecules. Drag force has following form:

$$f = \frac{3m_2 \rho_{11} C_D}{4d} C_c \frac{D_c}{\rho} \left( \frac{u_1 - u_2}{(u_1 - u_2)} \right),$$

where $C_D$ - drag coefficient, $m_2$ - particles volume concentration, $\rho_{11}$ - 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 (the sizes change from 10 nm to 100 microns). In this range of particle diameters 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 the 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 $Kn<0.01$) characteristic time of thermal relaxation describes by the following dependence $\tau_T^{cont} = d^2 \rho_{22} c_{p2} / 6 \lambda \mathbf{Nu}$. For free-molecular flow regime (at $Kn > 10$) [11]:

$$\tau_T^{fm} = \frac{\rho_{22} c_{p2} d}{6 \alpha p} \sqrt{\frac{8 \pi m_{\text{gas}}}{R}} \left( \frac{\gamma - 1}{\gamma + 1} \right),$$

where $Kn = \frac{\lambda}{d}$ - Knudsen number. Here $\rho_{22}, c_{p2}$ - the true density and heat capacity of the particles, $\mu$ - molar mass of ambient gas, $\alpha$ - the accommodation coefficient. In the range of Knudsen numbers $0.01 \sim 10$ there is a transitional flow regime [10]. Here we use an approximation formula of the form $\tau_T^{tr} = [(\log Kn+2)\tau_T^{fm} + (1-\log Kn)\tau_T^{cont}] / 3$.

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 models: for the hydrogen-oxygen mixture - model [6, 12, 13], taking into account 38 reactions for 8 components; for methane-oxygen mixture - model [5, 14], taking into account the 92 reaction for 15 components, for silane-air mixture - model [15, 16], taking into account 140 reactions for 25 components.

3. The calculation results

3.1. Hydrogen-oxygen mixture
First of all, let’s consider the processes of DW interaction in a hydrogen-oxygen mixture with inert nanoparticles. Figure 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: $D_{CJ} = 2750$ m/s in hydrogen-oxygen mixture, $D_{CJ} = 2440$ m/s in methane-oxygen mixture and $D_{CJ} = 1820$ m/s in silane-air mixture) vs the volume concentration of inert particles for the particle size ranging from 10 nm to 100 microns. The data for micro particles are taken from [6]. From figure 1 it is seen that in the case of DW propagation in mixture of a gas and particles with the diameter change 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, exists the two flow regimes: 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 [1-2, 5-6], in which the suppression means splitting of DW to frozen shock wave (SW) and lagging 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 the concentration limits of detonation, i.e. minimum volume concentration of inert particles that suppress the DW, in hydrogen-oxygen mixture 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 efficiency of DW supression in hydrogen-oxygen mixture in the transition from microparticles to nanoparticles does not increase, dependences goes at each other.

![Figure 1](image-url)  
**Figure 1.** The dependencies of DW velocity deficit in the stoichiometric hydrogen-oxygen mixture vs the inert particles volume concentration. Comparison of the effectiveness of DW weakening and suppression by micro- and nanoparticles.

### 3.2. Methane-oxygen mixture
Figure 2 shows the dependence of the 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 [5]. It is seen that all the above-described flow regimes in the hydrogen-oxygen mixture is valid for the methane-oxygen mixture. However, for a gas suspension with 1 micron particles, the decreasing of the DW velocity deficit is observed only to value $\eta = 0.8$, after which the failure and suppression of DW are occurs. In addition, the efficiency of DW suppression in methane-oxygen mixture in the transition from microparticles to nanoparticles does not increase too. Critical volume concentrations of inert particles are as follows: 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](image-url)

**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.

### 3.3. Silane-air mixture

It is seen in figure 3 that in the case of DW propagation in silane-air mixture and 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.

Besides that, it is seen, that the efficiency of DW suppression in silane-air mixture in the transition region (from 10 nm to 100 nm) particles does not increase, dependences goes at 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 – $m_2^* = 4 \cdot 10^{-2}$. 


4. Conclusions
The physical and mathematical models describing the processes of ignition, combustion and detonation in mixtures of hydrogen-oxygen, methane-oxygen and silane-air in the presence of inert micro- and nanoparticles were proposed. Based on these models the dependencies of detonation velocity deficit vs the size and concentration of inert micro - and nanoparticles were found. It was revealed that the two types of detonation flows exists in the mixture of a gas and nanoparticles, as well as in gas suspensions with micro particles: 1. stationary propagation of weakened 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.

Acknowledgments
The work was supported by Russian Science Foundation (project No. 16-19-00010) and Russian Foundation for Basic Research (grants No. 15-08-01947-a, No. 17-08-00634-a). Part of the work concerning calculations in the silane-air mixture were carried out on the basis of the RSF project, in the hydrogen-oxygen and methane-oxygen mixtures were carried out on the basis of the RFBR projects.

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