Three-Dimensional Structure of Detonations in Suspensions of Aluminum Particles

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Abstract

Recently we have used scarce available data on the detonation cell size in suspensions of aluminum particles in air and oxygen to adjust the kinetic parameters of our two-phase model of detonations in these mixtures. The calculated detonation cell width was found by means of two-dimensional unsteady simulations using an assumption of cylindrical symmetry of the flow in the tube. However, in reality the detonation cells are three-dimensional. In this work we apply the same detonation model which is based on the continuous mechanics of two-phase flows for 3D numerical simulations of cellular detonation structures in aluminum particle suspensions in oxygen. Reasonable agreement was obtained with the aforementioned 2D results on the detonation cell width. The range of tube diameters where detonations in Al/O2 mixture at a given particle size and concentration would propagate in the spinning mode is estimated (these results make a complement to our previous analysis of spinning detonations in Al/air mixtures). Coupling these results with the formerly obtained dependences of detonation cell size on the mean particle diameter can help to better plan the experimental studies of detonations in aluminum suspensions.

1 Introduction

Due to the lower reactivity of suspensions of aluminum particles both in air and in oxygen in comparison with typical gaseous explosives, the data on detonation cell sizes in these two-phase mixtures are scarce [1,2]. Hence a special care must be taken while planning both laboratory and large scale experiments with suspensions of aluminum particles, namely, the choice of initiation energy must be appropriate for the average size of aluminum particles, their concentration and characteristic dimensions of the tested mixture. Therefore, there is a need in improving prediction ability of detonation models for aluminum suspensions especially in what concerns the characteristic detonation cell width λ. Indeed, in gaseous explosives the detonation cell size serves well as a measure of reactivity of different mixtures and, for example, the critical diameter of detonation transmission from a tube to an unconfined space scales with λ.

Recently we have numerically simulated the detonation cell structures in Al/O_2 and Al/air mixtures [3] and have adjusted the kinetic parameters of the model [4,5] to fit the available data. This gives the following indications on the detonation cell widths: λ = 40 ± 10 cm in Al/air mixture at particle apparent density σ=0.5 kg/m^3 (richness r=1.6) and d_o =13.5 μm [1] and λ = 10 ± 1 cm in the stoichiometric Al/O_2 mixture at σ=1.5 kg/m^3 (r=1) and mean particle diameter d_o of 8.6 μm [2]. The same model [3] was applied also to simulate, for the first time, the spinning detonations in the Al/air mixture [6]. It is worth to note that Tsuboi et al. [7] have studied the problem of spinning detonations in corn-starch suspension in O_2 but in a zone of a limited longitudinal extension.

The present work was motivated by the fact that the aforementioned numerical studies [3] for Al/air mixtures were performed in the two-dimensional case assuming that the flow in the tube is axisymmetric, which implies however a quite specific form of detonation cells. Here, we apply the same model [3] to Al/O_2 mixture but directly in three-dimensional case. The effect of tube diameter on the cell structure was studied and the range of tube diameters where detonation propagates in the spinning mode is predicted for the considered size and apparent density of aluminum particles. Calculated detonation cell sizes compare favorably with the former estimates of λ obtained in 2D calculations under the assumption of cylindrical symmetry of the flow in the tube. Thus, taking into account that detonation cell width scales with the particle size d_o as $\lambda \propto d_o^n$ [3] where n=1.4, one can already make better design of experiments on detonation of aluminum suspensions. More precise predictions could be made by numerical unsteady multidimensional simulations.

2 The model and simulation results

The detonation model is based on the principles of continuous mechanics of multiphase flows [8] and is exactly the same as described in [3] but is applied here in 3D case rather than in 2D symmetrical one (our model describes aluminum particle burning similarly to [9]). Since spinning detonations in suspensions of Al in air were already analyzed before [6], we consider below only stoichiometric Al/O_2 mixtures with σ=1.47 kg/m^3 and mean particle diameter d_o =8.6 μm (corresponding to the experimental conditions of Ingignoli [2]). The ideal CJ detonation velocity D_{CJ}, pressure, particle velocity and density of this mixture are respectively 1592 m/s, 34.1 bar, 748 m/s and 5.24 kg/m^3.

