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Parameters for Attenuation and Suppression of Detonation Wave with Inert Particles

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The method of gas detonation wave attenuation and suppression by chemically inert particles injection before the leading shock front is considered. Parameters and cell size of a steady detonation wave are calculated. The minimum mass fraction and total mass of particles and the characteristic size of the cloud, which are necessary for detonation wave suppression, are calculated. Methane-, Cyclohexane-, Hydrogen- and Silane-air mixtures with particles of W, WC, Al_2O_3, SiO_2 and KCl are considered. Results of calculations quite good correspond to available experimental data. The process of suppression is more effective, if particles have high heat capacity and heat of melting. Among the particles under consideration Al_2O_3 and SiO_2 particles are better for detonation suppression.

Detonation limits for different chemical compositions of methane-air mixtures and mass fractions of SiO_2 particles are calculated. An increase of particles concentration leads to increase of the lower and decrease of the upper detonation limit. If a mass fraction of condensed phase is high enough, detonation wave propagation is impossible.

A steady detonation wave reflection from a rigid wall ($D \rightarrow D$ reflection) in cyclohexane- and silane-air mixtures with SiO_2 particles is considered. It is shown, that particles can drastically reduce pressure and temperature behind the reflected wave and therefore prevent crucial destruction of equipment.

The efficiency of detonation wave suppression at different relations between fuel and oxidizer is calculated. Methane- and cyclohexane-air mixtures with Al_2O_3 particles are considered. It is shown, that for every particles concentration the value of cell size has a minimum, which corresponds to a fuel-rich chemical composition. It means that for this relation between fuel and oxidizer the efficiency of detonation wave suppression by particles injection has a maximum.

1. Introduction

Chemically inert solid particles can be used for effective control of gaseous detonation. Theoretical and experimental investigation of detonation wave (DW) suppression in gaseous mixtures by injection of chemically inert particles ahead the wave front are very important for safety industry and very far to be completed.

An algorithm for calculation parameters and cell size of detonation wave in a mixture of a gas with chemically inert microparticles was presented in article of Fomin and Chen (2009). Results of calculations are used for analysis of the method of multifront detonation wave (DW) suppression by particles injection before the leading shock front. The ratio between the channel diameter and the detonation cell size was used to estimate the limit of detonation. The minimum total mass of the particles and the characteristic size of the cloud, which are necessary for detonation suppression, were calculated. It was shown, that such suppression is more effective, if the particles have high heat capacity, low melting point and high heat of melting.

But the model of Fomin and Chen (2009) was not compared with available experimental results. The validity of the model for a wide range of chemical compositions of gaseous mixtures and kinds of particles

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was not verified. Additionally, the following questions still need to be considered. Is it possible to reduce an impact of DW on the wall by the particles injection and therefore prevent crucial destruction of equipment, caused by detonation? How additions of the particles influence on pressure and temperature behind a reflected wave? How chemical composition of gas influences on DW parameters at different mass fraction of condensed phase? At which chemical compositions relative cell size is bigger and therefore the efficiency of DW suppression by particles injection is higher? How concentration limits of detonation wave depend on mass fraction of a condensed phase? Such problems will be considered here for a wide range of chemical compositions of gaseous mixtures and kinds of particles. Fomin and Chen model (2009) (with some modifications, see below) will be used.

2. Parameters and relative cell size of DW in gas-particles mixture

The typical results of calculations of DW parameters in gas-particles mixture is shown in Figure 1. A steady one dimensional DW in methane/O_2/N_2 mixture with WC, KCl, and Al_2O_3 microparticles is considered; α is the unitless mass fraction of condensed phase, u_D, P and T are DW velocity, pressure and temperature in Chapman-Jouguet (C.–J.) plane respectively, T_{sw} and P_{sw} are temperature and pressure behind the shock front, P_0 and T_0 are initial pressure and temperature.

