

The Influence of Shock Waves on the Vaporization and Combustion of Aluminum Droplets

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1 Introduction

Because aluminum (Al) is an energetic fuel additive for propulsion systems and because of the effectiveness of particle damping in suppressing combustion instabilities in rocket motors, aluminum particles have been widely employed in combustion applications [1]. The importance of aluminum in combustion systems has led to a large number of studies involving aluminum combustion specific to propulsion applications. However, aluminum is also being used as a fuel additive for heterogeneous explosives [2]. Most of the burning time correlations for Al particles [3, 4] were developed for propulsion applications where shock waves are not present and the relative velocity between the Al particles and the oxidizing gas is small. When subjected to high-speed flows produced by a detonation, Tanguay *et al.* [5] found that larger Al particles may burn in a kinetic-limited regime even though the same particles burn in a diffusion-limited manner in quiescent environments. Al particle burning-time correlations developed for propulsion applications cannot account for such behavior. Before detailed burning-time correlations in high-speed flows can be developed, basic mechanistic understanding must be obtained. In this paper, we illuminate some of the complex physics when a shock wave interacts with vaporizing Al droplets in inert and reactive environments through the use of direct numerical simulation techniques. Large, 230 μm -diameter Al droplets, which are diffusion-limited in quiescent conditions [3], are simulated to observe what effect shocks and high-speed flow has on the rate-limiting combustion mechanisms.

2 Numerical Model and Computational Setup

To accurately predict the influence shock waves have on the vaporization of Al droplets, a technique based on the level set method [6] was employed to separate the computational domain into gas-phase and liquid-phase regions. The model in the gas-phase region uses the two-dimensional reactive Navier-Stokes equations assuming an ideal gas. Nine species were considered: Al, O₂, O, N₂, AlO, Al₂O, AlO₂, Al₂O₂, and Al₂O_{3(l)} with a nine-step chemical reaction mechanism [7]. The liquid region representing the droplet uses the non-reactive Navier-Stokes equations with an isentropic equation of state that accounts for cavitation [8–10]. Phase change between the gas and liquid phases is based on the

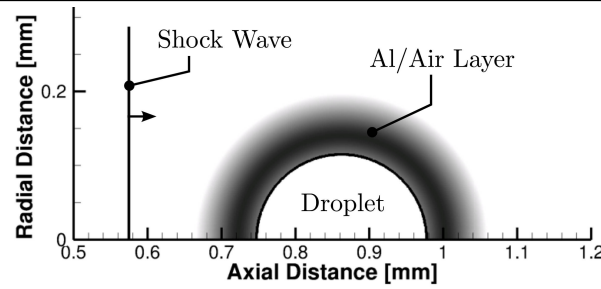


Figure 1: Initial conditions used in this study.

Schrage-Knudsen equation from kinetic theory [11]. Heterogeneous surface reactions are not considered because data useful for detailed numerical simulations are not available. Further details of the model and corresponding input parameters can be found in Houim [7] and Houim and Kuo [8].

The governing equations were solved using an operator split approach with fifth-order methods applied to the hyperbolic terms for the gas-phase [12] and liquid-phase [8] regions. Second-order conservative differencing was used for the viscous and diffusion terms in both regions. The gas-liquid interface was captured using the level set method [6] and was coupled with a variant of the ghost fluid method [13] that uses the exact solution to a gas-liquid Riemann problem that accounts for velocity and pressure jumps across the interface due to phase change and surface tension [8]. Details on the numerical methods used, including adaptive mesh refinement [14], and validation tests can be found in Houim and Kuo [8, 12].

The initial conditions are shown in Fig. 1. A shock wave with Mach number, M , propagates into air at 1 atm and 300 K and impacts a 230 μm -diameter Al droplet with an initial temperature of 2750 K. An Al/air layer that smoothly transitions from heated Al vapor at the surface to ambient air away from the droplet was used to minimize the strength of shocks arising from impulsively induced vaporization [8]. The top, left, and right boundary conditions are non-reflecting and the bottom boundary condition is an axis of rotation. The total height of the domain is 287.5 μm and the computational cell size, at the finest level of refinement, was $\Delta x = 0.898 \mu\text{m}$. The time-step size was determined using a CFL number of 0.5 based on the wave speed in the liquid phase region. The simulations consider two general environments: inert and reactive to compare and contrast between burning and non-burning situations.

