# Simulation of detonation wave passage through 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, oxygen, argon 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, presented in [1].

## 2 The influence of argon dilution on detonation velocity

The kinetic scheme, used for calculation of detonation processes in two-phase mixture, has been successfully verified in [1]. Ignition delay and DW parameters in stoichiometric hydrogen-oxygen mixture with argon additions have been calculated. Fig. 1 shows a high coincidence of theoretical and experimental [2] data. It can be seen, that increasing of argon mass fraction leads to decreasing of detonation velocity. Obviously, this is caused by an increasing amount of heat removed from the detonating mixture. As can be seen, our calculations with a 3% accuracy coincide with experimental data [2], in which the initial parameters are $p_0 = 0.2$ atm, $T_0 = 295$ K. If argon concentration is more, than 95%, DW suppression occurs. At such conditions classical DW structure transforms into frozen shock wave (FSW) and subsequent wave of ignition and combustion (WIC). Thus, it is shown that the used kinetic scheme describes the available experimental data with high accuracy. Therefore, it can be used for calculation of DW suppression by chemically inert particles.

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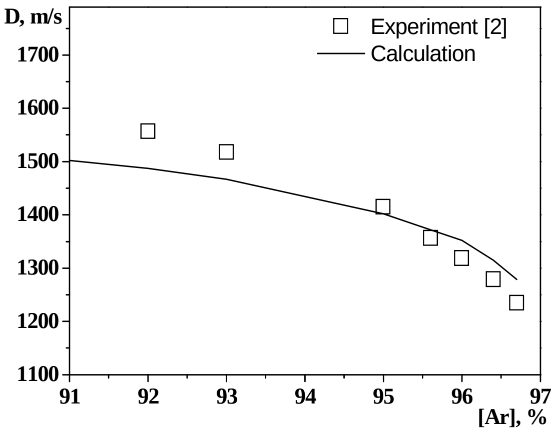


Fig. 1. The dependence of detonation velocity on argon mass fraction (comparison with experimental data, presented in [2]).

# 3 Influence of particles amount on detonation velocity

Parameters of DW in $2H_2+O_2$ mixtures with $SiO_2$ particles have been calculated. Condensed phase assumed to be chemically inert. The vapor pressure of the condensed phase assumed to be negligible small. Fig. 2 shows the calculated value – $\eta = D/D_{CJ}$ versus mass concentration of particles $\xi_2$; $D$ 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 experimental data of [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.

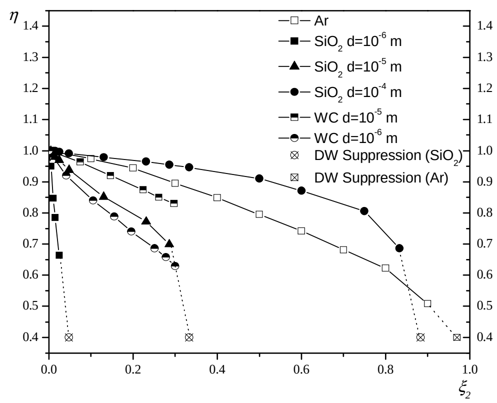


Fig. 2. The dependence of detonation wave velocity deficit on mass concentration of inert components.

# 4 Finite size of the 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 cloud, which quenches the DW. That is, the size of the cloud, that after the wave complex, consisting of FSW and WIC, exit from cloud, the initiation of DW did not happen.

Nonstationary DW propagation in a gas with cloud of particles has been considered. The aim of the calculations was to determine the minimum length of the cloud $L_*$ for successful quenching of DW. This length will be called as critical. DW propagation in a cloud of 10 μm and 100 μm particles with corresponding limiting volume concentrations $m_2^*$ has been calculated.

# 5 Subcritical size of the cloud

If $\overline{L} = L / L_* = 0.067 - 0.134$, where $L_*$ - critical size of the cloud, it would be determined later, then DW propagates without split into FSW and WIC. However, the characteristic triangular pressure profile of DW inside a cloud transforms, i.e. at such sizes of a cloud the decay of DW structure just starting. At the size of the cloud, greater than $\overline{L} = 0.134$, DW structure transforms into FSW and subsequent WIC. It means that *L* = 0.134 can be considered as subcritical length of the cloud, which leads to the splitting of the detonation front.

