Calculation of the shock waves interaction with various diameter spheres in hydrogen-air mixture

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Abstract. The results of modeling shock waves interaction with spheres are presented. The Mach number was chosen so as the temperature behind the shock waves front would not exceed the auto-ignition temperature of hydrogen in air. A mathematical model and a reduced kinetic scheme of chemical reactions verified previously were used. The dependences of the mixture time of ignition beginning along the width of the channel and its location from the Mach number of the shock wave were refined. The flow pictures for two spheres located one behind the other were obtained. The analysis of the results was carried out.

1. Introduction

The study of combustion initiation and stabilization by the shock waves interaction with spheres of different diameters is important both from the scientific and technical points of view. The investigation of combustion and detonation development and suppression covers a wide area of science connected with explosion safety, namely the development of the methods for suppressing gas detonation by inert particles. This problem is also interesting for studying the issues of combustion initiating at the micro level, as well as initiating and re-initiating detonation when interacting of the shock wave (propagating along a combustible mixture) with particles.

Currently, there are a lot of works devoted to this issue, which indicates the relevance of this problem for the whole world. To model the phenomena considered it is necessary to familiarize with a certain number of experimental and theoretical works devoted to combustion and detonation processes. For example, experimental and theoretical studies of the detonation initiation are presented in the works of A. A. Vasiliev [1], [2], [3], [4]. A special attention should be paid to the work [1]. This paper presents a large review of various combustion regimes when a high-speed body passes through combustible gas. The estimation of the energy required for initiating detonation in certain conditions was carried out. The analytical correlation between the aerodynamic characteristics of the high-speed body and the physicochemical parameters of the combustible mixture was proposed as a criterion for initiating gas detonation. The review of experimental data agreeing well with the theoretical approach proposed is presented.

Returning to the question of the shock waves interaction with particles, we should notice a number of works mainly devoted to the study of the shock and detonation waves passage through a cloud of particles. For example, the shock wave passage through a system of fixed bodies was experimentally investigated in work [5]. The results of study of the dynamics and physical conditions of the collective head shock formation in front of the spheres with the line of centers placed across the supersonic flow behind the transmitted shock wave are presented in this paper. Various types of shock wave structures were recorded in the experiments. The quantitative criterions of existence of these regimes and their transition to a common head shock were determined with using the local theory of interference of gas-
dynamic discontinuities. The criterions obtained were confirmed in a series of experiments on transient conditions.

Shock waves propagation in a cloud of particles was experimentally and theoretically studied in [6]. Use was made of continuous-discrete model of the laminar flow mixture of gas and particles for calculations. The qualitative restructuring effect of a supersonic flow behind the shock wave in the cloud of particles was obtained in the dispersed phase volume concentrations range of 0.1–3%.

In the work [7], parametric investigation of the influence of the shock wave interaction with the sphere located above the plate on lifting force of this sphere was carried out. The lifting force source is the secondary SW reflected from the flat plate and falling on the lower part of the sphere. This study was conducted in a non-viscous and viscous setting. In each case, the relation between the distance from the plate to the sphere and its diameter was investigated. As the sphere gets close the plate the lift coefficient increases. The influence of the falling SW Mach number was studied for the inviscid case. Reducing of the Mach number lead to increasing lift coefficient. In general, accounting viscosity results in a higher lift coefficient.

In the paper [8], the results of numerical simulation of the shock wave propagation in the air above the particle and array of aluminum particles for Mach numbers up to 10 are presented. A special feature of the mathematical model and the numerical algorithm is to be carried out of through calculation in the gas phase and inside the particles. The drag coefficient was calculated depending time and that the maximum drag coefficient decreasing at the Mach number increasing was shown. It was shown for array of particles that the shock wave amplifies when passing on each subsequent particle and the maximum of the drag coefficient increases. For the last particle normalized drag coefficient depending on the distance between the particles for two Mach numbers was established. The existence of distance between particles where the magnitude of the normalized resistance coefficient is maximum was shown. In [9], this approach was evolved for modeling particles deformation.

The present work considers the ignition and combustion of a hydrogen-air mixture by the passing shock wave interacting with fixed spherical particles. Such issue is very interesting from the viewpoint of explosion and fire safety, because the energy impact for ignition initiation of a combustible mixture less than for detonation initiation.

2. Problem formulation

The problem formulation was the same as in previous studies [10]. However, in addition to calculations of the shock wave interaction with one fixed particle, calculations for two particles with a diameter of 10 mm were carried out. The particles were located one behind the another (Figure 1).
The distance between the particles centers was varied from 30 mm to 50 mm. The computational domain was filled with stoichiometric hydrogen-air mixture with the parameters: static temperature $T_{st} = 300$ K, static pressure $P_{st} = 100$ kPa. The shock wave interacted with spheres was simulated in this area. The parameters of the mixture behind the shock front varied depending on the shock wave Mach number. Calculations were carried out for Mach numbers $M_{sw} = 2.65 \div 2.85$. The Mach number was chosen so as the temperature behind the front of SW did not exceed the auto-ignition temperature of hydrogen in air.

