Numerical Simulation of Detonation Cells in Hydrogen-Air Mixture with Suspended Aluminum Particles

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Introduction

We present preliminary results of 2D numerical gasdynamic study of detonation cell structure in hybrid two-phase hydrogen-air mixture with suspended aluminum particles of different size. The results are in qualitative agreement with observed effects of particles on detonation cell structure. Currently we attempt to get quantitative agreement with the experimental data by improving description of kinetics of gaseous reaction and of particle effect on composition of detonation products.

Description of the Problem

In the hybrid hydrogen-air mixtures with suspended aluminum particles two different reactions can occur behind the shock wave. First, rapid gaseous reactions take place, releasing H_2O (O_2 can be available in lean gaseous explosives). Oxidation of suspended aluminum particles by these species begins after ignition of particles. Both reactions are exothermic and thus can support detonation propagation. Non-monotonous character of heat release in hybrid mixtures can result in different modes of detonation wave propagation [1].

Gaseous reaction is described as one-step Arrhenius reaction. Results shown below correspond to a simple case of constant γ=1.4 and molecular weight of detonation products (μ_o=0.029 g/mole) and the CJ detonation velocity of D_0=1909 m/s, which represents some typical value for the lean mixtures studied experimentally in [2]. As for the ignition temperature of aluminum, we used T_{ign}=1350 K and assumed that particles are sufficiently fine to ignore temperature distribution inside particles. Burning time of aluminum particles was assumed to be proportional to square of initial particle diameter d_o.

To solve the system of two-phase 2D governing equations in slab geometry we used the LCPFCT technique [3] together with special adaptation procedure along longitudinal x-co-ordinate performed every time when shock front arrives sufficiently close to the right boundary of the computation grid. Most of the 2D plane results shown below are obtained using 375*300 grid with initial size of 0.25 m * 0.2 m, i.e. $\Delta x=\Delta y$=0.6667 mm.

The flow was initiated by a jump in a longitudinal distribution of pressure and temperature near the closed wall of the channel (distribution of flow parameters across the channel was initially uniform) able to provide successful initiation of the detonation in two-phase mixtures with particles of different diameters («fine» 3.5 μm and «coarse» 13 μm) and

particle concentrations up to 300 g/m^3. Difference in size of fine and coarse particles provides nearly 14-fold difference in burning time of considered particles.

Results of Calculations

Fig.1 shows tracks of maximum pressure calculated for 13-μm aluminum particles at particle concentration σ=300 g/m^3. Note that every soot plate is 0.8 m in length and that recording of tracks of maximum pressure on a new plate begins as soon as shock front arrives to the right boundary of the given plate. Therefore, rightmost part of every plate displays how non-uniform is the shock front. First plate shows how initially plane 1D flow is transformed into two-dimensional one as a result of formation of hot spots having purely numerical origin. Then detonation cell width gradually decreases with time as detonation velocity increases and approaches its quasi-steady value of 1832 m/s, which is significantly below the CJ detonation velocity in pure gas (D_0=1909 m/s). The cell pattern becomes quite regular after about 4.5 meters of detonation propagation.

