Mathematical modeling of the detonation wave and inert particles interaction at the macro and micro levels

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Abstract. Calculation technology for modelling of two-dimensional detonation flows in a system of the reacting gas mixture-inert particles has been developed. The problems associated with the cellular detonation suppression are researched. The interaction of the detonation wave with inert particles is modeled using the macro and micro approaches. First, the interaction with Al₂O₃ particles with a diameter of 100 μm and 1 mm at the macro level was investigated using a continuum approach. Values of the volume concentration resulting in a change of the detonation cell size, weakening of the detonation wave, and suppression detonation are obtained. Secondly, a simulation of the detonation wave interaction with particles at the micro level has been carried out. A wave structure of the flow near the particles is obtained and the mechanism of detonation suppression was shown at volume concentrations of particles close to those obtained in modeling at the macro level.

1. Introduction

It is known that detonation waves in gas and heterogeneous combustible mixtures have a cellular structure [1-2]. It has also been established that the addition of inert particles to an explosive mixture contributes to the suppression of detonation [3-12]. The interaction between detonation waves and inert particles have been studied mainly in one dimension, resulting in estimates of the effect of volume fraction, particle diameter, and their thermophysical properties on the ability to attenuate and suppress detonation. However, the nonuniform structure of the detonation cell undoubtedly influences the parameters of mixtures of explosive gases with chemically inert particles and the limiting detonation characteristics. It can be noted that the interaction of cellular detonation waves in gases and mixtures of gas with inert particles has been the subject of a few studies, e.g., [13-14]. Thus, it is of both theoretical and practical interest to investigate the detonation-wave parameters and estimate the detonation cell size in mixtures of combustible gases and inert particles.

The interaction of a detonation wave with inert particles is investigated in the work by means of two approaches. On the one hand, the modeling of the problem at the macro level is carried out, when the cellular detonation wave is suppressed by a cloud of stationary particles. On the other hand, the direct simulation of the detonation wave interaction with fixed particles at the micro level has been studied.

2. Mathematical model and numerical implementation

In the initial stage of the study, we consider the interaction of a cellular detonation wave with a cloud of inert fixed isothermal particles or a porous filter. This assumption is possible in the case of...
interaction with relatively large particles, where the velocity and temperature of the particles do not vary significantly during the passage of the detonation wave. To test this assumption, we estimated the velocity and thermal relaxation times for a single particle of alumina (Al₂O₃), sand (SiO₂), and tungsten carbide (WC) of diameter 1 μm ±1 mm in the gas flow behind a detonation wave. The calculations of the ratio of the velocity and thermal relaxation times of the particles showed that for alumina and sand particles, which have comparable densities and similar heat capacities, for diameters of 1-100 μm, the velocity relaxation time somewhat exceeds the thermal relaxation time. For tungsten carbide particles, having a high density and lower specific heat, the velocity relaxation time is about an order of magnitude higher than the thermal relaxation time over the whole range of diameters, with this difference decreasing somewhat with increasing diameter. The estimates allow us to judge the applicability of the process model used in this study. It can be seen from the tables that, for particles larger than 100 μm, the thermal and thermal relaxation time is an order of magnitude higher than the gas-dynamic time of transit of the detonation wave through the mixture. Thus, particles of this size can be considered fixed and isothermal.

The mathematical model includes the Favre-averaged Navier-Stokes equations for a multicomponent gas mixture with allowance for chemical reactions, supplemented by the SST modification of the k-ω model of turbulence. The interaction with fixed particles for the macro level problem was determined by means of a source term in the equations of momentum and energy. The solution was carried out in a two-dimensional formulation. As boundary conditions on the channel walls, standard no-slip conditions for velocities were set. The heat fluxes were equal to zero on the walls when solving the problem at the macro level in the continuum approach. The particle surfaces were assumed to be isothermal with a temperature of 300 K at the micro level.

As in any problem with chemical reactions, when modeling flows with detonation waves, the problem arises of choosing an appropriate kinetic scheme for description of the combustion process. A scheme with reduced or detailed kinetics can be chosen. The detailed kinetics allows for more accurately reproducing parameters such as the ignition delay time and burning time of the mixture, especially at the limiting modes, but it requires a great deal of computer time. In [15], three models of the chemical kinetics of hydrogen combustion in oxygen and three gas-dynamic models of the flow of the reacting mixture behind the front of the initiating shock wave were analyzed. In [16], the use of certain kinetic models of the hydrogen-air mixture is justified to describe detonation. The verification performed on the experimental data on the ignition delay time and on the velocity of the detonation wave made it possible to determine the kinetic parameters of the model. Based on the detailed and reduced kinetic mechanisms of nonequilibrium chemical transformations within the framework of the ANSYS Fluent software, a mathematical technology was developed to describe the spread of cellular detonation in the channels. It is shown that the detonation cell size corresponds to the experimental data. Chemical reactions in the gas phase at this paper were modeled by a reduced one-stage kinetic model. In [16], this kinetic scheme was verified by the experimental data on the ignition delay times and the detonation wave velocity under various conditions.

