MICRO-LEVEL MODELING OF THE DETONATION WAVE ATTENUATION BY INERT PARTICLES

by

Igor BEDAREV*

Khristianovich Institute of Theoretical and Applied Mechanics SB RAS,
Novosibirsk, Russia

Original scientific paper
https://doi.org/10.2298/TSCI19S2439B

A computational technology for direct modeling of the detonation waves interaction with a set of particles at the micro level has been developed. A simulation of the detonation waves passage through a system of particles with their different relative positions was carried out. Stoichiometric hydrogen air mixture is considered. The combustion process is described using a reduced kinetic mechanism. Estimates of the ratios between times of the velocity and thermal relaxation are obtained. Detailed shock-wave patterns of gas flow in the particles vicinity are obtained. The possibility of detonation failure at particles volume fractions of close to the concentrations obtained in modeling at the macro level has been revealed.

Key words: *detonation suppression, inert particles, mathematical modeling*

Introduction

The paper deals with to the problems of physical and mathematical description of phenomena in reacting heterogeneous media and the development of methods for studying shock-wave, explosive and detonation phenomena in a combustible gases and inert particles mixture. The construction of mathematical models of mechanics of reactive/inert heterogeneous media requires an accurate representation of the local characteristics of the flow field arising from the interaction of the gas phase and small particles of the dispersed phase [1]. When a shock or detonation wave passes through a cloud of particles, flow characteristics such as the particle drag, the dynamics of its heat exchange with the surrounding medium, and chemical transformations will depend on whether the flow velocity is subsonic or supersonic, *i. e.*, on which flow regime occurs. The flow regime around the particles depends, first, on whether a collective shock has been formed ahead of the cloud of particles or individual flow around each particle occurs and, second, on whether the particle is in the aerodynamic shadow of other particles [2, 3]. Therefore, it is important to analyze the influence of the flow around the particles on their drag and thermal and velocity relaxation using various gas flow models. In this case, it is advisable to consider different arrangements of the particles relative to the incident flow. This approach makes it possible to refine the integral empirical formulas for the drag and heat transfer coefficients and to more accurately determine the temperature conditions around the particles to describe their ignition and combustion. Detailed information on

* Author's e-mail: bedarev@itam.nsc.ru

the flow around the particles and their velocity and thermal relaxation allows a more accurate prediction of their ignition and combustion dynamics. The work is connected with the study of the phenomenon of detonation. Detonation can be used in perspective aircraft engines [4-6]. The relevance of our work is related to the problems of explosion and fire safety. It has been established that the addition of inert particles to an explosive mixture contributes to the detonation suppression [7-13]. Studies of the detonation waves and inert particles interaction are mainly carried out in a one-dimensional formulation and allow us to make estimates of the influence of the volume fraction, particles diameter, and their thermophysical properties on the ability to attenuate and suppress detonation. In [14], the suppression of cellular detonation by inert alumina particles (Al_2O_3) was investigated. It is shown that an increase in the particles volume fraction and a decrease in the particles diameter lead to inhibition of the detonation wave and the enlargement of the detonation cell. Particle volume fractions resulting in the failure of a cellular detonation wave are obtained. In the present work, the interaction of a detonation wave with an inert solid phase is investigated at the micro level. The aim of the work was a numerical study of the detailed interaction of passing detonation waves with a system of bodies to determine the dynamics of failure and re-initiation of detonation when it is interacting with inert particles.

Mathematical model and numerical implementation

Within the framework of the ANSYS FLUENT package of computer gas-dynamic analysis with the use of a 6DOF solver, we developed a computing technique for direct numerical simulation of velocity and thermal dynamics of an aggregate of several particles under the influence of a passing detonation wave. The Euler equations were used as a mathematical model for describing the gas flow in a vicinity of particles. In [15-17], this technology was used to direct modelling of the particles velocity and thermal relaxation behind shock waves. For the describing of the chemical transformations the reduced kinetic was used. Mathematical model and numerical approach verified in [18] on the ignition delay time, detonation wave velocity and detonation cell size.

