Numerical simulation of the suppression of cellular detonation by inert particles

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Abstract. The simulation of a cellular detonation wave propagating along a hydrogen-air mixture with a cloud of alumina microparticles was carried out. The gas dynamics was modeled by the system of Navier-Stokes equations describing the motion of a viscous compressible heat-conducting gas, with allowance for multicomponent nature of the gas mixture and chemical kinetics. A methodology has been developed for calculating detonation currents in ANSYS Fluent using the reduced kinetics. The reduced kinetics was verified by the size of the detonation cell. The interaction with inert particles with a diameter of 0.3÷100 μm and volume fraction of \(10^{-4}÷10^{-2}\) was investigated using a continuum approach. Values of the volume fraction resulting in a change of the detonation cell size, weakening of the detonation wave, and detonation suppression have been obtained.

1. Introduction

The problem of the mechanics of reacting heterogeneous media is investigated. It is associated with the development of methods for studying shock-wave, explosive and detonation phenomena in reacting mixtures of gases and microparticles. The problem is caused by questions of explosion and fire safety, in particular, by the development of methods for suppressing gas detonation by inert particles. It is known that the detonation wave in gas and heterogeneous combustible mixtures has a cellular structure [1-2]. It has also been established that the addition of inert particles to the explosive mixture contributes to the detonation suppression [3-6]. The study of the interaction of detonation waves and inert particles is mainly carried out in a one-dimensional formulation and allows estimating the effect of volume concentration, particle diameter, and their thermophysical properties on detonation attenuation and suppression. However, the non-uniform structure of the detonation cell undoubtedly influences the parameters of a blend of explosive gas and chemically inert particles and the limiting detonation characteristics. Thus, studies of the parameters of the detonation wave and an estimate of the size of the detonation cell in mixtures of combustible gases and inert particles are of scientific and practical interest.

2. Statement of the problem, mathematical model and computational technology

A cellular detonation wave interaction with a cloud of alumina microparticles (\(\text{Al}_2\text{O}_3\)) is simulated. The flow pattern is shown in Fig. 1. A cellular detonation wave was set as initial data in a two-dimensional channel with a length of 1 m and a width of 0.1 m. It propagated from left to right in a hydrogen-air mixture and ran into a cloud of inert particles. The cloud began at a distance of 0.2 m from the left border of the channel and filled the entire space to the right border. The canal was bounded by walls from all sides.
The gasdynamics of the detonation wave interaction with the solid phase was modeled by a system of two-dimensional Navier-Stokes equations, describing the motion of a viscous compressible heat-conducting gas, taking into account the multicomponent nature of the gas mixture and the reduced chemical kinetics [7]. The motion of the particles was described using a continuum approach. This model is valid for small volume fraction of particles and represents the equations of mass, momentum, and energy conservation for the solid phase. The system was supplemented by a source term to take into account the interaction of the phases. Particles were considered spherical. ANSYS Fluent software was used for modeling. The conservation equations for the particle phase and the source terms were programmed with the help of User Defined Functions. An implicit second-order scheme was used as a time approximation method. To approximate the convective terms over space, the AUSM flux vector splitting with the second order upwind scheme was involved. A quadrangular mesh was used in the calculations; it was dynamically adapted to the gasdynamic singularities of the flow in accordance with the density gradient. Figure 2 shows an example of a calculated mesh, obtained in the solution process, and a fragment illustrating the details of the adaptation technology. From the figure we see how the calculated grid is adjusted to the cellular structure of detonation.

**Figure 1.** Flow pattern.

**Figure 2.** Example of dynamically adapted mesh.

3. Calculations results.
As a result, a methodology was developed for calculating cellular detonation and its suppression in ANSYS Fluent using the reduced kinetics. The reduced kinetics is verified by the detonation cell size in stoichiometric hydrogen-air mixture at initial pressure $10^5$ Pa, temperature 300 K and sound speed 405 m/s. Further calculations were carried out under these conditions. Figure 3 shows the formation of a cellular detonation wave in a hydrogen-air mixture at two different base steps of the computational mesh. We note that the calculated mesh thickened 16 times in the regions of large gradients. The fields of pressure peaks at different instants of time are given in Fig. 3. A flat overdriven detonation wave was set in this calculation at the initial time moment. Under the action of infinitesimal perturbations it loses stability and propagates in a cellular mode. As the detonation wave moves, the cell becomes
coarser and a size in the range 10\textsuperscript{2}-20 mm is established. It can be seen that the average degree of irregularity characteristic of cellular detonation in the hydrogen-air mixture appears. The figure allows concluding about the solution convergence at a reduced mesh step and selecting 1 mm step for further calculations.