The ANSYS Fluent software was used to simulate the two-dimensional problem of propagation and suppression of a detonation wave. An explicit fourth-order Runge-Kutta scheme and an implicit second-order scheme were used for approximation in time. The explicit scheme was found to be preferred for calculations of inviscid flows. The calculations results show that the implicit scheme has a somewhat larger numerical dissipation than the explicit fourth-order method, which leads to a greater smearing of shock-wave fronts. However, due to constraints on the stability conditions, the use of the explicit scheme for problems with viscosity significantly increases the computation time. The viscous formulation in this case will require a too small time step from the point of view of feasibility of the calculation on a computer. Convective terms are approximated in space using a second-order AUSM upwind scheme.

In the calculations, we used a moving quadrangular mesh that thickened towards the surface of the body and adapted, as to the density gradient, to the gas-dynamic features of the flow (shock waves, contact discontinuities, rarefaction waves). In the vicinity of particles moving in the gas under the
action of the propagating shock wave the mesh moved together with the particles moving in the gas flow arising under the action of the shock wave. In constructing the mesh, the parameter \( y^+ \) on the particle surface was checked, which in all calculations did not exceed unity. Figure 1 shows an example of such a computational mesh adapted in the solution process for micro level problem. From this figure it is clearly seen how the computational mesh adapts itself to the features of the flow – the bow and hanging shock waves and the transmitted shock wave that arise in the flow in the vicinity of the particles system.

![Figure 1. Example of the dynamically adaptive computational mesh.](image)

3. **Formulation of the problem**

Plane overdriven detonation wave was used as the initial data to obtain a cellular detonation wave. Then cellular detonation wave was used at channel inlet, and a mixture of hydrogen and air and particles distributed in space were located in a low-pressure chamber (LPC) \( (p_0 = 1 \text{ atm}, T_0 = 296 \text{ K}) \), (Figure 3) for macro level problem. After the start of the calculation, the detonation wave moved from left to right and was attenuated by the presence of cold particles \( (\text{Al}_2\text{O}_3) \). At this stage of the study, the cloud of particles filled the entire LPC.

![Figure 2. Diagram of the computational domain for the macro level problem.](image)

The plane detonation wave with parameters close to the Chapman-Jouguet solution was set in the inlet section of the channel for solving the micro level problem. The flow diagram can be understood from Figure 1. From three to seven particles were arranged in a staggered order in the calculation area. The upper and lower boundaries of the computational domain were symmetry lines.

4. **Calculation results**

4.1. **Macro level problem**

Let us now consider the problem of the interaction of a cellular detonation wave with a cloud of inert fixed isothermal particles. The particles have a diameter of 100 \( \mu \text{m} \) and 1 mm. The left boundary of the cloud is at \( x = 0.2 \text{ m} \). The cloud occupies all the space to the right boundary of the computational domain. The diameter of the detonation cell for the stoichiometric mixture of hydrogen and air is approximately 15 mm; accordingly, three cells are accommodated within the channel width at the initial time. Figure 3 shows the maximum pressure field in time for particles with diameter \( d = 100 \mu \text{m} \) and volume fraction \( m_2 = 10^{-4} \). For this concentration, there is no significant change in the structure of the cellular wave. The number of cells is constant over the entire length of the cloud. Under these
conditions, the deficit of the detonation wave velocity is \( \eta = D/D_{CJ} = 0.93 \), where \( D \) is the DW velocity and \( D_{CJ} \) is the Chapman-Jouguet velocity.

**Figure 3.** Time history of the maximum pressure field during interaction with a cloud of particles for \( d = 100 \mu m \) and \( m_2 = 10^{-4} \).

Increasing the volume fraction of particles by an order of magnitude changes the structure of the cellular wave. Density isolines at different times are shown in Figure 4. At the time of 112 \( \mu sec \), three more cells are accommodated within the channel width, but at the time of 228 \( \mu sec \), the wave structure changes and the cell size increases.