The calculations were performed in a plane statement. A plane overdriven detonation wave was used as the initial data at domain inlet. An implicit second-order scheme was used for approximation in time. 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 present work, the particles were stationary, but the numerical method allows to take into account the movement of the particles and mesh in the their vicinity. 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.

Approximate estimates of the times of velocity and thermal relaxation particles in the flow behind the detonation wave

In the initial phase of the study, we estimated the ratio of the velocity and thermal relaxation times for single particles interacting with shock and detonation waves.

The model used included two ODE for the particle velocity and temperature:

$$\frac{\mathrm{d}U_p}{\mathrm{d}t} = \frac{3}{4}\frac{C_D\rho_g}{\rho_p d_p}\left(U_g - U_p\right)\left|U_g - U_p\right| \tag{1}$$

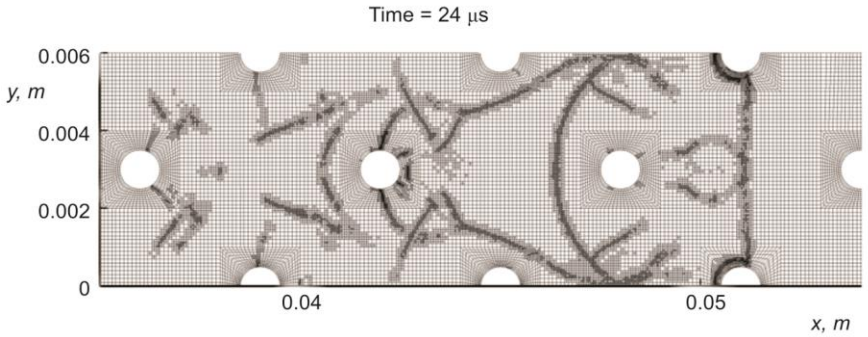

Figure 1. Fragment of a dynamically adapted computational grid

$$\frac{\mathrm{d}T_p}{\mathrm{d}t} = 6\frac{\mathrm{Nu}\lambda_g}{\rho_p c_{ps} d_p^2}\left(T_g - T_p\right) \tag{2}$$

here U_p, U_g, T_p, T_g – velocity and temperature of particle and gas, respectively, ρ_p, ρ_g – density of particle and gas, d_p – particle diameter, λ_g – gas thermal conductivity, and c_{ps} – particle heat capacity. In the approximate model, the drag coefficient C_D was calculated using the Henderson approximation and the Nusselt number using an empirical dependence on the Prandtl and Reynolds numbers.

We estimated the ratios of the velocity and thermal relaxation times for particles of different diameters in the flow behind a detonation wave in a stoichiometric hydrogen-air mixture. These calculations were performed for particles of alumina (Al_2O_3), sand (SiO_2), and tungsten carbide (WC) with a diameter of 1 μm to 1 mm. This type of particles is relevant to the study of the attenuation and suppression of detonation by inert particles. The thermophysical properties of detonation products and the temperature variation of the specific heat of particles as a function of temperature are taken into account. Figure 2(a) show the calculation results for alumina particles. It is evident that for alumina and sand particles having similar densities and specific heats (therefore, only the results for alumina are given), the velocity relaxation time is somewhat (about 1.5 times) greater than the thermal relaxation time for 1 μm particles, and for 100 μm particles, the times are nearly identical. For tungsten carbide particles, fig. 2(b), which have a high density and a lower specific heat, the velocity relaxation time is an order of magni-

