Propagation and Structure of Hybrid Aluminum-Hydrogen-Air Detonations: A Computational Approach

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1 Introduction

Dust explosions have long been studied to mitigate industrial hazards in environments such as coal mines and metal factories. These detonations can be categorized as heterogeneous (reactive particles with oxidizing gas), hybrid (both particles and gas reactive), or dusty (inert particles in reactive gas) mixtures [1, 2]. Among these, metal powder combustion, particularly aluminum, has gained attention due to its high energy density and potential applications in aerospace propulsion, such as enhancing specific impulse and suppressing combustion instabilities in solid rocket motors.

In propulsion, hybrid detonation systems, such as pulse detonation engines (PDEs) and rotating detonation engines (RDEs), capitalize on pressure-gain combustion for improved performance [3, 4]. Aluminum, in particular, has been shown to improve combustion efficiency and thrust when mixed with gaseous fuels [5–7]. Experimental studies using aluminum powder in detonation tubes have characterized critical phenomena, such as deflagration-to-detonation transitions and hybrid detonation wave structures [8–10]. However, computational investigations remain relatively limited, despite their ability to uncover phenomena that are not easily observed experimentally [2].

This study bridges the gap in computational analyses of hybrid detonation systems, focusing specifically on the underexplored influence of aluminum particle size on detonation dynamics. By addressing limitations in existing experimental and computational studies, this work provides new insights into pressure-gain combustion technologies.

2 Problem Description and Numerical Models

Figure 1 illustrates the numerical setup used in this study. The computational domain consists of a 10-cm long and 1-cm wide channel with both ends open (outflow boundary condition), with the top and bottom surfaces acting as periodic boundary conditions. The entire channel is filled with hydrogen and air with an equivalence ratio between 0.25 and 1, with an initial temperature and pressure of 300 K and 1 atm respectively. At the left boundary, a combination of three hotspots is used to mimic a directly-initiated detonation. The hotspots initially contain a stoichiometric mixture of hydrogen and air, with a

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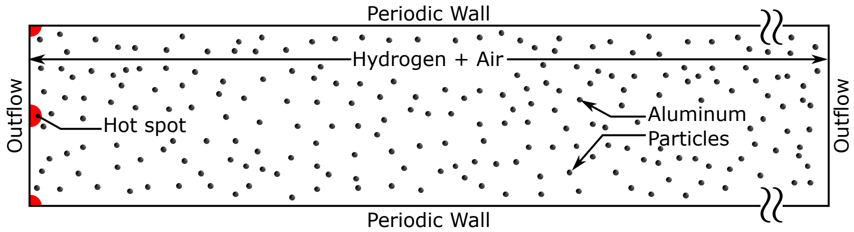

Figure 1: Initial and boundary conditions of the numerical setup.

temperature of 1500 K and pressure of 50 atm. In addition to the gas mixture, micron or sub-micron-sized aluminum particles are distributed uniformly throughout the channel. The particle volume fraction is varied between 0.002836% and 0.011344%, corresponding to a pure aluminum-air equivalence ratio of 0.25-1, to study the effect of particle concentration on the detonation. The aluminum particles are assumed to be spherical and monodisperse, with a constant heat capacity of 1177 J/kg.K, and a material density of 2700 kg/m^3 [7].

The coupled, multiphase, compressible, unsteady Navier-Stokes equations are solved using the University of Florida's HyBurn code. The governing equations for the solid phase are derived using a kinetic-theory approach within an Eulerian framework. Details of the complete equation set and numerical modeling approach can be found in [11, 12]. The solid phase model incorporates drag, convective heat transfer, particle-particle interactions, and inelastic collisions. The governing equations are solved using high-order Godunov methods.

The O'Conaire [13] detailed reaction mechanism (9 species, 21 reactions) is used for the gas-phase hydrogen-air reactions, which has been shown to work well for detonations applications [14]. For the Aluminum particle-air reactions, the Benkiewicz and Hayashi [15] model is used. Although this is a fairly simple model, it works well for aluminum-air detonation scenarios, resulting in detonation velocities and cell sizes that agree with experimental observations. To verify this, numerical simulations identical to the verification tests in [7] were performed. The results, shown in Figure 2, suggest that the detonation cell size is $\sim$40 cm which agrees well with [7], and the Chapman-Jouguet detonation velocity, D_{CJ}, is $\sim$1900 m/s, which is close to those reported in [16].

The AMReX massively-parallel library [17] for adaptive mesh refinement is used. For detonations, it is imperative that the half reaction length is appropriately resolved. To ensure this, a base resolution of 156 μm is used, along with 4 levels of refinement and a refinement ratio of 2 in each level. This results in a mesh resolution of $\Delta x = \Delta y \approx 10$ μm at the finest level, which ensures at least 10 computational cells in the half reaction length of hydrogen-air detonations.

