Limits of shock wave ignition of hydrogen–oxygen mixture in the presence of particles

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Abstract. It is a well known fact that the cloud of non-reacting particles in the flow weakens or even suppresses the detonation. Contrary to this phenomenon there are experimental data showing that the presence of solid particles in the combustible mixtures shorten significantly the ignition delay time. In other words particles could promote the initiation of detonation. This paper analyzes numerically the phenomenon of detonation initiation behind the shock wave in the combustible mixture containing only one solid particle. Numerical results demonstrate a significant degree of lowering of ignition limits. Namely, it is shown that it becomes possible to ignite the gaseous mixture much earlier due to the shock wave interaction with solid particle surface. It is found that ignition arises in subsonic region located between the particle and the bow shock front.

1. Introduction
Nowadays the detonation of gas–particle suspensions is of great research interest. The issue of the detonation of such mixtures is relevant for prevention of catastrophic emergency explosions, for example, in coal mines. It is important as well for justification of safety measures on the nuclear power plants. Determination of ignition mechanisms and possible paths of its control are among the fundamental scientific tasks in the line with more widely discussed issue of definition of quantitative characteristics of combustion waves initiation. One of the early works, devoted to these phenomena is [1], where in particular it is mentioned, that about 90% of all total world energy is produced by flaming of different fuels. It is significant that the International Energy Outlook 2013 (IEO2013) [2] projects that this fraction will not fall below 80% until 2040 and will combined with growth by 56% of world energy consumption between 2010 and 2040.

Among the contemporary data devoted to the detonation behavior in gas–particle suspensions the issues concerning detonation initiation and sustained propagation are of primary interest. Paper [3] proposed the model of hydrogen–oxygen detonation attenuation and suppression according to which the detonation speed decreases due to the inert solid particles addition. In [3] it was shown that detonation speed considerably decreased with reduction of particles size and growth of their volume concentration. The considered effect could be suitable for safety control on the detonation-hazardous objects. Another important issue considered in [4] concerns the model of ignition of aluminum particles suspensions in shock and detonation waves. The dependencies of ignition temperature on the shock wave parameters, the size and concentration of particles and the oxidizer content are defined in [4]. Paper [5] represents a review on shock wave initiation of dust–gas mixtures ignition. Ignition of dust particles by the incident and reflected
shock waves is considered and the dependencies of the ignition characteristics on the particles properties are obtained. The review [5] concerns experimental studies of issues of spontaneous detonation and detonation initiation by particle and their numerical treatment. In particular in [5] the opacity of the flashing mixture is observed that makes impossible experimentally to clarify the details of process of ignition of the single particle. In the experiments devoted to study ignition in the rapid compression machine [6] it was obtained that prior to the gaseous mixture ignition the micro particles occasionally suspended in the reactive atmosphere were ignited. In [7] the formation of ignition kernels inside shock tube reactor were also coupled with the presence of particles artificially suspended in the gaseous mixture by experimentalists. As these particles were able to provide local additional energy due to friction or due to catalytic reactions they induced local ignition events.

Although there are a lot of information on the solid microparticles effect on detonation initiation and propagation phenomena there are still no clear understanding of the particular role of single particles in these processes. Due to this the aim of this paper was to analyze in details the behavior of compressed mixture flow in the vicinity of solid particle surface. Recently in [8] we analyzed numerically the interaction of the shock wave with a single particle in non-reactive gas that allowed us to visualize temperature fields forming in the vicinity of solid particle surface. It was observed that the gaseous mixture is subjected to additional heating in the region between frontal surface of the particle and the bow shock wave as well as in the wake behind the particle. Here we decided to enrich the data obtained earlier and considered the case of reactive mixture that allowed us to visualize ignition phenomenon itself and estimate possible decrease in ignition delays and lowering in ignition limits.

