High Explosive-Driven Shock-to-Detonation Transition in Confined Al-air Mixtures

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Abstract

Numerical simulations are carried out using a robust, two-phase simulation strategy to investigate SDT (Shock-to-Detonation Transition) in Al-air mixtures triggered by a high explosive (HE). An Al ignition model based on Boiko's data that was recently applied to investigate two-phase explosions, is used for this study. It is found that stronger HE charges give smaller detonation velocity deficits at the end of the tube. In particular we are comparing our numerical results with experimental findings of Borisov et al. In the final paper, we will also study the effect of the HE mass and Al concentration on the structure of the detonation wave.

1 Introduction

Deflagration-to-Detonation Transition (DDT) in both Aluminum-air and Aluminum-oxygen mixtures have been studied in the literature for over four decades, both experimentally and numerically. One of the earliest experimental studies on confined DDT in aluminum-oxygen mixtures was undertaken by Strauss [1], where Al was ignited by exploding silver wires placed at the top of the tube. Both granular Al particles of mean diameter 5 μ m and flakes of size ~ 40 μ m were considered and it was observed that mixtures containing 48–64% by mass of aluminum powder detonated, with the run to detonation distances being 0.5–1.6 m, decreasing with increasing aluminum concentration. Detonation was in the spinning mode and detonation speeds of 1550 m/s and pressures of 31 atm were reported for both granular Al and flakes.

Later, experiments on the detonation of flake and spherical Al particles in air were carried out by Tulis & Selman [2] in a vertical detonation tube. Ignition was achieved with the detonation of ~ 2.8 g of RDX or tetryl placed 0.6 m outside the tube, and spinning detonation was reported in the Al-air mixture. They observed that flake Al particles with a surface to mass ratio of 3–4 m²/g readily detonated with velocities of ~ 1650 m/s and pressures of 5 MPa. For 5 μ m spherical Al particles, detonation was subdued, with a maximum detonation velocity of 1350 m/s and detonation pressure of 3 MPa. Furthermore, they concluded that for flake Al particles the induction time between the initial shock and the reaction zone is $\sim 1 \mu$ sec, but is as long as 14 μ sec for spherical particles.

Extending on the above study, Tulis & Selman [3] undertook experiments on unconfined detonation of Al-air mixtures for both flake and atomized particles. A 100 g C4 charge was used to disseminate 4.54 kg of Al particles, forming a two-phase cloud about 6 m in diameter and 1 m in height in a time span of about 25 ms. Subsequently, the main charge, placed 0.5 m from the test device, was detonated to ignite the particle cloud. It was reported that atomized Al particles did not detonate, albeit minor blast overpressure enhancement was observed. For the flake Al particles, however, detonation was induced, and the blast wave overpressure was significantly higher than that of a C4-only explosion. Their key conclusions are that only particles with high surface-to-mass ratios, e.g., 3-4 m²/g, could undergo DDT, and that HE charges as large as 2.27 kg are required to ignite the unconfined cloud in order to have a DDT.

DDT of Al particles in both air and oxygen was experimentally and theoretically investigated by Borisov et al. [4] in a 12.2 cm dia. tube. Spherical Al particles of dia. 1–33 μ m, and flake Al particles of 1 μ m thickness and *** Corresponding author: kaushikb@lbl.gov** 1

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10–15 μ m in length, were studied, and were ignited using a high explosive (HE). The detonation propagated in the spinning mode in the Al-air/oxygen mixtures and it was observed that for flake Al particles, the variation of the energy of detonation initiation with Al concentration is U-shaped, with the minimum energy corresponding to $\sim 330 \text{ g/m}^3$ of Al (stoichiometric proportion) in the two-phase mixture, and the minimum energy of detonation initiation being 3.4 MJ/m² (corresponding to 12 g of the explosive charge). For spherical particles, the detonation initiation energy was much lower than flakes, and monotonically decreased with increase in Al concentration. Both lean and rich limits were reported, corresponding to Al concentrations of ~ 210 and 400 g/m³, respectively for flakes, and ~ 140 and 750 g/m³, respectively for spherical Al particles. Only clouds with particles smaller than 10 μ m were susceptible to DDT. Detonation velocities were typically around 1750–1800 m/s for both flake and spherical Al particles; for flakes this was nearly independent of concentration, and for spherical particles this increased with concentration, with the slowest detonation velocities being at the lean limit. The detonation pressures were 33–35 atm for flakes and independent of Al concentration; for spherical particles, this increased from 19 to 27 atm with the increase in Al concentration. They also attempted to ignite a large cloud of 3.5 μ m spherical Al particles in an unconfined setting, but without success. Finally, they compared their experimental results with simple steady 1D theory and obtained reasonable agreement.