3 Results and Discussion

To understand the effect of aluminum particles on the hydrogen-air detonations, first a base case needs to be established. One case was setup with stoichiometric hydrogen-air mixture (equivalence ratio, $\phi_{H_2} = 1$) without any particles. Figure 3(a) shows the numerical soot foil results which indicate a cell size, λ, of $\sim$ 2.7 mm, which aligns closely with the 2.8 mm reported in [18]. Note that the cell size was calculated by finding the mean λ for the cells in the regular section of the smoke foil, i.e., between $x = 0.07$ and 0.095 m. From here on, all reported λ will follow the same method, unless stated otherwise. Decreasing ϕ_{H_2} to 0.8 results in an increased λ of $\sim$7 mm (figure 3(b)), which is slightly smaller than the 10 mm reported in [18], suggesting higher reactivity in the Benkiewicz model [15], which warrants further investigation in the future. One possible way to correct this would be to add an

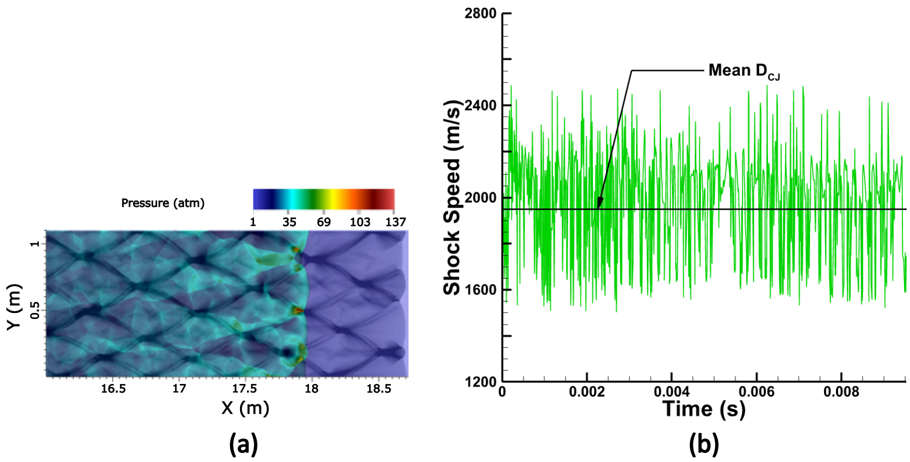

Figure 2: Numerical results of Al-air cellular detonations with 13.5 μm particles and mass loading of 0.5 kg/m^3 showing (a) overlay of numerical smoke foil on the pressure field and (b) speed of the leading shock.

ignition delay model and needs to be investigated in the future. As the ϕ_{H_2} is decreased further to 0.25, the detonation fails, as expected, because the height of the channel is not enough to support the much larger detonation cells that would form at this equivalence ratio.

Let us consider the case of $\phi_{H_2} = 0.8$ as the base case for now, since this produces a stable detonation, and see what happens if we add aluminum particles to it. There are a variety of different particle sizes we can choose from, however, we only consider a size range of 0.1-10 μm, which have been reported to produce interesting hybrid detonations [2]. Adding 1 μm particles, with an aluminum-air equivalence ratio (ϕ_{Al}) of 0.25, reduces λ to 0.5-1.4 mm (figure 3 (c)) and increases D_{CJ} (figure 4 (a)) by ~200 m/s, while making the cells slightly irregular, which aligns with [2]. This indicates that the fuel-air mixture is more reactive than the base case without particles.

If we increase the particle size to 10 μm, however, the cells become highly irregular (figure 3 (d)). It is difficult to estimate the mean cell size range due to large differences in sizes which can be as small as 0.2 mm to sometimes larger than 7 mm. The shock speed plots imply that the D_{CJ} is similar to, but slightly lower than the base case. These observations indicate that the aluminum particles do not not contribute to the detonation. The reason that the 10 μm-particles behave so differently than the 1 μm-particles is due to the significantly reduced surface area-to-mass ratio, which leads to slower energy release. The lower reactivity of larger particles has been studied in great details by several researchers. In the context of detonations, the larger particles start to ignite outside the reaction zone of the ZND detonation and beyond the Chapman-Jouguet (C-J) sonic plane, and thus, do not alter the base H_2-air detonation structure. This is often referred to as pseudo-gas detonation [2]. The D_{CJ} is slightly lower because the gas loses energy to the colder particles via conduction, even though they do not contribute to the reactions. The effect is similar to adding inert particles in a gaseous combustion to reduce the energy release rate. In case of deflagrations, the effect is much stronger as the combustion occurs much more slowly which gives more time for heat conduction to sap the energy away from the gas. Once beyond the C-J sonic plane of the H_2-air detonation, the particles may still react if there is enough left-over oxygen. This often leads to a second detonation wave to form which has been observed by Zhang et al. [8, 9]. However, in these simulations, we do not observe a second wave, likely because the channel is fairly small, and the larger particles would need a lot more time to form a second detonation wave. This is a topic of interest for future research.