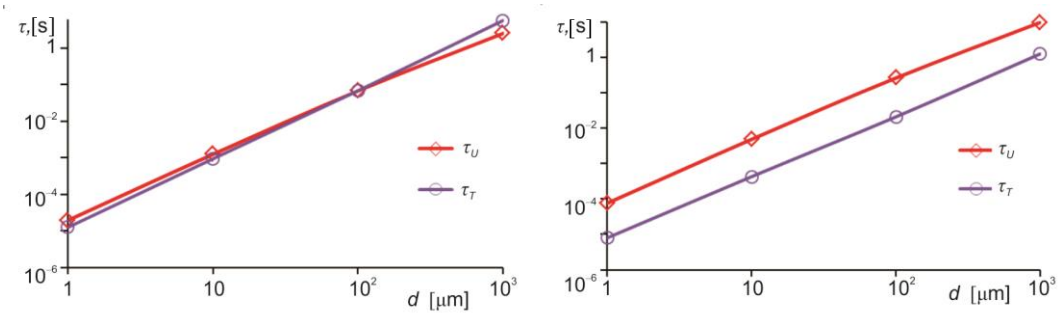

Figure 2. Relaxation times *vs.* particle diameter for alumina (*a*) and tungsten carbide (*b*) particles in the flow behind a detonation wave

tude greater than the thermal relaxation time in the whole range of diameters, with this difference slightly decreasing with increasing particle diameter. The estimates suggest that particles larger than 100 μm interacting with a detonation wave can be considered motionless and isothermal since the velocity and thermal relaxation times exceed the gas-dynamic time of interaction with the detonation wave by more than an order of magnitude.

Results

Simulation of the plane detonation wave passing on stoichiometric hydrogen-air mixture through a grid of fixed particles with 1 mm diameter is performed. Calculations for particles located in a staggered manner at different relative distances between the particles $k = l/d$ (l – distance between particles, d – particles 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 3 shows pressure flowfield for detonation wave interaction with three particles at $k = 10$ at different times. This distance between the particles corresponds to a volume fraction ~10^{-2}. Note that the upper and lower boundaries of the computational domain are symmetry lines. We