Later, Ingignoli et al. [5] undertook experiments and computations to investigate unconfined detonation of Aloxygen mixtures. An Al-oxygen suspention in a polyethylene bag of 0.7 m diameter and 1 m height, was detonated by exploding a TNT charge of variable mass (up to 150 g) at the top of the bag. Both atomized Al powder of 3.5 μ m mean diameter and flakes 1 μ m in thickness and up to 25 μ m in longitudinal size, were considered; the Al-oxygen mixture was 1.6–2.7 times rich. Although detonations were observed, the shock velocity was normally much lower than the CJ value, and the reaction zone was not close enough to the shock front to permit coupling. The authors' effort to obtain soot plate records of detonation cells was inconclusive. 1D numerical analysis was also carried out which revealed that only particles smaller than 2 μ m and clouds larger than 2 m diameter, can detonate.

Zhang et al. [6] undertook experiments on DDT in Al-air mixtures using a detonation tube 0.3 m in diameter and 40 m in length. They considered two different ignition sources: (1) a stoichiometric H_2-O_2 detonation wave ignited by 9 spark plugs at the upstream end wall of the ignition section; and (2) a 300 J pyrotechnical igniter that consisted of a primer pill with an exploding wire and a small 35 mg nitro charge, for a weak initiation. Anthraquinone-air, cornstarch-air and Al dust-air mixtures were investigated. For Al flakes of size 36 μ m \times 36 $\mu m \times 1 \mu m$, the distance required for the flame and shock wave to couple, normalized by the tube diameter, varied from 120 to 49 as the Al cloud concentration was increased from 200 to 500 g/m³. The detonation velocities were \sim 1800 m/s and compare well with the past experiments of Borisov et al. [4]. Later, Zhang et al. [7] investigated the detonation of 100 nm and 2 μ m Al particles in air at elevated pressures using a 13 m long, 80 mm diameter tube. While the 100 nm Al particles could detonate at 1 atm, the 2 μ m particles could do so only at 2.5 atm. From this they concluded that Al combustion is not diffusion limited and must also depend on the chemical kinetics at the particle surface. Spinning detonation was observed, as evidenced by pressure oscillations in their measurements. In addition, for 2 μ m Al particles at 2 atm initial pressure, a "dust quasi-detonation" was reported wherein the shock velocity is significantly lower (in this case ~ 40 %) than the Chapman-Jouguet detonation value. Later, Zhang et al. [8] performed experiments to investigate unconfined Al-air DDT. Two types of Al particles were used: atomized Al with a mean diameter of 2–3 μ m (loading mass 47.6 kg), and Al flakes (31.5 kg). A 21.3 g/m, 6.1 mm diameter PETN cord was exploded to disperse the Al particles into a cloud 18 m in length and 3 m \times 3 m in cross section, giving rise to a suspension with an average Al concentration of 670 g/m^3 for the atomized particles and 290 g/m³ for the flakes. Then, the Al-air cloud was ignited at one end using 8 kg C4. It was reported that although DDT phenomena was observed for both atomized and flake Al, detonation was established only in the latter, with peak pressures of 4–8 MPa and shock velocities of 1460-1530 m/s. In addition, the authors used kinetics-limited 1D and 2D models to predict DDT in unconfined Al-air mixtures.