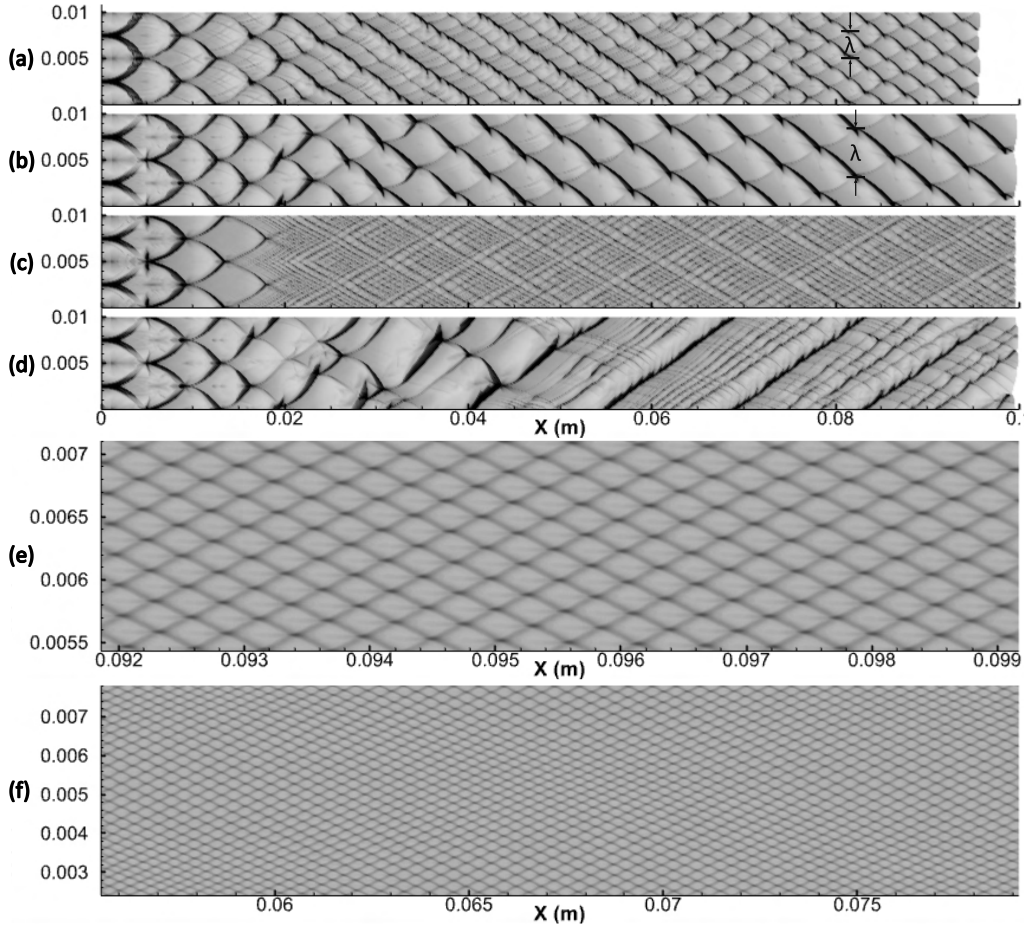

Figure 3: Numerical soot foils of cellular detonations for (a) $\phi_{H_2} = 1$; (b) $\phi_{H_2} = 0.8$; (c) $\phi_{H_2} = 0.8$ with 1 μm Al; (d) $\phi_{H_2} = 0.8$ with 10 μm Al; (e) $\phi_{H_2} = 0.8$ with 0.1 μm Al; and (f) $\phi_{H_2} = 0.25$ with 0.1 μm Al particles. Note that figures (e) and (f) are zoomed in to be able to visualize the smaller cells.