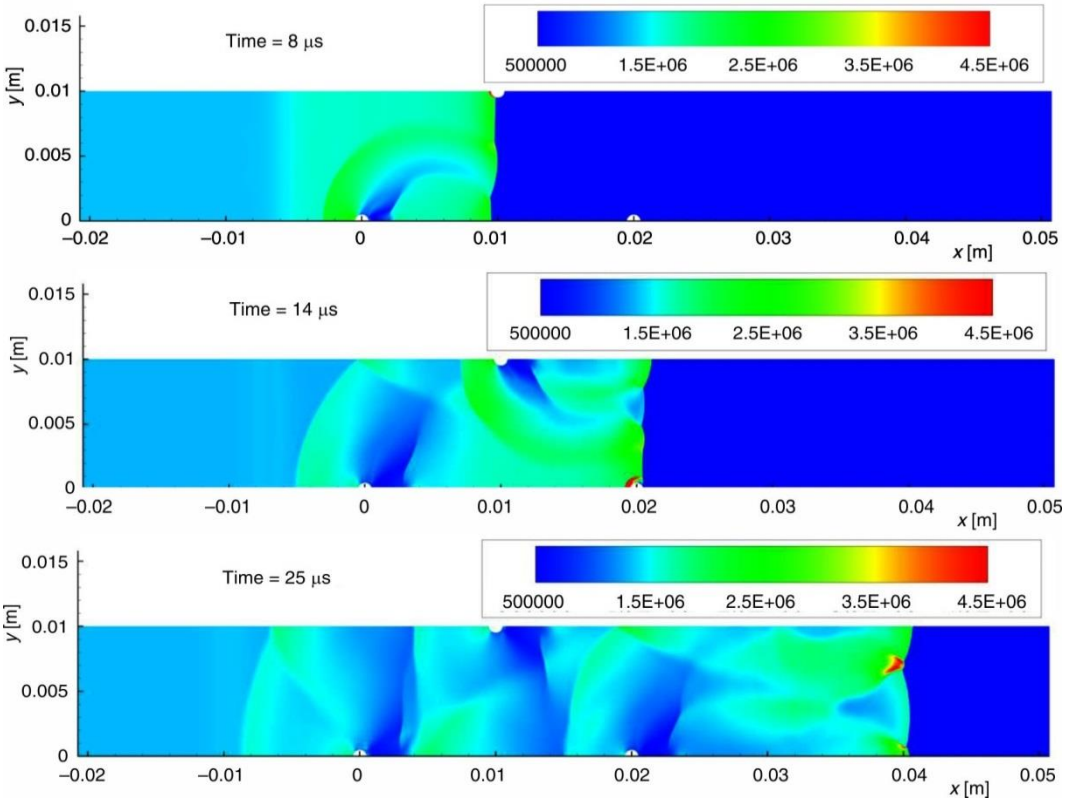

Figure 3. The pressure flowfield at different times for three particles at $k = 10$
(*for color image see journal web site*)

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 ~10^{-1}) and the length of the *cloud* is increased (up to 64 particles), a separation of the detonation wave front into a shock wave and a combustion wave is occurred. Figures 4 and 5 shows the pressure and temperature fields at different times. Pressure flowfields show an attenuation of the detonation wave in a particle cloud. We can see a significant pressure decrease in the cloud and immediately behind it. The separation can be observed at the time of 30 μs, 45 μs, and 60 μs in fig. 5. It should be noted that detonation suppression is observed at a same particles volume fraction in [14] where for modeling of the detonation wave interaction with inert particles was used a macrolevel approach with continuous solid phase. Than the combustion wave overtake the shock wave (75 μs) and the re-initiation of detonation takes place (90 μs). With an increase of the *cloud* length it is possible to completely suppress detonation without re-initiation.

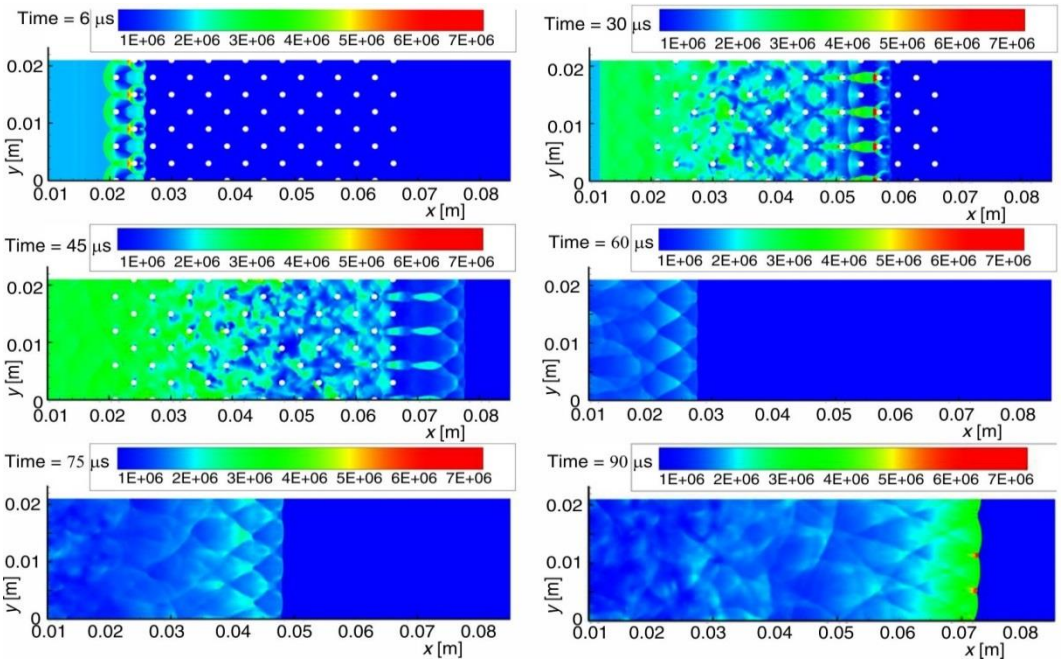

Figure 4. The pressure flowfield at different times for 64 particles at k = 3
(*for color image see journal web site*)