Many numerical/theoretical studies on DDT in Al clouds have also been undertaken. Veyssiere & Khasainov [9] undertook a 1D numerical study of detonations in gaseous mixtures of hydrogen, ethylene or acetylene containing Al particles. They showed that a steady double-front detonation (DFD) can propagate, where the first front is supported by the heat release from the gases, and the second by the heterogeneous reactions between the Al particles and the gaseous products. The time delay between the two fronts was computed for different Al particle concentrations and compared well with past experiments. Later, Veyssiere & Khasainov [10] investigated DDT in hydrogen-air gaseous mixtures with suspended fine Al particles. The differences in the order of magnitude of the characteristic induction and combustion times of gaseous mixtures and solid particles gives rise to nonmonotonic heat release behind the leading detonation front. They showed that three different steady propagation regimes may exist: Pseudo-Gas Detonation (PGD), Single-Front Detonation (SFD) and Double-Front Detonation (DFD). Among other things, they also investigated the effect of particle size, heat loss effects and gaseous composition on the structure of the propagating detonation front. This study clearly demonstrated that multiple detonation regimes exist in hybrid two-phase mixtures.

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Benkiewicz & Hayashi [11] undertook 2D numerical simulations of multi-headed, steady detonations in Aloxygen mixtures using an adaptive mesh refinement technique. They concluded that the detonation of 2.5 μ m particles evolves into a two-headed mode of propagation, and is independent of Al concentration for lean mixtures. For 1 μ m Al particles, the detonation cell size is much finer, and it evolves initially in a 11-headed mode which later transitions to a 8.5-headed mode in a 12 cm high tube. This study clearly demonstrated that multidimensional numerical simulations can also capture transverse effects in the propagation of steady detonations in two-phase mixtures.

One-dimensional numerical studies on detonation in Al-air mixtures have been carried out by Fedorov & Khmel [12], identifying different self-sustaining detonation regimes: normal CJ detonations, weak detonations with an internal sonic point, and weak detonations with an intersonic final equilibrium state. These studies were later extended to the investigation of 2D cellular detonation formation in stoichiometric Al-oxygen mixtures [13], where the authors determined the transverse size of the detonation cell for different particle sizes in the range 1–10 μ m. Then, they also numerically investigated detonation in bidisperse Al-oxygen mixtures [14] and concluded that the detonation in such mixtures is not ideal, and the steady-state portion of the structure is limited by the equilibrium-frozen sonic point. In addition, they postulated that for bidisperse suspensions, a "hard" initiation in the fine particles and "soft" in the coarse is possible, which gives rise to the existence of unsteady two-front structures.

2 Formulation

A heterogeneous two-phase continuum model based on Nigmatulin [15] is used for the study and is summarized in [16, 17]. Both phases have separate velocities and temperatures and interact through source terms that account for inter-phase mass, momentum and energy transfer. A recently proposed Al ignition model [18, 19] based on Boiko's data [20, 21] is used for the analysis; this empirical model is robust and also accounts for Al cloud concentration effects, unlike most other counterpart models used in contemporary literature. For the present the mass transfer rate from Al solid to vapor is assumed to be diffusion-limited; in the future, however, a hybrid combustion mechanism [22] can be employed where the mass transfer accounts for both the diffusion as well as the kinetic regimes of Al burning. Quadratic equations of state expressions are used for each species [23], based on the CHEETAH code. Robust second-order Godunov schemes are used to solve the governing equations for the gas [24–26] and particle phases [27]. Adaptive mesh refinement (AMR) is used to resolve the finer scales in the flow [28]. The overall approach is consistent with ILES [29]. More details on the numerical simulation strategy can be found elsewhere [16, 17].

3 Preliminary Results and Discussion

Preliminary simulations are carried out to study SDT in Aluminum-air mixtures inside a rectangular tube of dimensions 4.2 m \times 12 cm \times 12 cm. The left side of the tube is an outflow, while the other five sides are free-slip walls. A 1400 \times 40 \times 40 base grid is used with 3 levels of refinement corresponding to refinement ratios of 2 each. The tube is filled with flake Al-air mixture corresponding to an ambient concentration of 330 g/m³, which is the stoichiometric value for Al-air mixtures; the Al flake particle size is 2.5 μ m. We investigate the effect of initiation energy on the SDT. To this end, cubic PETN charges corresponding to different mass (\sim 3–15 g) are placed 12 cm inside the tube from the open end. The blast wave from the PETN charge ignites the Al-air mixture and initiates shock-induced combustion which slowly evolves to a detonation, propagating to the right. Since the left end of the tube is open, only about half of the energy from the explosive charge is used in the initiation of the SDT. We terminate the simulation when the detonation wave reaches the right end of the tube.