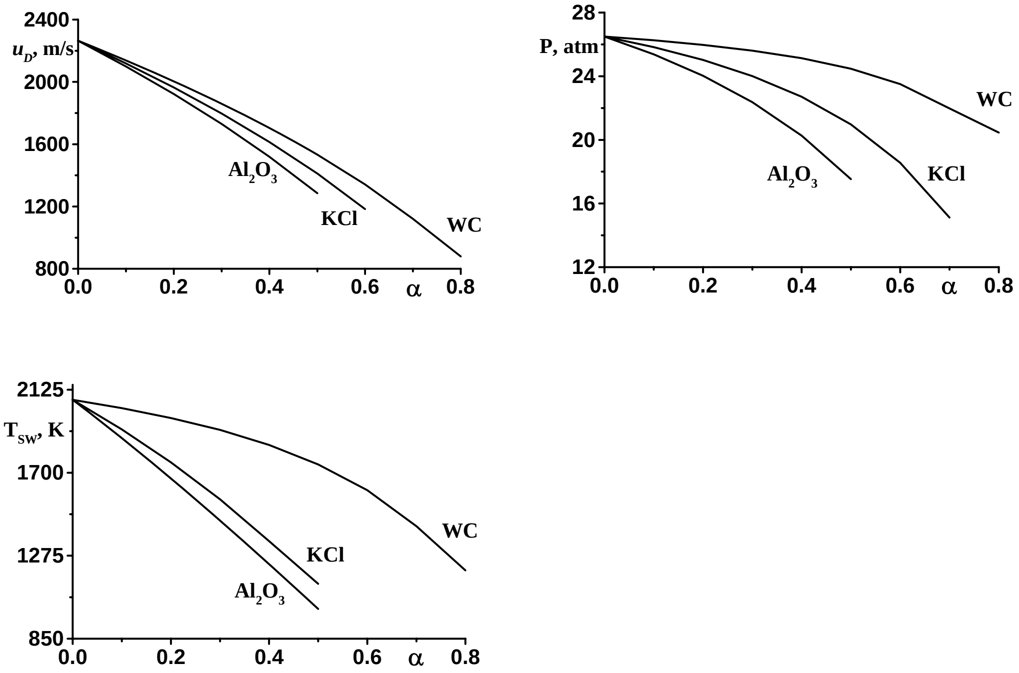

Figure 1: DW parameters in $CH_4 + 2O_2 + N_2$ mixture with Al_2O_3 , KCl and WC microparticles; $P_0 = 1$ atm, $T_0 = 273$ K

Energy losses due to heating of particles are determined by corresponding increase in enthalpy of condensed phase. The increase in enthalpy of Al_2O_3 is greater than that for KCl and WC, heated to the same temperature. As a result, as is seen from Figure 1, DW parameters in mixture with WC and KCl (i.e., the wave velocity, pressure, and temperature behind the leading shock front and in C.-J. plane) are higher than the corresponding parameters of mixture, containing Al_2O_3 particles. Similar results have been obtained for cyclohexane-, hydrogen- and silane-air mixtures.

3. Minimum total mass of a cloud; comparison with experimental data

Note the minimal total mass of particles that should be injected into the tube to suppress DW and the corresponding longitudinal size of the cloud as M and H. In Fomin and Chen (2009) model it was assumed that $F = L = a$, where L, F and a are the longitudinal size of the cloud after compression, the distance between the leading shock front and C.-J. plane and the transverse size of detonation cell respectively. In the frames of the present work it is assumed that $F \approx 3a$ and, owing to transition processes, caused by detonation wave penetration into the cloud, $L \approx 3F$. Such changes increase the accuracy of M and H calculations as compare with corresponding formulas of Fomin and Chen (2009) model. The value M, calculated in the frames of the algorithm, presented here, is shown in Figure 2; η is the unitless molar fraction of the fuel in the gas, d is a tube diameter (d = 16.4 mm). Calculations: SiO_2 microparticles; experimental results (Laffitte and Bouchet, 1959): potassium bitartrate 10–20 μm particles. Black triangles and squares correspond to experiments and calculations respectively. As can be seen, the calculated value M quite good corresponds to the available experimental results.