Conclusions

Estimates were obtained for the ratios of the velocity and thermal relaxation times of micron-sized particles of different chemical composition interacting with detonation waves. It is shown that for particles of sand and alumina, the times of velocity and thermal relaxation are close to each other and for tungsten carbide particles, the velocity relaxation time is substantially higher than the thermal relaxation time. For large particles velocity and thermal

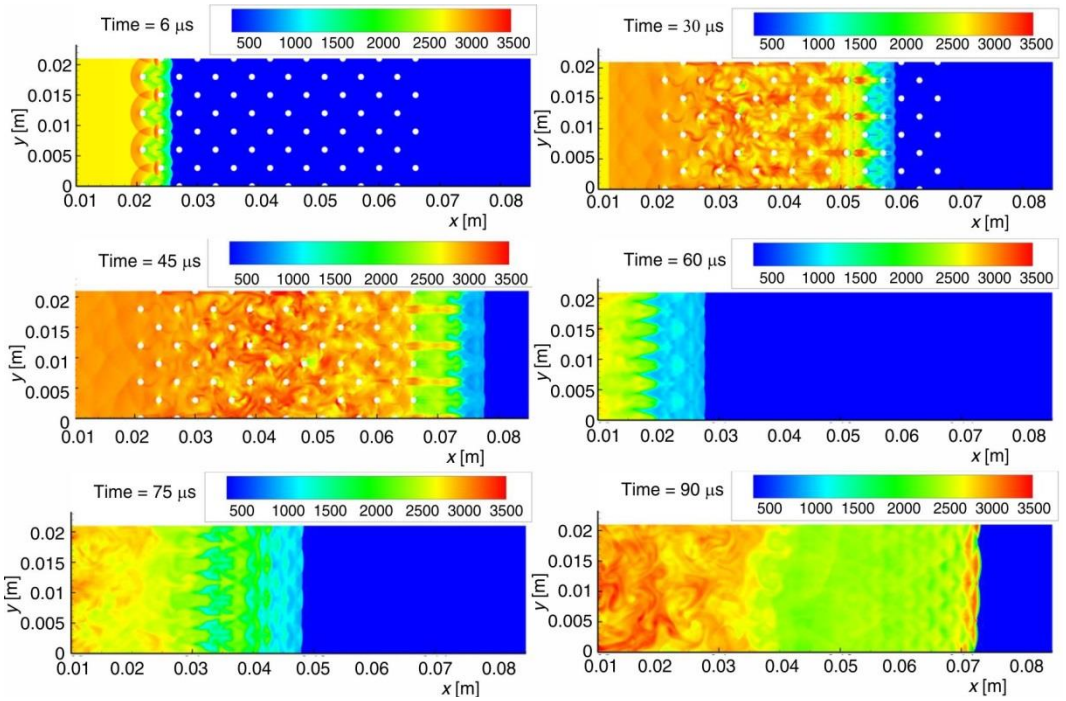

Figure 5. The temperature flowfield at different times for 64 particles at $k = 3$
(*for color image see journal web site*)

relaxation times of inert particles exceed the gas-dynamical time of interaction with the detonation wave by more than an order of magnitude. These estimates allowed concluding that particles larger than 100 μm can be considered motionless and isothermal. 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.

Acknowledgment

This work was partially supported by the Russian Foundation for Basic Research (Grant No. 17- 08-00634).