2. Problem setup
To achieve clear understanding of the single particle effect on the ignition phenomenon we studied numerically the following idealized problem. A 160-µm particle was placed in the flow of compressed gas behind the shock wave generated in the shock tube as a result of discontinuity decay. Schematically the problem setup is presented in figure 1. Before initial time instant a diaphragm of zero thickness splitted the tube into two regions: driver section filled with high-pressurized helium and driven chamber filled with test mixture—stoichiometric hydrogen–oxygen mixture at specified initial pressure $P_0$. Both gases were at initial temperature $T_0 = 300$ K. Two series of calculations were carried out with initial pressure of test mixture $P_0 = 0.1$ bar and 1.0 bar. In case $P_0 = 0.1$ bar $P_1$ was varied in the range 30–80 bar that corresponded to the certain ranges of pressure and temperature of the gas behind the shock wave: $P_a = 1.34–1.74$ bar and $T_a = 883–1045$ K. In case $P_0 = 1.0$ bar the considered range of compressed gas parameters was $P_a = 13.5–17.3$ bar and $T_a = 886–1048$ K. In such a way the diapason of temperatures near the self-ignition limit was studied at near-normal ($P_a = 1.34–1.74$ bar) and elevated ($P_a = 13.5–17.3$ bar) pressures.

Boundary conditions on the tube walls and particle surface were assumed to be adiabatic in our calculations. In addition the particle was assumed to be motionless. It should be noted that adiabatic approximations is acceptable only when duration of the process does not exceed time of the temperature relaxation $t_t \approx R^2/\chi$, where $\chi$—coefficient of thermal diffusivity of the particle, m²/s; $R$—particle radius. Immovability approximation can be used only if duration of the process is not longer than time of velocity relaxation $t_v = m/(6\pi\eta R)$, where $m$—the mass of the particle, $\eta$—dynamic viscosity, Pa·s. In view of considered problem setup in such a way we studied the processes taking place in the neighborhood of the particle after arrival of the shock wave front during time interval much more smaller than both times of relaxation. In such formulation of the problem heat conductivity and thermal capacity of the particle were excluded. To check the assumptions, quantitative estimation of heat absorbed by the particle from the flow were carried out in order to analyze how the temperature field changes if the
Figure 1. Problem setup: 1—driver gas under high pressure; 2—diaphragm of zero thickness; 3—test mixture.

specified properties of the particle will be taken into account. The calculations shown that the heat absorbed by the particle is much less than that gained due to the braking action of the particle. Therefore temperature field does not change significantly whether heat conductivity and thermal capacity of the particle are taken into account or not.

The radius of the shock tube was chosen in such a way to avoid effects of oblique reflected shocks on the processes evolving in the vicinity of 160-µm particle.

The calculations were performed using the code based on the Lagrange–Euler algorithm also called as “coarse particles method” [9] recently used to study a wide range of combustion and detonation related phenomena (see e.g. review [10]). The equations of state for fresh mixture and combustion products were assigned by interpolation of data taken from NASA tables [11]. Chemical kinetics of hydrogen–oxygen combustion is described by well proved reduced scheme consisting of only nine reactions [12]. Chosen kinetics scheme reproduces with a good accuracy both qualitative and quantitative features of ignition and burning of hydrogen–oxygen mixture.

To confirm the acceptability of the code for numerical analysis of shock–particle interaction we tested the code using a simplified problem on the determination of maximum heating generated in the flow by its full stop and reflection from completely rigid wall. The obtained results occurred to be in a good accordance with the analytical estimations for ideal gas [13]. A good agreement between pressure values obtained analytically and numerically is shown in figure 2. Numerically obtained temperature values occurred to be a bit smaller (about 5%) compared with analytically predicted.

3. Results
Consider first the simplest one-dimensional case of ignition behind the incident shock wave driven by expanding driver gas. The exothermal reaction in such a case starts far behind the shock front since the gas directly ahead the contact surface is in compressed state for longer time period, so the progress of reaction in this region achieves transition to exothermal stage earlier. Ignition delay in one-dimensional simplified problem corresponds to that realized at $T_a$ and $P_a$. In case when the 160-µm particle is put into the flow a high temperature region is formed between the particle and the bow shock which forms ahead of the particle as it is shown
Figure 2. Dependence of pressure ($P_r$) behind reflected shock on pressure ($P_a$) behind incident shock.

Table 1. Limits of shock wave ignition of stoichiometric hydrogen–oxygen mixture.

| $P_0$, bar | $P_1$, bar |
|------------|------------|
| Without particle | With particle | In reflected shock |
| 0.1 | 65 | 20 | 7 |
| 1 | 750 | 350 | 100 |

in figure 3. The particular mechanism of energy thermalization in this region is associated with flow deceleration when interacting with particle. As well there is a heated region in the wake behind the particle that is related with the dissipation in the shear layers. It should be noted that in considered cases corresponding to near-ignition conditions (i.e. high enough temperatures) the flow formed behind the incident shock wave is supersonic. Therefore the regions of higher temperature corresponds to the regions of flow deceleration down to subsonic velocities. These regions are visualized in figure 3 with the use of sonic line where the local value of Mach number equals 1.0.