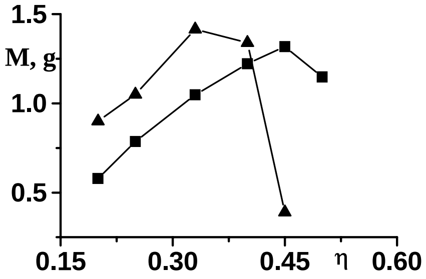

Figure 2: The minimum mass of particles, leading to detonation suppression. Mixture $\eta CH_4 + (1 - \eta)O_2$, $P_0 = 1$ *atm*, $T_0 = 298$ *K*

4. Detonation wave reflection from a rigid wall in gas-particles mixtures

A problem of DW reflection from a rigid wall in gas/chemically inert particles mixtures is considered (Figure 3a). A steady one-dimensional DW with constant C.-J. parameters behind the leading front impacts a rigid wall. As a result, reflected wave occurs. The gaseous phase behind the reflected wave front is in a state of chemical equilibrium. Such kind of reflection in gaseous mixtures called D → D reflection. The same term for DW reflection in gas/particles mixtures is used here.

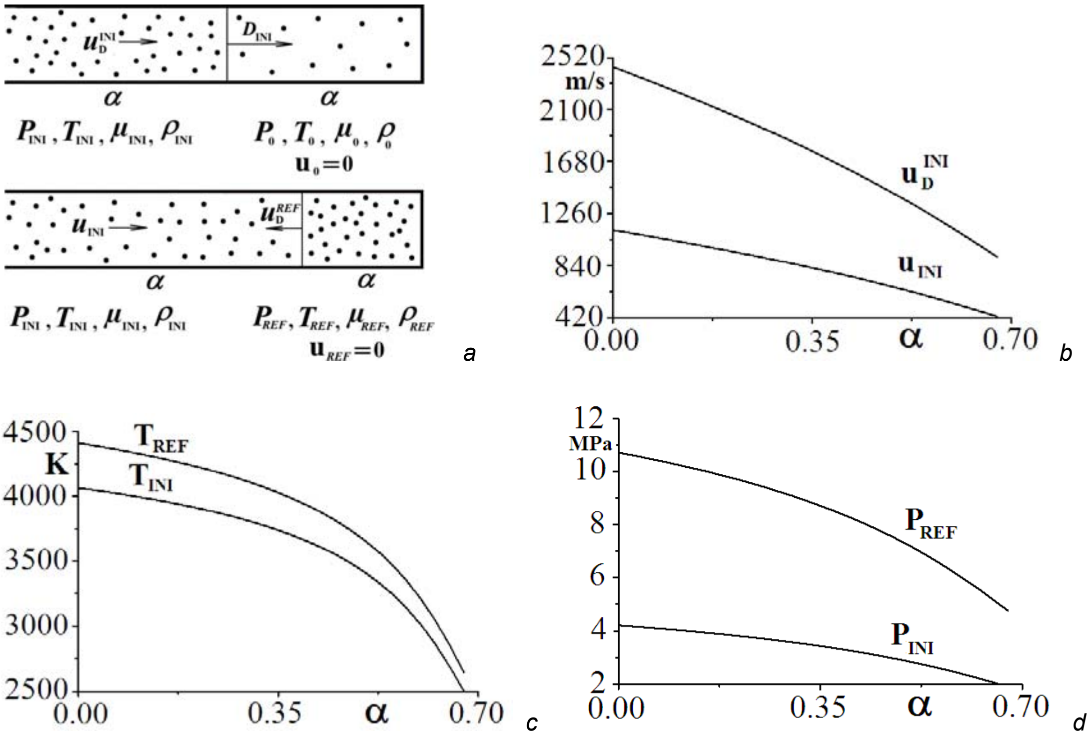

Figure 3: D → D reflection of DW in $0.1C_6H_{12} + 0.9O_2$ *mixture with* Al_2O_3 *microparticles*