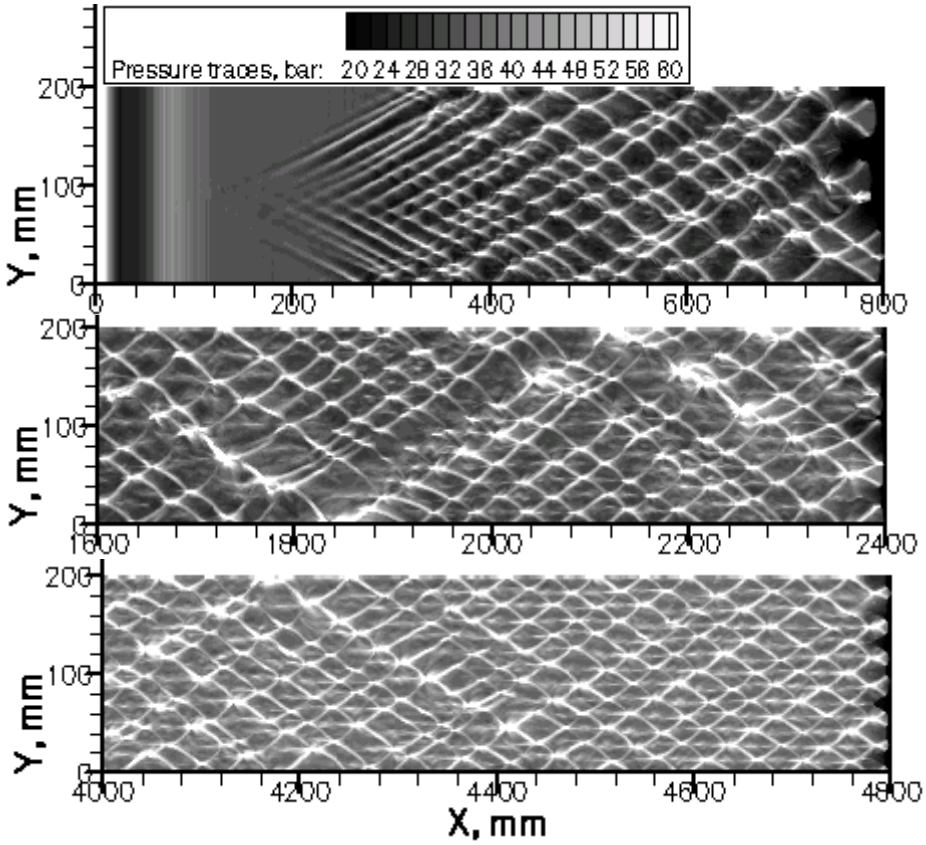

Figure 1. Tracks of maximum pressure for coarse 13-μm aluminum particles at σ=300 g/m^3.

Fig. 2 compares distributions of pressure near the shock front at t=1 and t=2 ms for the run considered above. At t=1 ms one can see a dark band just behind the shock with a thickness of about 20-30 mm, which indicates that a strong secondary shock travels behind the leading front. Results of 1D calculations presented below also display the secondary shock but at a much larger distance behind the leading shock. No secondary shock is observed in pure

gas. Fig.2 shows that the distance between the secondary shock and leading front decreases with time. Furthermore, the overall pressure level behind the secondary shock increases with time due to reaction of aluminum particles. Thus, coarse aluminum particles decrease propagation velocity of the leading detonation front. This propagation regime is classified as the double-front detonation (DFD), described earlier [1].