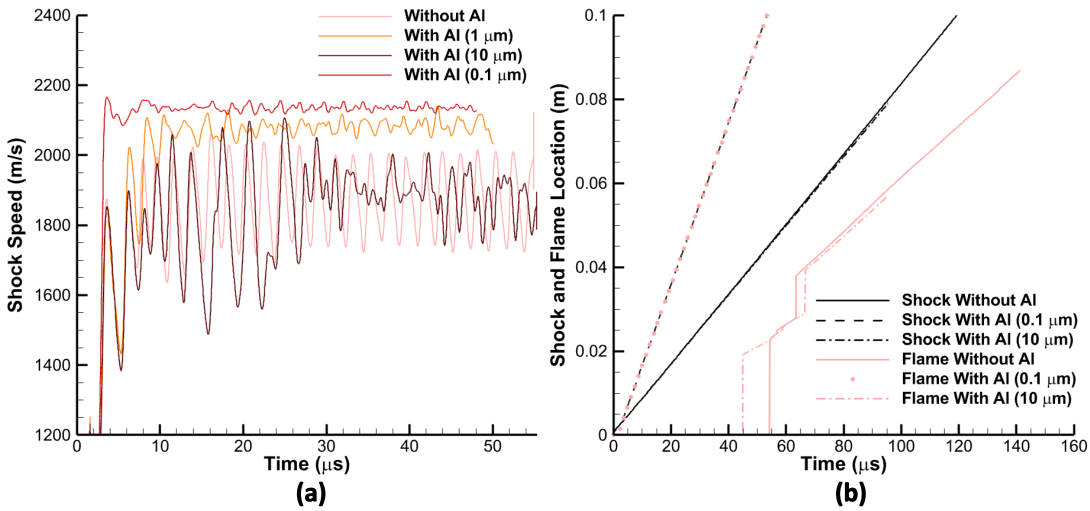

Figure 4: Plots of (a) leading shock speeds for $\phi_{H_2} = 0.8$ without Al, with 1 μm Al, with 10 μm Al, and with 0.1 μm Al particles; (b) shock and flame speeds of $\phi_{H_2} = 0.25$ without Al, with 0.1 μm Al, and with 10 μm Al particles.

On the contrary, if we reduce the particle size to sub-micron levels of 0.1 μm, the detonation behavior completely changes. In figure 3 (e) we see that the cell size becomes significantly smaller than the base case ($\sim$0.24 mm) and the cells are highly regular. The D_{CJ} is considerably higher than the base case at $\sim$ 2150 m/s, which is also higher than the 1 μm-particles case. Once again this makes sense, because the smaller particles react much more quickly and effectively. Additionally, in this case, the Al-air reactions dominate over the H_2-air reactions. This becomes more evident if we look at the numerical smoke foil of a pure Al-air detonation with $\phi_{Al} = 1$. For the pure Al-air case, the cell size is $\sim$ 0.17 mm, which is much closer to the cell size in the hybrid case. In fact, in this case, the hydrogen reduces the reactivity of the particles by reacting and removing oxygen available for the particles. A detailed analysis of this hypothesis is beyond the scope of this work, but is of primary interest for future work.

Another interesting case to study is to start with the base case of $\phi_{H_2} = 0.25$ and add 0.1 μm-particles to it at the same ϕ_{Al} of 0.25. The first observation is that the detonation does not fail, and instead produces highly uniform and tiny cells, with a cell size of $\sim$ 0.28 mm (figure 3 (f)). Thus, even with a small amount of added aluminum particles, the highly lean H_2-air detonation can sustain a stable detonation. On the other hand, addition of 10 μm-particles to the same mixture, does not help with detonation propagation, once again suggesting that the larger particle size do not participate in the detonation. The comparisons of the flame propagation behavior of these three cases can be seen in figure 4 (b). The base case (without particles) and the 10 μm-particle cases clearly show that the flame and shock fronts are separated right from the start, implying detonation failure, whereas the same for the 0.1 μm-particles are coupled together which is an indication of detonation propagation. This has important implications on lean mixture detonations. In various scenarios where gaseous fuel supply is limited (such as in outer space), detonation-based engines can continue to operate with addition of a small quantity of reactive metal particles of the appropriate size such as sub-micron sized aluminum, that may be mined in-situ on other celestial bodies.

4 Conclusions

This study computationally investigates the propagation and structure of hybrid aluminum-hydrogen-air detonations, emphasizing the role of aluminum particle size and concentration. The findings highlight significant variations in detonation behavior based on particle characteristics. Smaller particles (≤ 0.1 μm) significantly enhance detonation reactivity, producing smaller, regular cell sizes compared to larger particles (≥ 10 μm), which behave as pseudo-gas detonation systems [2]. Notably, the addition of appropriately sized aluminum particles enables the sustenance of detonations in lean hydrogen-air mixtures, underscoring their potential in extending operational ranges in propulsion systems.

These results provide valuable insights into hybrid detonation dynamics, suggesting practical applications in aerospace propulsion, particularly in environments where fuel resources are constrained. Future work should investigate complex particle interactions, ignition delays, and larger domains to refine hybrid detonation models.

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