Mass fraction of particles and parameters of initial detonation wave (velocity u_D^{INI}, temperature T_{INI}, pressure P_{INI}, mixture velocity u_{INI}, density ρ_{INI} and molar mass μ_{INI} of gas) assumed to be known. Parameters of reflected wave (velocity u_D^{REF}, pressure P_{REF}, temperature T_{REF}, mixture velocity u_{REF}, density ρ_{REF} and molar mass μ_{REF} of gas) should be calculated. The following system of algebraic equations is used: conservation equations of (a) mass, (b) momentum and (c) energy, (d) equation of state, (c) equation of chemical equilibrium and (d) traditional condition, that behind the reflected wave velocity of a mixture equals to zero. Thus, the number of equations equals to the number of variables.

Results of calculations of D → D reflection in mixture $0.1C_6H_{12} + 0.9O_2$ with Al_2O_3 microparticles are presented in Figure 3(b-d), α is the unitless mass fraction of condensed phase. As can be seen, particles can essentially reduce parameters of reflected wave and therefore prevent crucial destruction of equipment, caused by detonation. For example, as can be seen from Figure 3c, if mass fraction of particles increases from 0 to 0.675, a temperature behind reflected wave decreases in 1.67 times. Attenuation of pressure in this case is even more effective: its value decreases in 2.25 times (Figure 3d).

5. The influence of gas composition on DW suppression by particles injection

The efficiency of detonation wave suppression in gas-particles mixtures with different stoichiometry and mass fractions of condensed phase can be analyzed. The results of calculation of DW parameters in cyclohexane/oxygen and CH_4/oxygen mixtures with Al_2O_3 and SiO_2 microparticles and different stoichiometric relation between fuel and oxidizer are presented in Figures 4-6; η is the unitless molar fraction of the fuel in the gas, α is the unitless mass fraction of condensed phase, a_P is the transverse cell size in gas without particles, $P_0 = 1$ атм, $T_0 = 298$ K. As can be seen from Figures 5 and 6, at fixed concentration of the particles the value a/a_P has the minimum. Such minimal value corresponds to the lowest efficiency of detonation wave suppression (because the minimum value of the relative cell size corresponds to the maximum values of M and α_*). For example, if $\alpha = 0.5$, then a/a_P has the minimum value at $\eta = 0.1625$ (stoichiometric mixture corresponds to $\eta = 0.1$). It means that for this stoichiometry the efficiency of detonation wave suppression by particles injection is minimal too. An increase of the value a/a_P in fuel-lean and fuel-rich mixtures means that the efficiency of detonation suppression by particles injection increases too. But for fuel-rich mixtures such effect is not so essential.