3 Results

A time sequence for $M=2$ and $M=4$ shock waves interacting with the 230 μm -diameter Al droplet in a non-reactive environment are shown in Fig. 2. Details of the cavitation bubble formation and collapse that occurs during the first 0.175 μs of the simulation are not shown for the sake of brevity, but can be found in Houim and Kuo [8]. As the shock wave travels over the droplet, the pressure and high-speed flow simultaneously compresses the Al vapor layer and strips it off the surface. Pressurization of Al vapor near the surface does not change the equilibrium vapor pressure (since p_{sat} is governed by the droplet surface temperature which is unchanged by the shock), but the equilibrium mass fraction is drastically reduced. There is now more Al vapor near the droplet surface than the new phase equilibrium condition allows. Thus, Al vapor locally condenses on the droplet surface, which produces a significant decrease in the evaporation mass flux [shown in Fig. 3(a)] when the shock wave first impacts the droplet at about $t = 0.25 \mu\text{s}$ and $t = 0.125 \mu\text{s}$ for the $M=2$ and $M=4$ cases, respectively.

What is perhaps surprising is that the rate of convection from the high speed gases behind the shock wave is not strong enough to make up for the reduction in vaporization rate produced by the decrease in equilibrium vapor mass fraction between the shocked and quiescent cases. From quasi-steady, diffusion

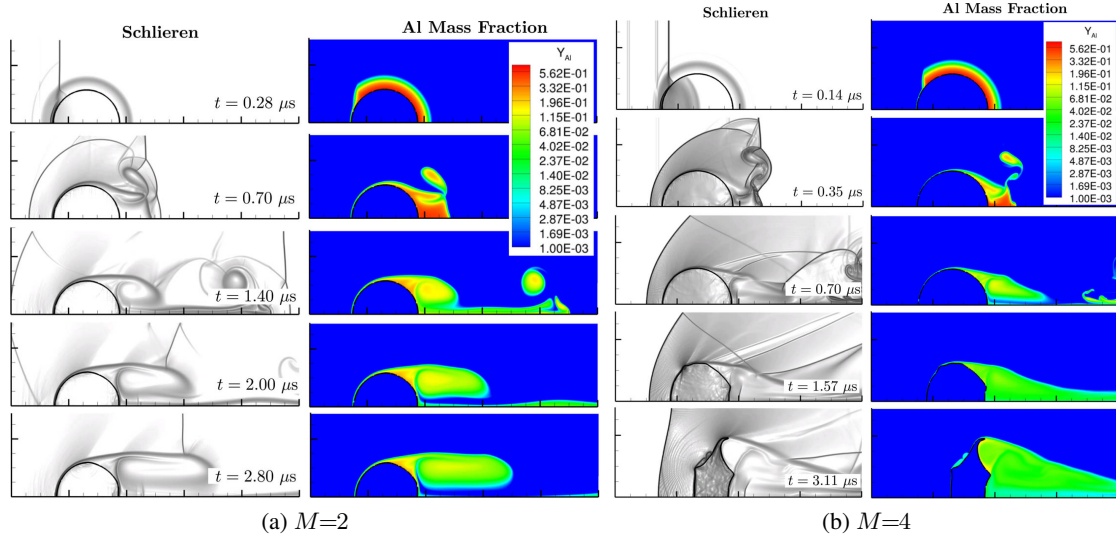


Figure 2: Time sequence of computed Schlieren ($|\nabla\rho|$) and Al vapor mass fraction fields for (a) $M=2$ and (b) $M=4$ shock waves interacting with a $230\text{ }\mu\text{m}$ -diameter Al droplet in a non-reactive environment. The Schlieren field in the droplet was multiplied by a factor of 25 to increase visibility. Reproduced from Houim [7] and Houim and Kuo [8].

limited droplet vaporization theory [15] and the Ranz-Marshall correlation [16], the ratio of the droplet vaporization rate from a quiescent condition to a post-shock condition is approximately [7, 8]:

$$\frac{\dot{m}''_{\text{shock}}}{\dot{m}''_{\text{quiescent}}} = \frac{\ln(p_{\text{shock}}) - \ln(p_{\text{shock}} - p_{\text{sat}})}{\ln(p_{\text{quiescent}}) - \ln(p_{\text{quiescent}} - p_{\text{sat}})} (1 + 0.267 Re_d^{1/2} Pr^{1/3}), \quad (1)$$

where Re_d and Pr are representative Reynolds and Prandtl numbers.

Depending on how a representative Reynolds number and average pressure are computed, the ratio of the vaporization rate is around 89% for the $M = 2$ case and between 75% and 105% for the $M=4$ case. Thus, diffusion-limited theory is consistent with the computed results, even in magnitude, as long as convective enhancement is taken into account.

Contour plots of temperature and some species mass fractions for a $M=2$ shock interacting with an Al droplet in a reactive environment are shown in Fig. 4 and the vaporization mass fluxes are shown in Fig. 3(b). Unlike the purely vaporizing droplet, high speed flow behind the $M=2$ shock increases the vaporization mass flux from the quiescent case by about 25% as shown in Fig. 3(b). This increase is caused by higher Spalding transfer numbers for a burning droplet compared to a vaporizing droplet and is predicted from diffusion-limited droplet combustion theory [15]. However, the magnitude of the increase between the $M=2$ and the quiescent reacting cases is overpredicted by a factor of 2 to 6.