Schematics of the pressure, temperature, and the density of the fuel (Al gas), Al combustion products and the PETN driver are shown in Fig. 1 along the centerline at 2 ms time instant for a 15.2 g PETN booster charge. Cellular structures are evident near the leading front. The peak temperatures are \sim 4200 K—the flame temperature for Al-air mixtures. Pockets of fuel are also convected downstream, where they will burn slowly as they mix with the limited oxidizer, if any, that is available downstream from the detonation front. The HE driver products only extend to about one-third of the tube and so are not in competition with Al for oxidizer in the vicinity of the detonation front. We observe interesting shear patterns at the interface due to baroclinic effects.

Schematics of the pressure (bar), temperature (Kelvin) and Al combustion products (g/cc) in the vicinity of the detonation front at the 2.05 ms time instant are shown in Figs. 2, 3 & 4 respectively for HE masses 3.4 and 15.2 g. The peak pressures and temperatures are slightly higher for the stronger initiation, albeit only by a very small amount. The flame is highly turbulent, as evident from the temperature and products schematics.



Figure 1: Structure of SDT in Al-air mixtures: (a) pressure; (b) temperature; (c) fuel; (d) products; (e) driver.



Figure 2: Pressure schematic at 2.05 ms time instant for HE masses (a) 3.4 g; (b) 15.2 g.

The pressure traces along the centerline are presented in Fig. 5 at time instants 1 and 2 ms. The peak pressures are on the order of \sim 70 bar at the von Neumann spike. A compression wave is caused due to subsequent interactions of the early blast wave that reflects from the side walls, and this trails behind the leading detonation front, as seen in Fig. 5 (a). Subsequently, this wave merges with the leading detonation wave, thereby augmenting the pressure behind the front. We also note that the motion of the transverse waves at the front are not synchronized for the different test cases. The pressure equilibriates to ~ 10 bar on the left side of the tube, far away from the detonation front.

The profiles of solid Al mass remaining $(mass_{Al})$ in the tube is plotted in Fig. 6 (a); as evident, the consumption of Al is non-linear at very early times due to the 3D spherical blast from the charge, after which it transitions to a linear trend as the planar detonation wave propagates along the tube; the respective Al mass consumption rates, $mass_{Al}$, are plotted in Fig. 6 (b) and as evident the rate is higher for a stronger HE mass, but tends to asymptote beyond ~ 12 g. The x - t diagram of the leading detonation front is shown in Fig. 7 (a); the leading front attains a straight line trajectory with time for all the cases considered; we compute the least-square slope of these trajectories to determine the detonation velocity, shown in Fig. 7 (b). As evident, the front attains velocities in the range 1600-1700 m/s and the detonation velocity deficit is smaller for a stronger HE charge (the CJ value is 1830 m/s); furthermore, the trend is almost linear with the HE mass used in the initiation.

In the final paper, we will investigate lean and rich Al-air ratios as well and investigate the dependence of the initial HE charge mass on the propagation of the leading detonation front.

4 Conclusions

Two-phase simulations are carried out to investigate SDT in Al-air mixtures with the detonation being initiated by a HE. Our simulation model demonstrates that stronger HE charges result in slightly faster detonation velocities and Al mass consumption rates. In the final paper, we will also study other Al-air ratios and deduce the effect of the HE mass on the structure and propagation of the detonation wave.

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Figure 3: Temperature schematic at 2.05 ms time instant for HE masses (a) 3.4 g; (b) 15.2 g.



Figure 4: Al combustion products schematic at 2.05 ms time instant for HE masses (a) 3.4 g; (b) 15.2 g.

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Figure 5: Pressure profiles along the centerline for different HE charge masses (identified in the legend) at time instants (a) 1 ms and (b) 2 ms.



Figure 6: Profiles of (a) mass_{Al} and (b) $mass_{Al}$.

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Figure 7: (a) x-t diagram and (b) detonation velocity.

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