Consider now the numerical results obtained for the case $P_0 = 0.1$ bar and correspondingly $P_a \sim 1.0$ bar. One-dimensional simulations showed that in tube 0.6 m long the ignition does not take place below the temperature $T_a = 994$ K ($P_a = 1.61$ bar). This means that the ignition delay in this case is much greater than the time during which the flow of compressed gas passes the distance of 0.6 m length. At the same conditions but in presence of particle this limit goes down to $T_a = 820$ K ($P_a = 1.19$ bar). In case of elevated pressures ($P_a \sim 10.0$ bar) the ignition limit occurs to be higher—$T_a = 909$ K ($P_a = 14$ bar) in presence of particle. The fact that the
Figure 3. Schematic diagram of particle–gas interaction in supersonic flow.

ignition limit goes up with the increase in initial pressure is well known and related with the peculiarities of hydrogen–oxygen combustion kinetics (see e.g. [14]). One can easily obtain that at higher pressures the ignition limit is displaced to the region of higher temperatures.

Table 1 represents the comparison between the regime parameters (initial pressures of test mixture and driver gas) sufficient for hydrogen–oxygen mixture ignition in the driven section of 0.6 m length: $P_0$—pressure in low pressure chamber, $P_1$—pressure in high pressure chamber. One can clearly see that the ignition possibility increases noticeably with the addition of single 160-µm particle into the flow. The intensity of the shock wave necessary to ignite mixture in the tube of given length decreases by two or even three times. Generally speaking the basic mechanism of ignition in case of compressed flow interaction with a particle is the deceleration of the flow. Although it should be noted that in contrast to the case of flow deceleration by the solid wall the criterion of ignition in case of flow–particle interaction is stricter. The initial pressure of driver gas sufficient for hydrogen–oxygen mixture ignition behind the shock reflected from the solid wall is presented in the third column of table 1.

When the particle location relative diaphragm is varied, the limit of ignition becomes somewhat smaller in terms of temperature and pressure if the particle is set on larger distance from the diaphragm. This effect is obviously related with later arrival of the contact surface to the particle. For this reason the test mixture in the vicinity of particle is at high temperature during longer time period.

Figure 4 represents the temperature field evolution at subsequent time instants that illustrates the evolution of ignition phenomenon in the vicinity of particle. One can observe that ignition of test mixture arises inside the subsonic region. After successful ignition the combustion spreads outwardly from the ignition kernel including the direction opposite to the bulk flow. The latter fact indicates that the speed of combustion front propagation is at least higher than the sonic speed in the compressed mixture. This allows to propose that such a reaction wave is able to form a detonation wave propagating at least in the direction opposite to the bulk flow. The mechanism of such combustion wave propagation can be related with the fact that adjacent layers of the mixture are already heated up to near critical temperature and the reaction inside them has already started. Additional energy transfer out from the combustion zone could promote
Figure 4. Ignition and propagation of combustion wave. Frames correspond to flow patterns in consecutive time instants. Time interval between frames is 0.1 $\mu$s. Black line shows sonic line.

the exothermal reaction in these layers. As a result such a combustion wave would propagate and even accelerate that in number of cases could lead to the combustion wave speed increase up to the sonic speed in the combustion products and subsequent onset of detonation.
4. Conclusions
Obtained results clearly illustrate the possibility of early ignition event arising in the shock–induced flow in presence of single solid 100-µm particle. The ignition takes place in the heated region which origins are related with energy thermalization inside the regions of flow deceleration. The discussed phenomenon is of paramount interest for the issues of explosive safety when the dust particles always presenting in the environment could affect significantly the processes of explosion evolution. Thus the dynamical processes such as shock waves could be effectively intensified via the additional mechanisms associated with their energy thermalization inside localized regions. As well the discussed phenomenon is of interest for fundamental studies in the field of chemical kinetics where the occasional solid particles could play a role of ignition kernels and disturb the obtained data.

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