In comparison to the inert environment, the rates of phase change are much higher and the Al vapor mass fraction near the surface of the droplet is lower when chemical reactions are considered. For example, at a time of $2\text{ }\mu\text{s}$ the partial pressure of Al, p_{Al} , at the front stagnation point is 74.0 kPa for the inert case, while p_{Al} is much lower for the reacting case with a value of 46.9 kPa. The saturated vapor pressure for either case is 82.3 kPa. Thus, there is a very large 43% deviation from equilibrium condition for the reacting case while the deviation for the inert case is quite modest at 10%. One of the primary reasons for this deviation is due to rapid chemical reactions between Al vapor and air creating a very thin concentration boundary layer, which, in turn, increases the rate of mass transport away from

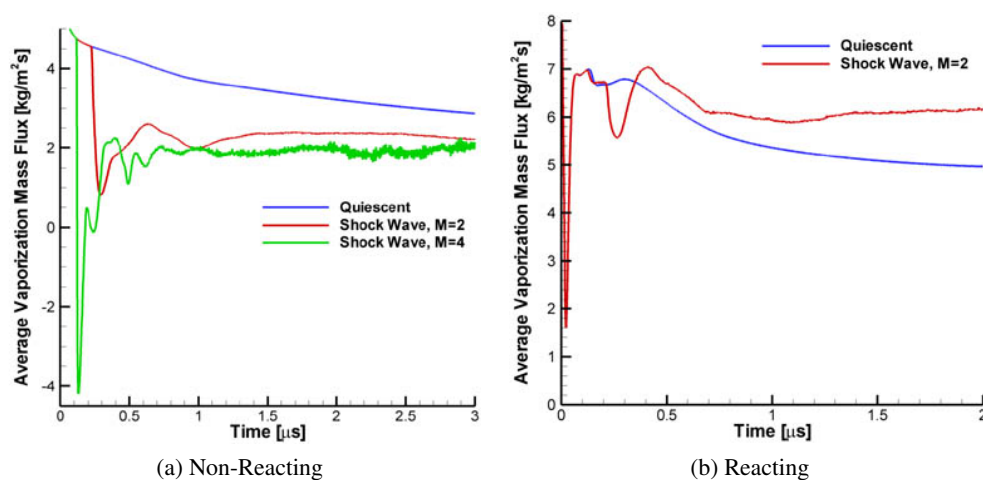


Figure 3: Computed average vaporization mass flux as a function of time for (a) non-reacting cases and (b) reacting cases. Reproduced from Houim [7] and Houim and Kuo [8].

the surface. However, the vapor generation rate at the surface computed from the Schrage-Knudsen equation [11] cannot keep up with the increased vapor transport rate away from the surface. Thus, p_{Al} decreases at the surface. This not only increases the rate of vapor generation (by over a factor of 4 at the front stagnation point) but also decreases the mean concentration gradient across the boundary layer. Eventually, the increase in the rate of vapor generation at and the decrease in vapor transport from the surface equilibrate.

Diffusion-limited droplet combustion theories typically assumes the vapor concentration at the surface is always at the phase equilibrium condition, which, in turn, implies that the vapor generation rate can be infinitely fast. Thus, correlations based on diffusion-limited assumptions are only valid when the difference between the equilibrium and actual vapor pressure at the surface is small and in quasi-steady conditions. However, the vapor generation rate is not infinitely fast as discussed above and the conditions are rapidly changing around the droplet in these simulations. When the vapor partial pressure at the surface is significantly different from the phase equilibrium condition, diffusion-limited assumptions are no longer valid and the burning mode of the droplet is in a transitional regime between diffusion-controlled and kinetic theory-controlled combustion. In such cases it is likely that direct attack of the Al droplet surface via heterogeneous surface reactions becomes significant. This is especially true at higher pressures when the equilibrium vapor mass fraction becomes significantly reduced. Since surface reactions were not modeled, the definition of kinetic theory-limited combustion in this work is different from the traditional chemical kinetic-limited combustion regime reported in literature [4] when chemical reactions become the rate limiting process rather than the rate of vapor generation at the surface. More work needs to be done to determine fundamental surface reaction mechanisms and their parameters for liquid Al with respect to various oxidizing species before they can be included in detailed numerical simulations.