When FSW enter into gas behind the cloud, ignition behind its front does not occur, because the gas temperature is below the critical temperature of ignition (500 K). However, when WIC enters into gas behind the cloud, its velocity rapidly increases, and it catches of FSW. As a result, a sharp increase in pressure and temperature occurs and overdriven DW forms (velocity 2982 m/sec, $\eta$ = 1.09). This overdriven regime subsequently goes into the Chapman-Jouguet mode (Fig. 3).

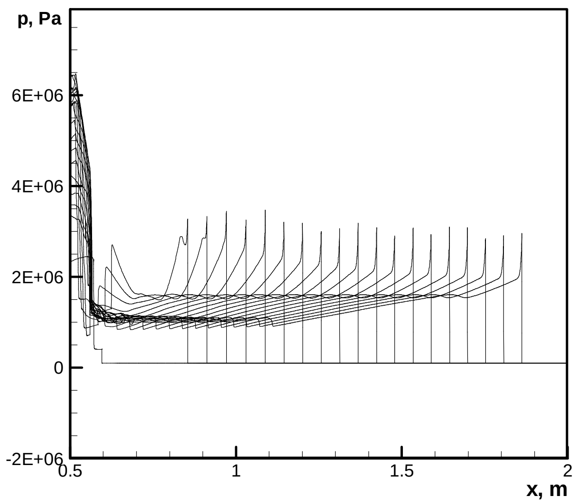


Fig. 3. The decay of DW structure into FSW and WIC in the cloud of particles, subsequent reinitiation of DW and evolution of overdriven DW into Chapman-Jouguet mode. Subcritical length of the cloud ($\overline{L} = 0.33$), $d = 100$ μm.

So, if cloud length is less than critical, then DW suppression by cloud of particles is not observed.

# 6 Critical size of the cloud

For the size of the cloud, larger than the critical, a wave of combustion, moving behind the front of FSW, propagates nonstationary; stationary propagation regimes are not observed. After the split of DW on FSW and WIC, velocity of WIC inside the cloud decreases. For example if $\overline{L} = 1.66$, then WIC velocity decreases from 380 m/sec to 200 m/sec in case of 100 μm particles and to 260 m/sec in the cloud of 10 μm particles. DW reinitiation behind the cloud does not occur.

Clouds with subcritical size does not quench the DW. If the particle cloud size is equal to $\overline{L} = 0.66$ reinitiation behind the cloud occurs, but if the particle cloud size is equal to 30 cm DW quenching occurs. Fig. 4 shows the pressure profiles in LPC after the complex consisting of FSW and SW, which is retained after quenching WIC, exit from a cloud of particles with diameter of 100 μm. It can be seen, that the amplitude of the SW is gradually reduced. Its velocity is equal to 1168.6 m/sec. In this case, SW pass through the gas mixture, the temperature behind it front is 500 K, far below the critical temperature of ignition ($T_* = 850$ K). We assume therefore that the critical value is $L_* = 30$ cm.

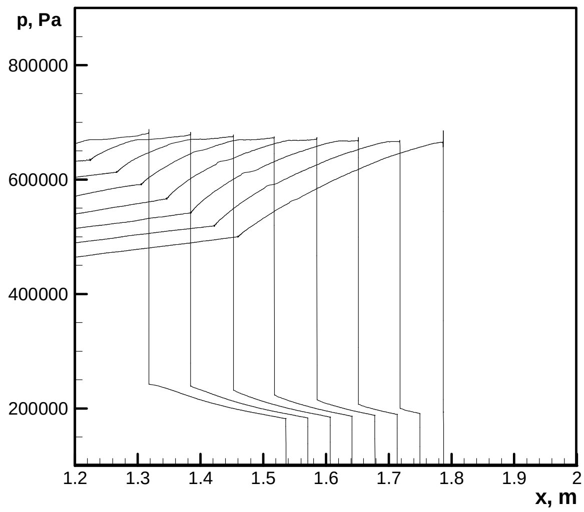


Fig. 4. Pressure profiles of the wave behind the cloud. Critical size of the cloud ($\overline{L} = 1$); $d = 100$ μm.

# 6 Conclusions

1. Physical and mathematical model to describe the suppression / attenuation of detonation in a mixture of hydrogen and oxygen, based on detailed kinetics, by adding inert particles, was proposed. Based on it, the detonation velocity deficit depending on the size and concentration of particles was found. The critical mass and volume concentrations of particles were identified.
2. In the problem of suppressing the detonation of finite size particle cloud with a constant volume concentration equal to the critical value for an infinite cloud, the minimum length of the particle cloud/filter was defined, such that after the complex - frozen shock + wave ignition and combustion exit from the filter deflagration to detonation transition is not observed.

# References

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