**Figure 4.** Density isolines at different times for particles with \( d = 100 \mu m \) and \( m_2 = 10^{-3} \).

This is confirmed by the maximum pressure picture shown in Figure 5. In the channel cross-section at \( x = 0.6 \) m, an irregular cellular detonation propagation regime is observed, and at \( x = 0.9 \) m, one and one-half cell is accommodated within the channel width. The velocity deficit in this case is \( \eta = 0.89 \).

**Figure 5.** Time history of the maximum pressure field during interaction with a cloud of particles for \( d = 100 \mu m \) and \( m_2 = 10^{-3} \).

Increasing the volume fraction of particles to \( 10^{-2} \) leads to rapid failure and quenching of detonation. The results of the calculations are shown in Figure 7 and 8. Detonation failure is observed already at a time of 70 \( \mu s \) and at \( x = 0.27 \) m. At a time of 260 \( \mu s \) and at \( x = 0.41 \) m, the cellular detonation degenerates into a shock wave without further re-initiation.

**Figure 6.** Density isolines at different times for particles with \( d = 100 \mu m \) and \( m_2 = 10^{-2} \).
Interaction with a cloud of particles $d = 1$ mm is shown in Figure 8, 9. The maximum pressure field in time for volume fraction $m_2 = 5\cdot10^{-2}$ and $m_2 = 10^{-1}$ are presented. The volume fraction value for detonation suppression increases with growing of the particles diameter. Cell size increases and the deficit of the detonation wave velocity is $\eta = 0.75$ at volume fraction $m_2 = 5\cdot10^{-2}$ (Figure 8). Detonation suppression occurs at volume fraction value $m_2 = 10^{-1}$ (Figure 9).

**Figure 7.** Time history of the maximum pressure field during interaction with a cloud of particles for $d = 100$ μm and $m_2 = 10^{-2}$.

**Figure 8.** Time history of the maximum pressure field during interaction with a cloud of particles for $d = 1$ mm and $m_2 = 5\cdot10^{-2}$.

**Figure 9.** Time history of the maximum pressure field during interaction with a cloud of particles for $d = 1$ mm and $m_2 = 10^{-1}$.

4.2. **Micro level problem**

Simulation of the plane detonation wave passing through a grid of fixed particles with 1 mm diameter is performed. Calculations for three, five, and seven particles located in a staggered manner at different relative distances between the particles $k = l/d$ ($l$ – distance between particles, $d$ – particle diameter) are done. Analysis of shock-wave configurations in the flow behind detonation wave has shown that, depending on the transverse distance between the particles, different modes of shock waves interaction can arise. The collective configuration of shock waves is realized at small distances. As the distance between the bodies increases, a transition from a collective flow around the particles to an individual flow around each particle (first, with Mach interaction and then with regular interaction of shock waves) occurs. Figure 10 shows pressure field for detonation wave interaction with three particles at $k = 5$ at different times. This distance between the particles corresponds to a volume fraction $\sim 10^{-2}$. Note that the upper and lower boundaries of the computational domain are symmetry lines. We can observe the formation of a collective shock wave in front of the particles in this figure. The collective shock wave passes through a regular (time 14 μs) and Mach (25 μs) interaction at the process of its formation. Particles are a source of perturbations for a plane detonation front. A plane detonation wave is transformed into a cellular-like wave at a time of 25 μs. Detonation suppression is not observed for this case.

When the distance between particles is reduced to $k = 3$ (corresponds to a volume fraction $\sim 10^{-3}$) and the length of the “cloud” is increased (up to 7 particles), a separation of the detonation wave front into a shock wave and a combustion wave is occurred. Figure 11 shows the temperature fields at different times. The separation can be observed at the time of 18 μs in Fig. 11. Than the combustion wave...
overtake the shock wave and the re-initiation of detonation takes place. With an increase of the “cloud” length it is possible to completely suppress detonation without re-initiation.

Figure 10. The pressure flowfield at different times for three particles at $k = 5$.

Figure 11. The temperature flowfield at different times for seven particles at $k = 3$.

5. Conclusions

- Within the framework of the ANSYS Fluent software, a mathematical technology was developed to describe 2-D cellular detonation wave interaction with inert particles.
- The values of the particles volume fraction are obtained resulting in a change of the detonation cell size, weakening of the detonation wave, and detonation suppression.
- A technology for modeling the interaction of a detonation wave with particles at a micro level has been developed. A wave structure of the flow near the particles is obtained. The mechanism of detonation suppression is shown at volume concentrations of particles close to those obtained in modeling at the macro level.

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