![Figure 3. Formation of cellular detonation in a hydrogen-air mixture.](image)

Further, to analyze the problems associated with the study of the cellular detonation suppression by inert particles, calculations of the detonation wave interaction with a cloud of alumina particles are carried out for different diameters and volume fractions. The values of the particles volume fraction resulting in detonation wave failure are obtained. Fig. 4 shows the results of modeling the passage of a cellular detonation wave through a particles cloud with a diameter of 100 \(\mu\)m. The fields of pressure maxima in time are given for the volume concentrations of particles \(m_2 = 10^{-4}, 10^{-3}, 10^{-2}\). For a small volume fraction, there is no significant change in the structure of the wave. The cells number remains unchanged over the entire length of the cloud. An increase in the particles volume fraction leads to a change in the structure of the cellular wave and an increase in the cell size. An increase in the particles volume fraction up to \(m_2 = 10^{-2}\) leads to detachment, quenching of the detonation, and its degeneration into a shock wave.

Fig. 5 shows the detonation wave velocity as a function of time at a particles concentration \(m_2 = 10^{-4}\) for different diameters in comparison with the velocity of the detonation wave without the particles presence in the fuel mixture (bold line). It is seen that as the particles diameter decreases, the detonation wave velocity is reduced, and detonation failure is not observed for a given volume fraction for all diameters. Because of the detonation cell enlargement with a decrease in the particle diameter, there is a growth in the nonuniformity of the detonation wave velocity profile.

![Figure 4. Fields of pressure peaks in time for particles with a diameter of 100 microns at a volume fraction of \(m_2 = 10^{-4}, 10^{-3}, 10^{-2}\).](image)
Figure 5. Detonation wave velocity for particles of different diameters at $m_2 = 10^{-4}$

The velocity distribution of the detonation wave at various volume fractions for 10 μm particles is shown in Fig. 6. Reduction of the particles diameter serves to achieve detonation failure even at a volume fraction of $5 \cdot 10^{-4}$. Figure 7 shows a summary of data on the detonation wave velocity deficit ($\eta = \frac{D}{D_{CJ}}$ where $D$ is the average velocity of the detonation wave, and $D_{CJ}$ is the Chapman-Jouguet velocity, $D_{CJ} = 1870$ m/s for these initial conditions), depending on the diameter of the particles at different volume concentrations. At $m_2 = 10^{-4}$, as noted above, the average detonation velocity reaches a constant value as the particle diameter decreases. However, as can be seen from Fig. 5, the local velocity oscillations for 1 μm and 0.5 μm particles are significantly different. This is due to the growth of the detonation cell size with its diameter decrease. In the case of 0.5-μm particles, one half of the cell is accommodated within the width of the channel. Further reduction of the diameter does not lead to a change in the flow pattern because of very rapid velocity and thermal relaxation of fine particles. It should be noted that at a particle concentration $m_2 = 10^{-5}$ detonation failure was observed already for 100 μm particles. This graph allows determining the flow regimes and the parameters of the particles cloud leading to detonation failure.

Figure 6. Detonation wave velocity as a function of volumetric fraction at $d_p = 10^{-5}$ m.
Figure 7 The detonation wave velocity versus diameters and volume concentrations of particles.

4. Conclusions
A calculation technique to describe 2-D cellular detonation wave suppression by inert particles was developed using the ANSYS Fluent software package.

The values of the particles volume fractions and their corresponding particle diameters leading to the change of detonation cell size, attenuation and suppression of a cellular detonation wave in a hydrogen–air mixture have been obtained.

5. References
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