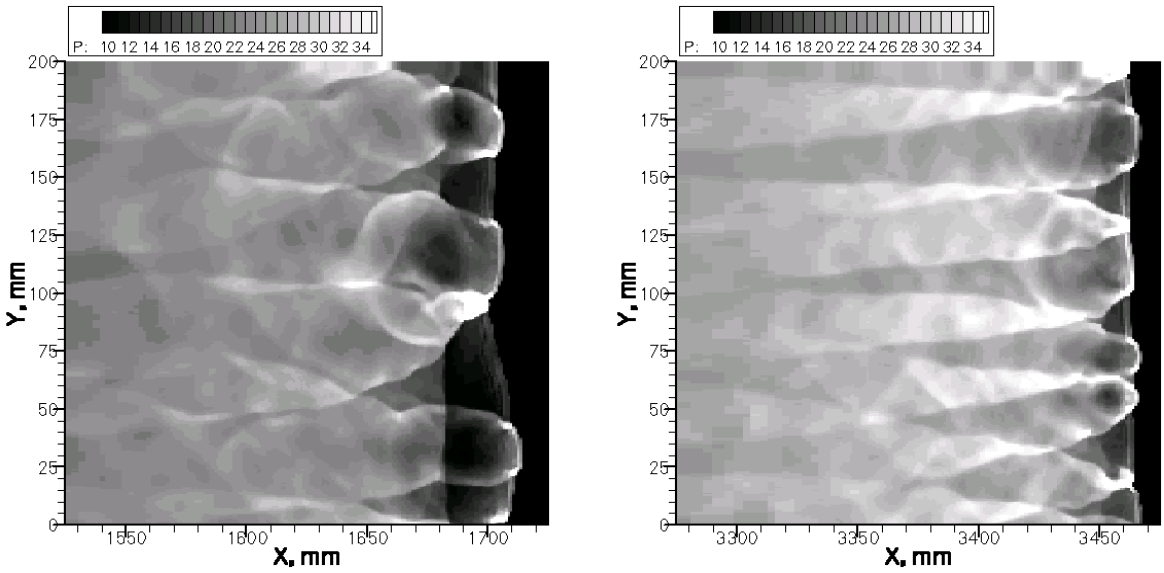

Fig.2. Pressure map at t=1 (left) and t=2 ms (right) for 13-μm particles at σ=300 g/m^3.

Fine 3.5-μm particles at σ=300 g/m^3 significantly increase detonation velocity in comparison with D_0. In this case one can expect that cell size should be noticeably smaller than in pure gas. Therefore, we performed this run using two times finer grid: Δx=Δy=0.3333 mm. Fig. 3 shows that cell pattern quite rapidly becomes regular and cell width is significantly smaller than with coarse 13-μm particles. The detonation velocity at the end of the second plate is D=2121 m/s i.e. 10 m/s lower than steady detonation velocity predicted by 1D calculations at the end of 10-m shock tube. In this case there is no secondary shock and, hence, particles burn inside the leading heat release zone of single-front detonation (SFD, see [1]) and increase amplitude of the leading wave.

Discussion

To explain the aforementioned results let us analyze 1D profiles of pressure P and Mach number (relative to the shock front, i.e. $M=(D-u)/c$) presented in Fig. 4. Here thick solid lines show P and M profiles in pure gas at t=1 and 2 ms. Thin solid gray lines correspond to coarse 13-μm particles at σ=300 g/m^3 at t=1 and 2 ms. Hence, addition of coarse particles decreases detonation velocity and results in formation of secondary shock. The leading detonation zone, just behind the leading shock, is subsonic since it corresponds to M<1. One can see that the flow behind the secondary shock becomes subsonic again, which is typical of double-front detonations. With coarse but inert particles (see dash lines) no secondary shock is formed behind the leading wave and detonation velocities for reactive and inert coarse

particles do not differ. However, for reactive particles the amplitude of the secondary shock is significantly lower than that of the leading wave and this shock does not affect tracks of maximum pressure presented in Fig.1. Indeed, though some bright points can be seen near the secondary shock (see Fig.2), their intensity is lower than that of triple points at the leading front and thus trajectories of secondary points cannot be seen in Fig.1.