The problem was solved using the flux-corrected technique [10] coupled with a grid adaptation along the tube axis thus ensuring the best numerical resolution in the leading detonation zone where basically $dx=dy=dz$=0.5 mm. Total number of meshes along the tube axis was N_x=1000, while N_y and N_z were varied proportionally to the tube diameter keeping $N_y = N_z$.

Detonation was initiated by means of a point explosion at the closed left end of the tube. Up to a detonation run distance of about 1 m, we have considered a plane one-dimensional flow. This early stage of the flow allows one to adjust the initiation energy and to get a quasi-steady detonation regime within a reasonable run distance. Then, this 1D solution was cloned to fill up the whole section of the 3D tube which was considered in a Cartesian frame of reference. Thus, at the beginning, the 3D solution looks like a mono-dimensional one. However, accumulation of truncation errors with time leads to a formation of "hot spots" (i.e. triple points) which after some transient period result in formation of the detonation cellular structure. The cellular structures shown below correspond to self-sustained detonations propagating at the velocity which is close to the ideal CJ value (no losses are taken into account).

In small tubes with diameter $d\leq$20 mm the detonation remains close to a one-dimensional case. In larger tubes when tube circumference becomes comparable with λ, the detonation after some propagation distance begins to spin either in counter-clockwise or clock-wise direction. The spinning mode is observed in a domain of tube diameters ranging from 25 mm to 75 mm. In all spinning cases the detonation pitch is about 4d due to the fact that in the case of the Cartesian grid the tube circumference always equals 4d rather than πd (consider as an example a tube cross-section with N_y=N_z=3 and 4).

If the tube diameter exceeds 75 mm, the detonation propagates in the multi-headed mode. Figure 1 displays the cellular structure in the form of traces of maximum pressure on the surface of the tube and on a diameter cross-section for tubes with diameter d equal 50, 80 and 150 mm. One can see that the cell size λ is of about 100 mm that reasonably agrees with the former estimation. The grid convergence tests with two times smaller mesh cells give the same range of tube diameters where spinning detonation is observed and do not change the size of detonation cells.

Figure 2 shows 3D maps of pressure at 4 instants of time in the case of tube diameter 50 mm in the form of 2D distributions of pressure on two orthogonal planes (*Y*=0 and *Z*=0) and isocontour surface corresponding to 60 bars. One can note non-uniformity of the detonation front, its progression (every 25 μs) in the longitudinal *X*-direction and rotation in the clock-wise direction.