3. Mathematical model

As in the previous paper [10], the problem considered was solved in a 2-D axisymmetric formulation. Use were made of Favre-averaged Navier-Stokes equations for multicomponent gas mixture supplementing by an SST modification of the $k-\omega$ turbulence model as a mathematical one. The reduced Arenius kinetic scheme including one gross reaction of hydrogen burning in air was used for the chemical kinetics simulation. In the work [11], this kinetic scheme was verified according to the experimental data on the ignition delay and the propagation velocity of the detonation wave under different conditions.

The ANSYS Fluent software package, which well proved itself in our previous works on the interaction of shock and detonation waves with microparticles, was used as a solver. In the non-stationary formulation, implicit second-order scheme for temporal approximation, and the AUSM flux vector splitting method with a second-order upwind scheme for spatial approximation were used.

In [12], the mathematical model presented and the calculated algorithm were subjected to additional verification against experimental data [13] on the detonation cell size and detonation modes. Comparative analysis showed that the approach used allows us to model complicated detonation processes, and in addition to qualitative agreement between the calculated and experimental flow pictures we achieved a quantitative agreement between detonation cell sizes.

A detailed quadrangular orthogonal grid was used. For convenience, the computational grid was divided into blocks in which the grid was constructed separately. Such way allows us to avoid unnecessary condensations, reduce the total number of grid nodes without increasing the grid step.

4. Calculations results

At the beginning, the calculations of the shock wave interaction with a single sphere with diameter $d = 10$ mm for Mach numbers 2.7 and 2.8 were made to specify dependences of the mixture time of ignition beginning of the over the entire width of the channel and its location from the Mach number of the shock wave obtained in [10]. Figure 2 presents these dependencies.

![Figure 2](image)

**Figure 2.** Dependencies of time and position of hydrogen-air mixture ignition at $d=10$ mm.

a) $L = f(M_{sw})$. b) $t = f(M_{sw})$. 

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Equations approximating the dependencies obtained:

\[ t = 5.8857M_{sw}^2 - 34.647M_{sw} + 51.221 \]  
\[ L = 3.7143M_{sw}^2 - 22.049M_{sw} + 32.748 \]

Further, the simulation of the SW interaction with two particles with a diameter of 10 mm spaced 30mm from each other was conducted. Figure 3 shows simulation results for Mach number 2.85.

Figure 3. Static temperature fields for Mach number 2.85 at different time.

Comparing the results for one and two spheres shows that adding a second sphere, at the distance of 30 mm, does not influence the character of the flow (time of ignition beginning changes slightly). As in the case with single a sphere in spite of the quite high temperature behind the head shock, the ignition begins in the wake of the sphere. The ignition area is slightly wider, however, this is not enough to intensify the combustion. The time and place of hydrogen-air mixture ignition beginning over the entire width of the channel remain practically unchanged.
A similar situation is observed with increasing Mach number. Figures 4 shows the simulation results for Mach 2.75 and 2.85. Increasing Mach number of the shock wave makes it possible to accelerate the ignition process. However it is not possible to achieve a more intense combustion in comparison with the case for one sphere.

![Figure 4](image.png)

**Figure 4.** Static temperature fields for Mach number 2.75 (a) and for Mach number 2.65 (b) at different time.

With increasing the distance between the spheres to 50 mm the flow pattern does not change substantially. Figure 5 shows the simulation results for Mach number 2.85.

![Figure 5](image.png)

**Figure 5.** Static temperature fields for Mach number 2.85.
By analogy with the previous case, adding a second sphere at a farther distance does not change the nature of the flow in the range studied of Mach number (Figure 6-7). Intensification is achieved by increasing mixture parameters behind the shock front.

![Figure 6. Static temperature fields for Mach number 2.65.](image)

![Figure 7. Static temperature fields for Mach number 2.75.](image)

It does not make sense to represent the calculation results for a sphere with 1 mm diameter, because in [10] it was found that such sphere is too small to initiate combustion and the present paper shows that adding the second sphere does not influence on the combustion intensification of hydrogen-air mixture.

As a result, it can be concluded that adding a second sphere and changing the distance between them does not lead to any significant consequences. Thus, the determining parameters for the intensification of combustion in the interaction of a SW with a particle are the Mach number of the shock wave and the particle size.
5. Conclusions
The problem of the shock wave interaction with two particles arranged one behind the another was solved using a previously developed mathematical model and mathematical technology for its implementation based on the ANSYS Fluent package.

The equations approximating the dependences of the onset time and the ignition position of the hydrogen-air mixture over the entire width of the channel are refined.

It was revealed that the presence of a second sphere, as well as a change in the distance between the spheres, does not change the nature of the flow and does not allow us to significant intensification of the ignition and combustion of the mixture.

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Nomenclature
- $T_{st}$ - static temperature;
- $P_{st}$ - static pressure;
- $M_{sw}$ - shock wave Mach number;
- $L$ - location of ignition beginning of the over the entire width of the channel;
- $t$ - time of ignition beginning of the over the entire width of the channel.

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