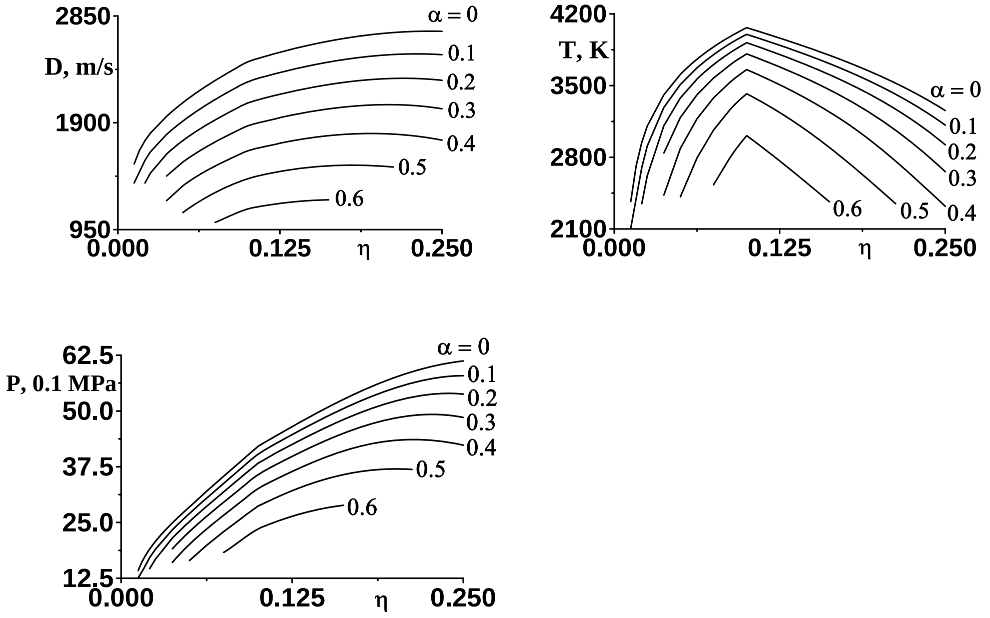

Figure 4: C.-J. parameters of DW at different stoichiometry and mass fraction of microparticles. Mixture: $\eta C_6H_{12} + (1 - \eta)O_2$ with Al_2O_3 microparticles

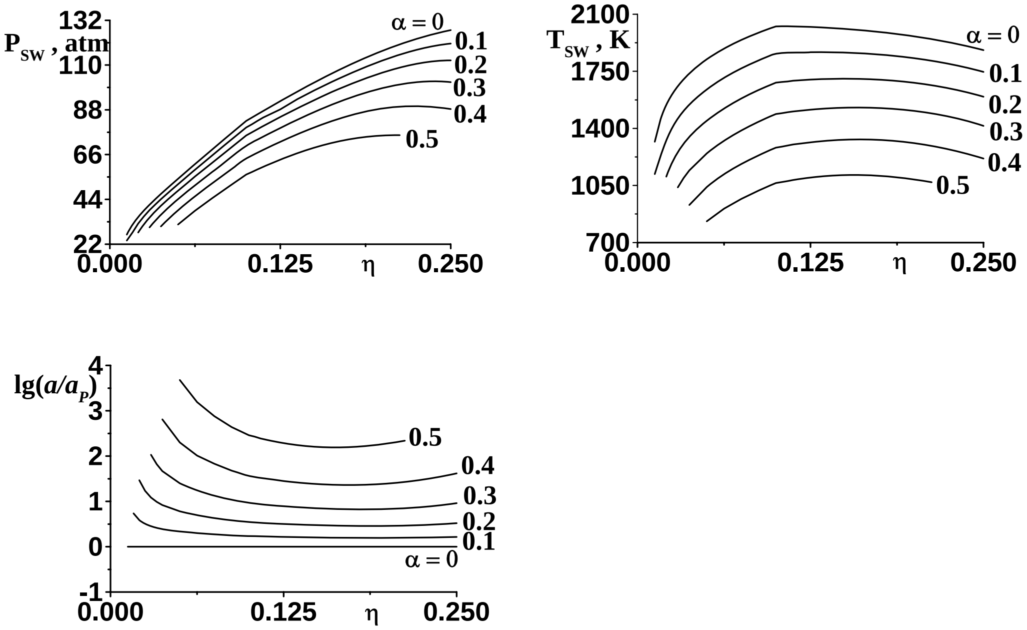

Figure 5: Von Neumann spike parameters and relative detonation cell size at different stoichiometry and mass fraction of condensed phase. Mixture ηC_6H_{12} + $(1 – \eta)O_2$ with Al_2O_3 microparticles