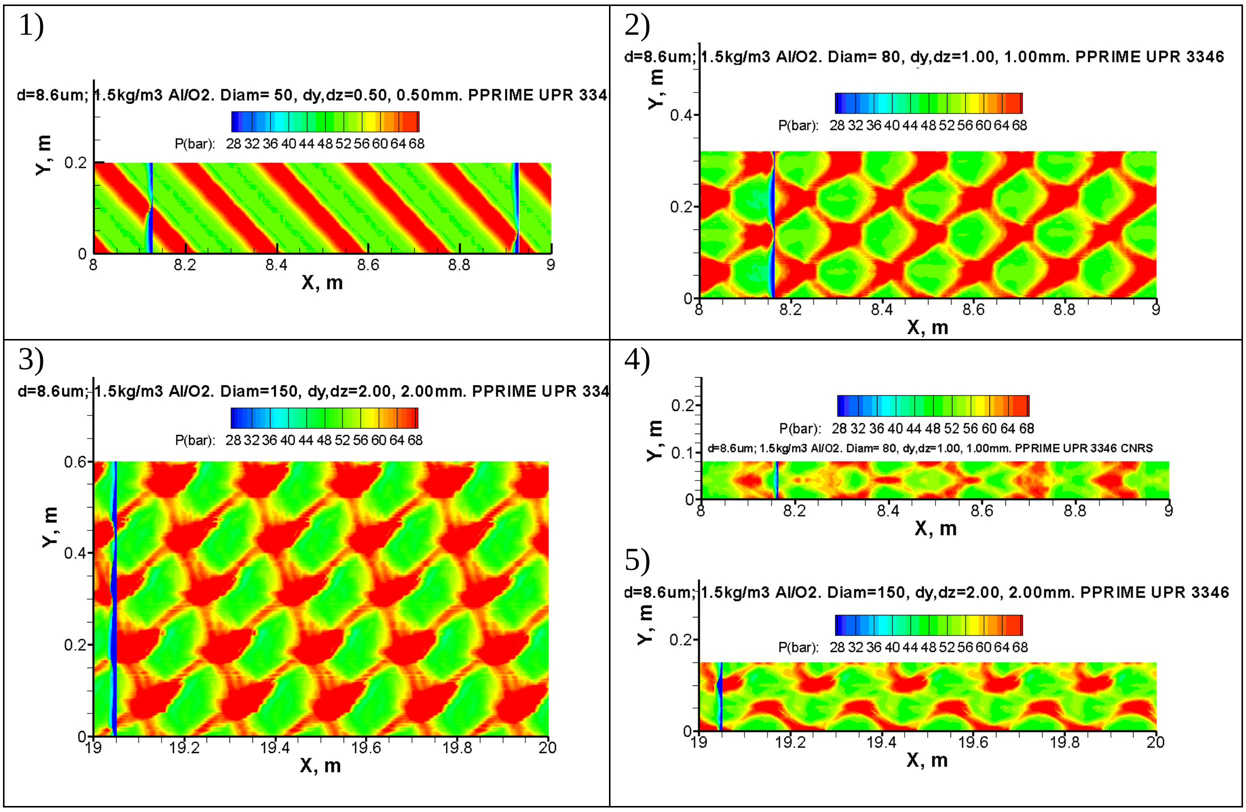

Figure 1. Traces of maximum pressure on the tube surface (1, 2 and 3) and on the diameter cross-section (4 and 5) at tube diameter of 50mm (1), 80 (2 and 4) and 150 mm (3 and 5)

Figure 3a displays for the 50-mm diameter tube the profiles of the mean gas velocity averaged over the tube cross-section $\left|U_{mean}(x)\right| = \frac{1}{S}\int_{-r}^{r}\int_{-r}^{r}\sqrt{U_x^2+U_y^2+U_z^2}\,dydz$ where $S=\int_{-r}^{r}\int_{-r}^{r}dydz$ is the area of the tube cross-section with a radius *r* (only those meshes at *X*=const are taken into account here which fall inside the circle with this radius). One can see that after some transient period the detonation propagation becomes autonomous since the particular form of the mean absolute velocity profile behind the CJ point (where Al particles are already burnt) reasonably match the Taylor-Zeldovich rarefaction wave behind a steady detonation: *U*=0 until *X*=*Dt*/2 and then grows linearly up to the CJ value. As expected, an abrupt change of the slope of $\left|U_{mean}(x)\right|$ curve occurs when particle velocity is close to its CJ value. From Figure 3b showing the variation of a longitudinal mesh size one can conclude that the numerical resolution in the leading detonation zone is sufficiently fine.

Figure 3c displays profiles at *t*=5.6 and 5.8 ms of the pressure $P_{mean}(x)$ averaged over tube cross-section along with the pressure along the tube axis (*y=0, z=0*) and that along two lines on the tube surface: (*y=r, z=0*) and (*y=0, z=r*). Figure 3d shows for comparison the profiles of mean gas density averaged over the tube cross-section and that at the same three lines. In both cases one can see that strong oscillations of main flow parameters take place behind the detonation front over the distance of about 8-12 tube diameters or 2-3 spin pitches (however, oscillations of mean gas density decay noticeably slower that those of mean pressure). These oscillations along with a large difference between the mean gas density and that at the characteristic lines confirms that transverse oscillations are induced by the front of the spinning detonation, which is in agreement with acoustic theories of spinning detonations [11, 12, 13]. Figure 3e shows however that kinetic energy of transverse motion of gas is quite small compared to that of longitudinal motion. Figure 3f displays for completeness the particle density and radius profiles along the same characteristic lines as above.