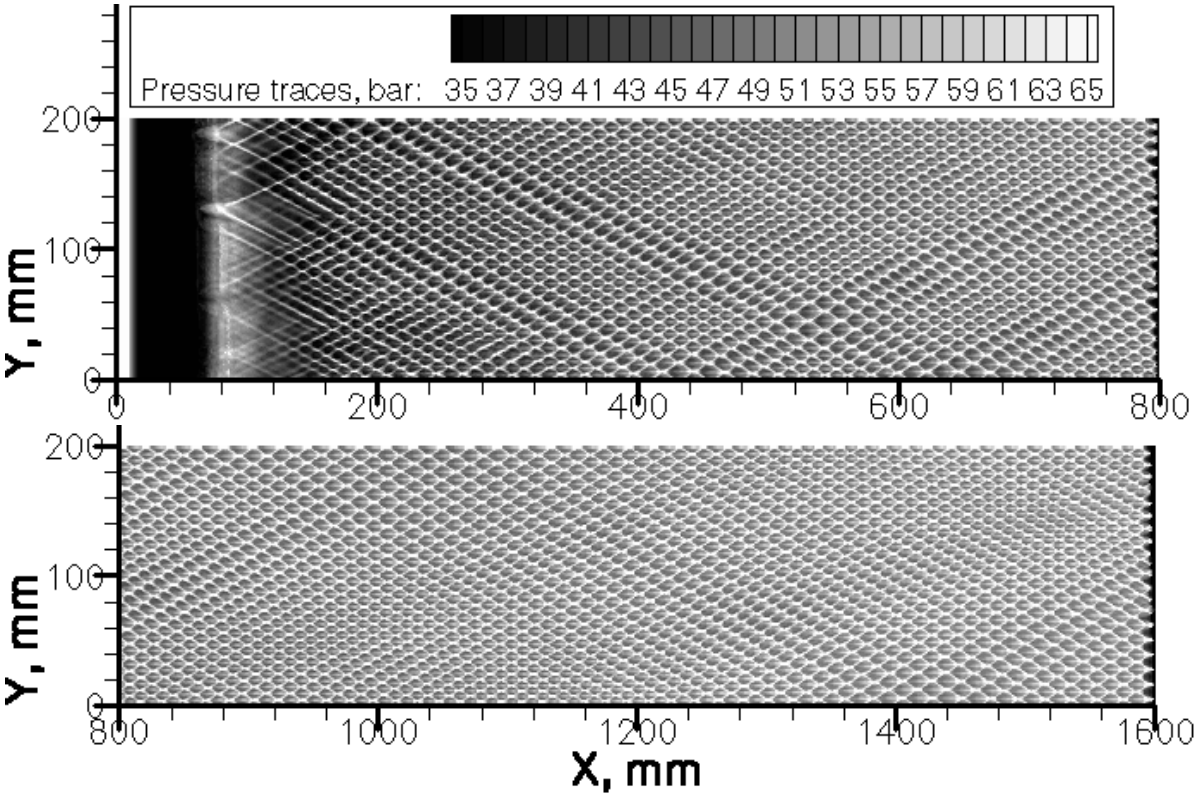

Fig.3. Maximum pressure tracks in the case of fine 3.5-μm particles at σ=300 g/m^3.

Dash-dot curves in Fig.4 correspond to fine 3.5-μm particles at σ=300 g/m^3. These particles burn nearly 14 times faster than 13-μm particles and the secondary heat release zone quickly catches up with the leading one increasing detonation velocity and pressure. At the same time, detonation zone thickness (where M<1) also grows, that means that global reaction becomes slower. Despite this fact, Fig.3 demonstrates that resulting cell size in hybrid mixture with fine particles is significantly smaller than in pure gaseous mixture. This conclusion agrees with observation [2].

The proposed model provides qualitative agreement with practically all experimentally observed trends [2] and improves existing knowledge of detonations of hybrid mixtures with aluminum. However, we continue our studies to achieve quantitative agreement with experimental data, including dependence of cell width in pure gas on pressure.