References

[1] Fedorov, A. V., *et al*., *Dynamics and Ignition of Gas Suspensions* (in Russian), Novosibirsk. Gos. Tekh. Univ., Novosibirsk, Russia, 2006
[2] Blagosklonov, V. I., V. M. *et al*., Interaction of Hypersonic Multiphase Flows, *Journal of Applied Mechanics and Technical Physics, 20* (1979), 5, pp. 571-578
[3] Boiko, V. M., *et al*., Collective Bow Shock Ahead of a Transverse System of Spheres in a Supersonic Flow Behind a Moving Shock Wave, *Fluid Dynamics, 39* (2004), 2, pp. 330-338
[4] Roy, G. D. S., *et al*., Pulse Detonation Propulsion: Challenges, Current Status, and Future Perspective, *Progress in Energy and Combustion Science, 30* (2004), 6, pp. 545-672
[5] Frolov, S. M., *et al*., Continuous Detonation Combustion of Hydrogen: Results of Wind Tunnel Experiments, *Combust., Expl., Shock Waves, 54* (2018), 3, pp. 357-363
[6] Wang, Z., *et al.*, Numerical Simulation of the Nozzle and Ejector Effect on the Performance of a Pulse Detonation Engine, *Thermal Science, 22* (2018), 3, pp. 1227-1237

[7] Kazakov, Yu. V., *et al*., Normal Detonation Regimes in Relaxing Media, *Combust., Expl., Shock Waves, 25* (1989), 1, pp. 109-115
[8] Tropin, D. A., *et al*., Mathematical Modeling of Detonation Suppression in a Hydrogen-Oxygen Mixture by Inert Particles, *Combust., Expl., Shock Waves, 46* (2010), 3, pp. 332-343
[9] Fedorov, A. V., Tropin, D. A. Determination of the Critical Size of a Particle Cloud Necessary for Suppression of Gas Detonation, *Combust., Expl., Shock Waves*, *47* (2011), 4, pp. 464-472
[10] Tropin, D. A., Fedorov. A. V., Physicomathematical Modeling of Detonation Suppression by Inert Particles in Methane-Oxygen and Methane-Hydrogen-Oxygen Mixtures, *Combust., Expl., Shock Waves, 50* (2014), 5, pp. 542-546
[11] Tropin, D. A., Fedorov, A. V., Mathematical Modeling of Detonation Wave Suppression by Cloud of Chemically Inert Solid Particles, *Combustion Science and Technology, 186* (2014), 10-11, pp. 1690-1698
[12] Fedorov, A. V., Tropin, D. A., Modeling of Detonation Wave Propagation through a Cloud of Particles in a Two-Velocity Two-Temperature Formulation, *Combust., Expl., Shock Waves, 49* (2013), 2, pp. 178-187
[13] Fedorov, A. V., *et al*., Modeling of Reflection of Detonation and Shock Waves from a Rigid Wall in Mixtures of a Reactive Gas and Chemically Inert Particles, *Journal of Engineering Physics and Thermophysics, 85* (2012), 3, pp. 614-619
[14] Bedarev, I. A., Fedorov, A. V., Modeling the Suppression of Cellular Detonation in a Hydrogen- Air Mixture by Inert Particles, *Proceedings,* XXV Conference on High-Energy Processes in Condensed Matter, AIP Conference Proceedings, AIP Publishing, Novosibirsk, Russia, 2017, Vol. 1893, 030136
[15] Bedarev, I. A., Fedorov, A. V. Computation of Wave Interference and Relaxation of Particles After Passing of a Shock Wave, *Journal of Applied Mechanics and Technical Physics, 56* (2015), 5, pp. 750-760
[16] Bedarev, I. A., Fedorov, A. V., Modeling the Dynamics of Several Particles Behind a Propagating Shock Wave, *Technical Physics Letters, 43* (2017), 1, pp. 1-4
[17] Bedarev, I. A., Fedorov, A. V., Direct Simulation of the Relaxation of Several Particles Behind Transmitted Shock Waves, *Journal of Engineering Physics and Thermophysics*, *90* (2017), 2, pp. 423-429
[18] Bedarev, I. A., *et al*., Application of Detailed and Reduced Kinetic Schemes for the Description of Detonation of Diluted Hydrogen-Air Mixtures, *Combust., Expl., Shock Waves, 51* (2015), 5, pp. 528-539

Paper submitted: September 1, 2018
Paper revised: November 1, 2018
Paper accepted: December 1, 2018