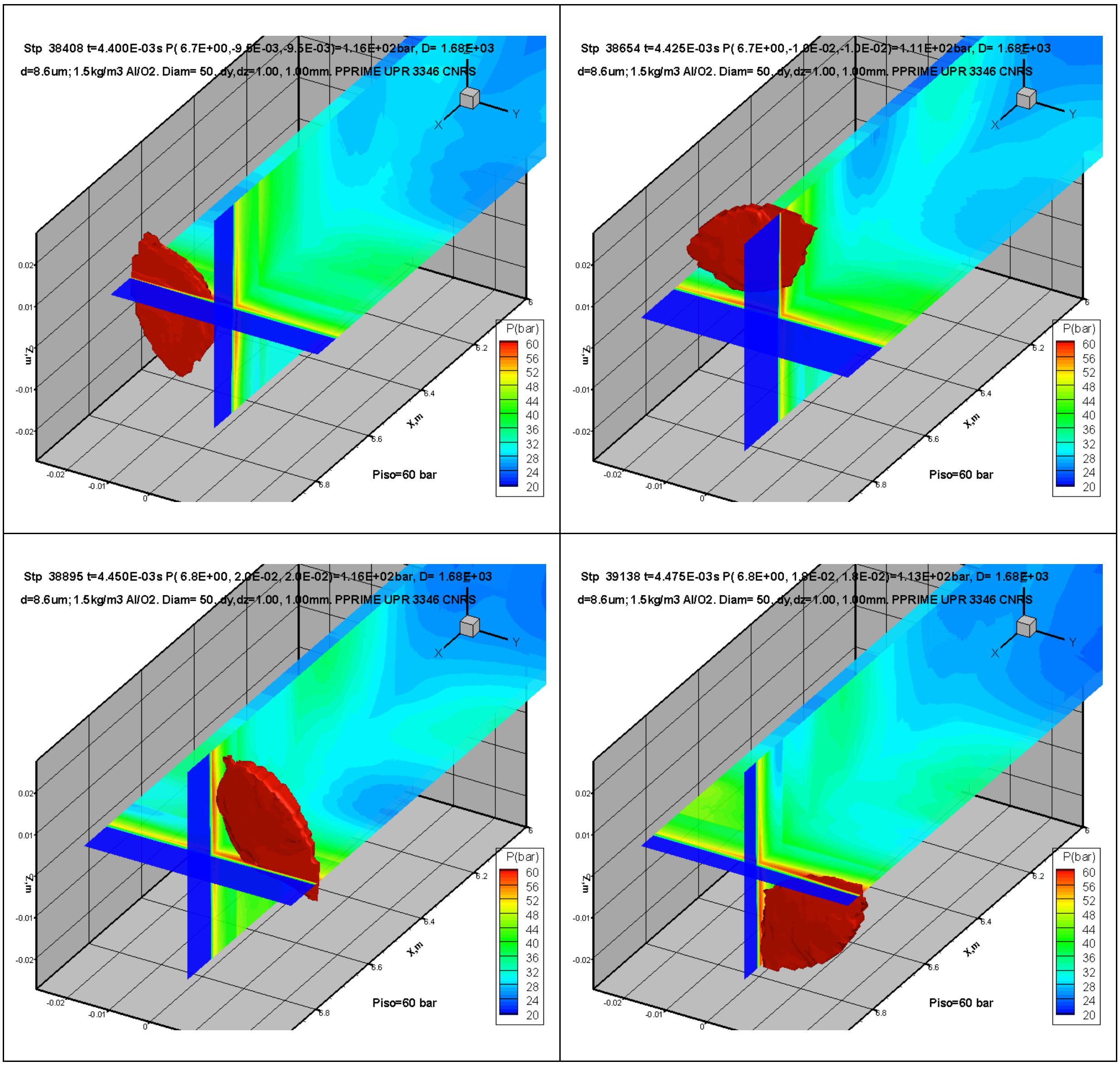

Figure 2. Pressure fields in a 50-mm diameter tube at t=4.400, 4.425, 4.450 and 4.475 ms.

Conclusions

Three-dimensional numerical study of detonation cellular structure in the stoichiometric mixture of aluminum particles with oxygen has shown that cell width agrees reasonably with our former estimations which were based on the 2D cylindrically symmetric simulations. For a given aluminum particle concentration and mean size the range of tube diameters where detonations propagate in the spinning mode is found. Coupling these results with the formerly obtained dependences of detonation cell size on the mean particle size, one can better plan the experimental studies of detonations in aluminum suspensions.