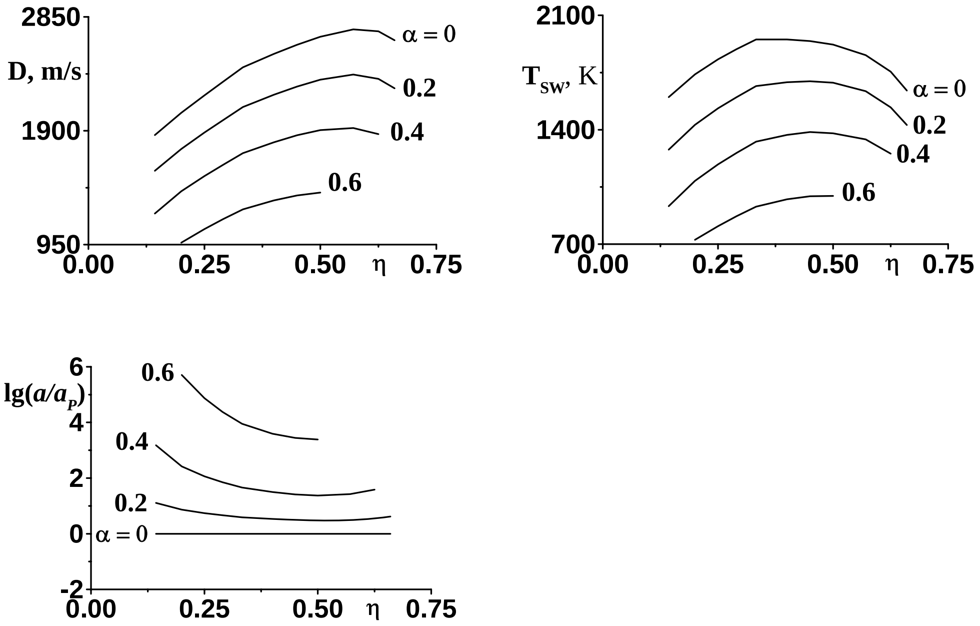

Figure 6: DW parameters and relative cell size at different stoichiometry and mass fraction of condensed phase. Mixture ηCH_4 + $(1 – \eta)O_2$ with SiO_2 microparticles

6. Detonability limits of DW in gas-particles mixtures

The algorithm for calculation the detonability limits in gaseous mixtures (see, for example, Vasil'ev, 2012) can be used for calculation the existence region of detonation waves in the gas-particles mixtures too. For this purpose, equation $a = \pi d$ and detonation cell size as a function of chemical composition of a mixture and mass fraction of a condensed phase should be used (Fedorov et al., 2012).

Methane/oxygen gaseous mixture with SiO_2 microparticles will be considered. The algorithm for calculation detonation wave parameters and relative cell size, presented here, will be used, P_0 = 1 атм, T_0 = 298 K, d = 16.4 mm. The relative cell size as a function of the chemical composition of the mixture and mass fraction of the condensed phase is shown in Figure 6, η is the unitless molar fraction of the fuel in the gas. Detonation cell size in pure methane-oxygen gaseous mixture can be found in Vasil'ev et al. (2000) article. Equation $a = \pi d$, Figure 6 and Vasil'ev et al. (2000) article allow us to calculate the detonation limits in the heterogeneous mixture under consideration (Figure 7). Results of calculations qualitatively correspond to the available experimental data (Wolanski et al., 1988).

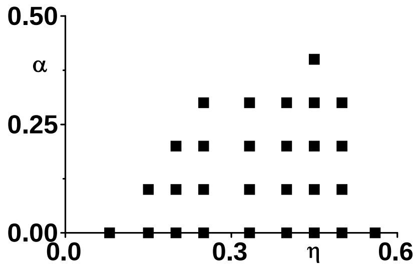

Figure 7: The existence region of detonation wave. Mixture $\eta CH_4 + (1 - \eta)O_2$ with different mass fractions of SiO_2 microparticles. Black squares correspond to the existence region of detonation wave

7. Conclusions

C.-J. parameters, cell size, limits and D → D reflection of DW in mixtures of combustible gas with chemically inert microparticles are calculated. The method of attenuation and suppression of multi-front DW in gas by particles injection is analyzed. The algorithm for estimation the minimal total mass of particles and characteristic size of the cloud, which are necessary for successful quenching of DW is presented. Results of calculations quite good correspond to the available experimental data.

It is shown, that the efficiency of detonation suppression is more effective for fuel-lean mixtures. D → D reflection of DW is considered. According to calculations, particles can essentially reduce pressure and temperature behind the reflected wave.

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