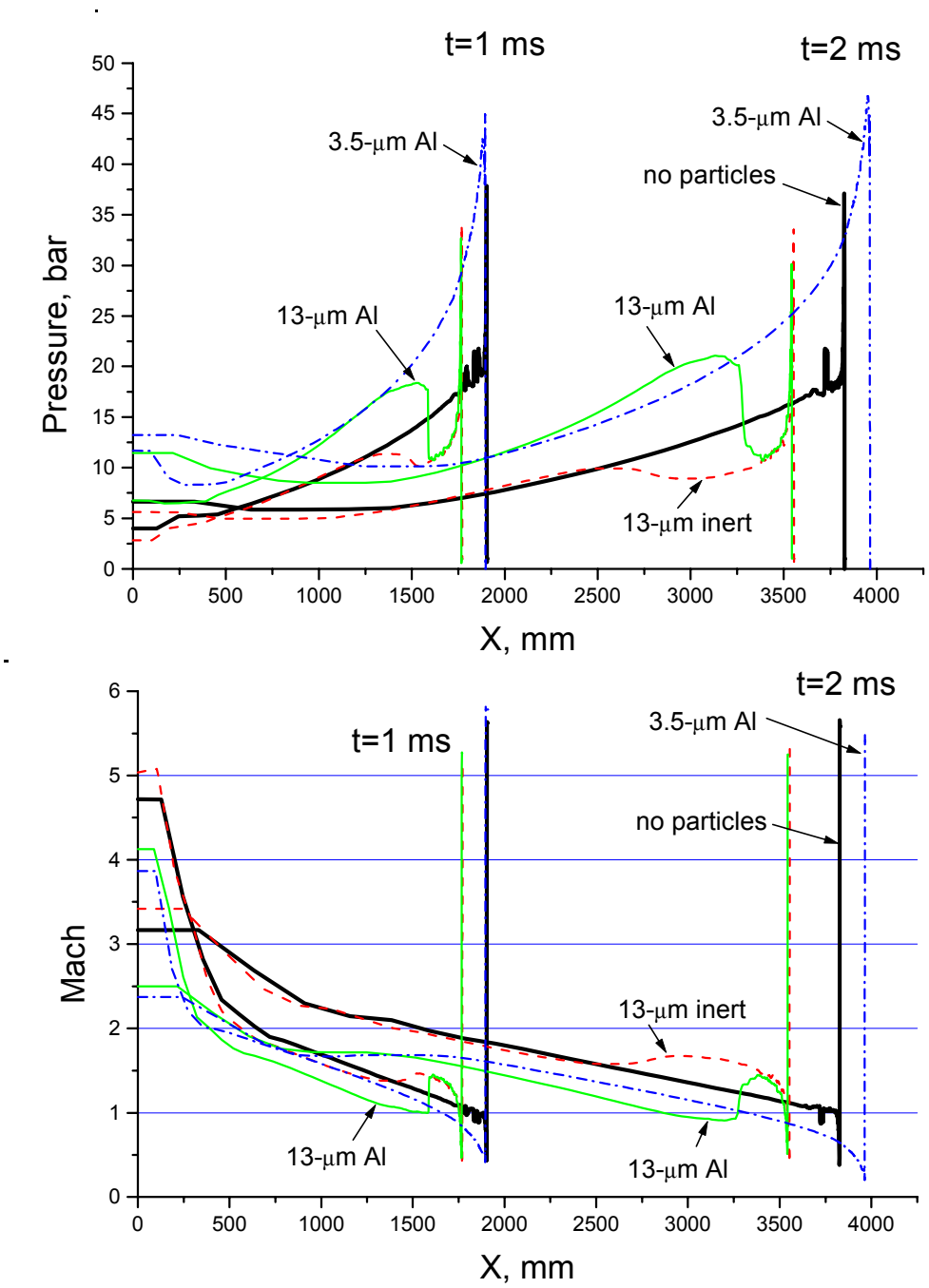

Fig. 4. 1D profiles of pressure (above) and Mach number at t=1 and 2 ms for σ=300 g/m^3.

Acknowledgements. This work was supported by the INTAS (project INTAS-OPEN-97-2027).

References

1. Khasainov B.A., Veyssiere B. (1996) *Initiation of detonation regimes in hybrid two-phase mixtures.* Shock Waves, V. 6, pp. 9-15.
2. Ingignoli W., Veyssiere B., Khasainov B.A. *Detonation Of Hydrogen-Based Gaseous Mixtures With Suspended Aluminum Particles.* Proceedings of the 17th International Colloquium on Gasdynamics of Explosions and Reactive Systems, CD-Rom ISBN 3-932217-01-2, n°151, Heidelberg, July 25-30, 1999.
3. Oran E.S., Boris J.P. (1987) Numerical Simulation of Reactive Flow. ELSEVIER, New York-Amsterdam-London.