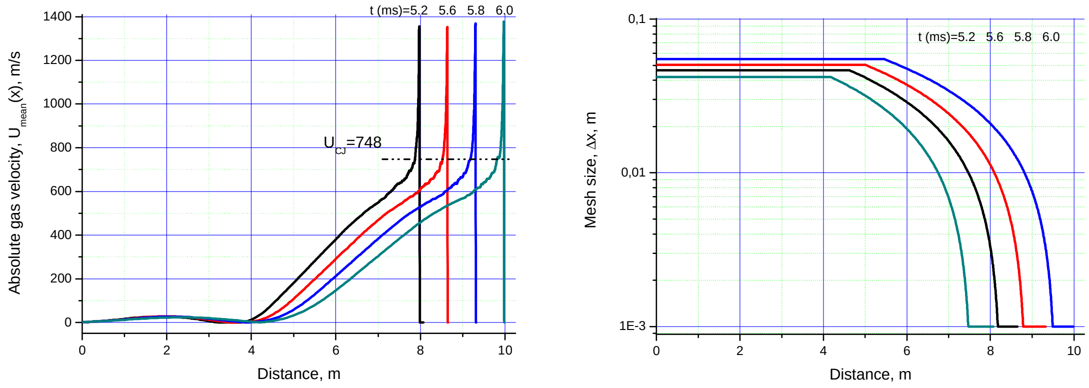

Figure 3a. Left: profiles of mean gas phase velocity U_{mean}; b) right: longitudinal mesh size.

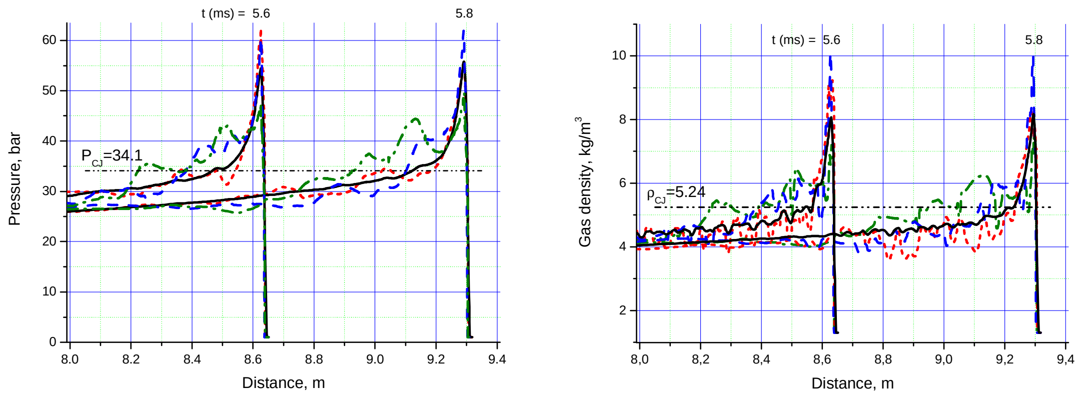

Figure 3c. Left: profiles of mean pressure averaged over tube cross-section (black lines), of pressure along the central line (red), and at tube surface at y=0 (magenta) and z=0 (blue lines); d) right: profiles of gas density corresponding to those of pressure.

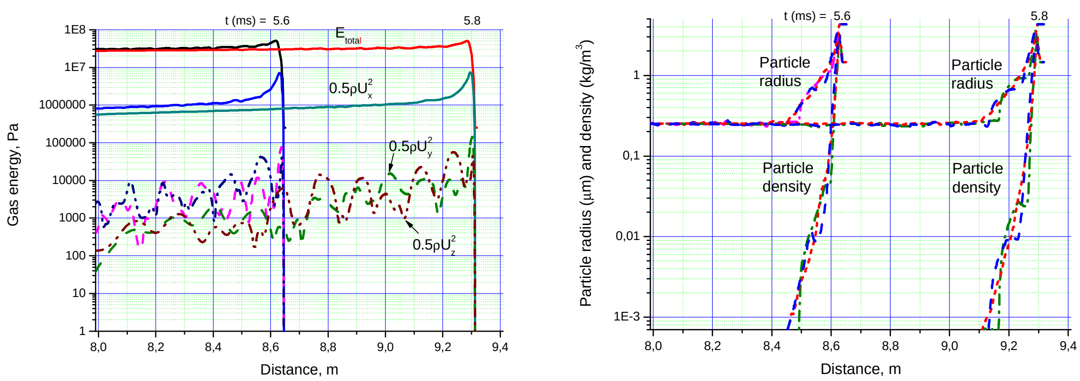

Figure 3e. Profiles of averaged gas energy: total one, kinetic energy of longitudinal and transverse motion; f) profiles of particle density and radius along the same characteristic lines as above. Tube diameter d=60 mm.

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