The partial pressure of Al vapor at the top of the droplet at a time of $2 \mu s$, where the boundary layer is much thicker than at the stagnation point, is 73.3 and 69.1 kPa for the inert and reactive simulations, respectively. Both cases are relatively close to the saturation pressure of 81.9 kPa. Thus, vaporization is likely governed by mechanisms closer to a diffusion-limited regime in regions where the boundary layer is thick such as the rear portion of the droplet. This is opposite to the front portion of the droplet which is transitioning to kinetic theory-limited mechanisms due to the thin boundary layer and much higher pressures. In high-speed flows it is likely that vaporization on some portions of the droplet surface are

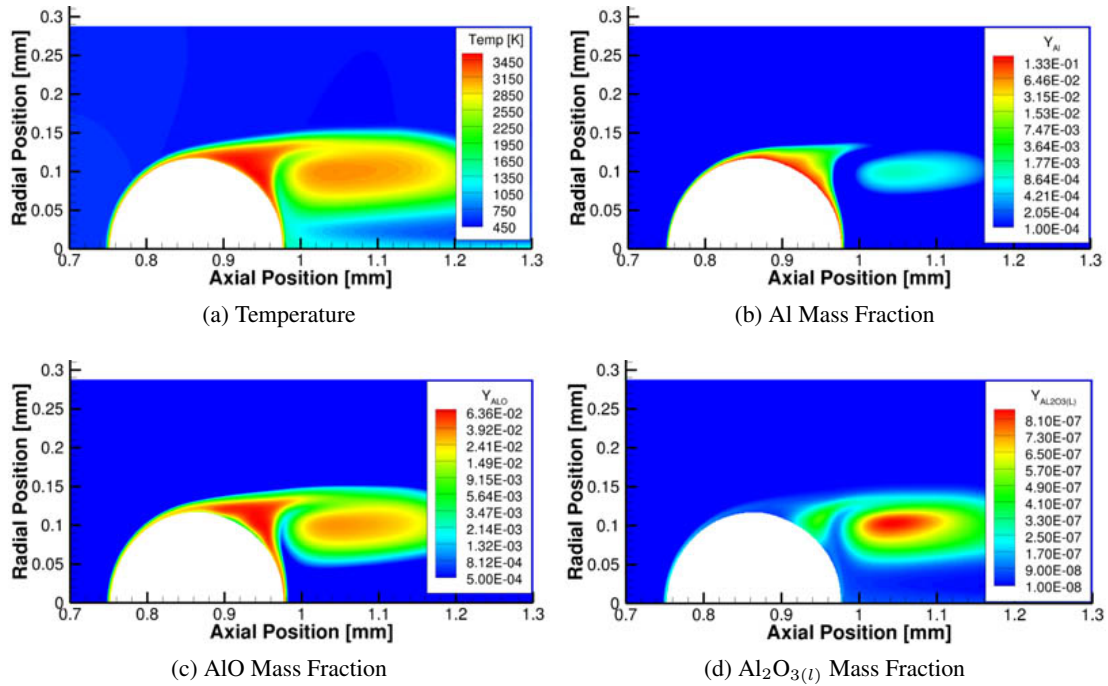


Figure 4: Computed temperature and mass fraction fields for a $M=2$ shock wave interacting with an Al droplet at a time of $2.13 \mu\text{s}$. Reproduced from Houim [7] and Houim and Kuo [8].

governed by diffusion-limited mechanisms while other portions may be transitioning to kinetic-limited mechanisms. The reason that diffusion-limited theory was successful in predicting the vaporization trends for the inert case is due to the relatively small 10% deviation from the phase equilibrium condition at the front stagnation point. This creates a situation where the diffusion-limited assumption is a reasonable approximation over the entire droplet surface. However, if smaller droplets with a diameter on the order of 10 to 50 μm are considered, the diffusion-limited vaporization approximation may breakdown in these high-speed flows even for purely vaporizing droplets. If very small droplets, with a diameter on the order of 1 μm , are considered the diffusion-limited assumption may no longer be valid even for purely vaporizing droplets in quiescent environments due to very small diffusion length scales.

Using diffusion-limited combustion theory on burning droplets that are in a kinetic-limited or even a transitional regime overpredicts the rate of phase change as discussed above. Overprediction of the Al droplet burning rate using diffusion-limited combustion theory and departure of surface vapor mass fraction at the front stagnation point from the phase equilibrium condition provides some evidence that burning of large Al droplets in high speed flows can transition to a kinetic-limited regime. This observation is in agreement with the recent experimental results of Tanguay *et al.* [5].

4 Conclusions

In this work direct numerical simulations of shock waves interacting with vaporizing 230 μm -diameter aluminum droplets in inert and reactive environments were performed. Aluminum particles of this size typically burn in a diffusion-limited manner in quiescent conditions [3]. It was found that the compressed, high-speed flow behind the shock wave decreases the vaporization rate of an Al droplet in an inert environment in comparison to a quiescent condition. The magnitude of this decrease is well predicted using diffusion-limited droplet vaporization theory in conjunction with the Ranz-Marshall corre-

lation. The same cannot be said for shocks interacting with Al droplets in reactive environments, where the net consumption rate of the droplet was increased in the post-shock flow, which is overpredicted using simplified theory. The reason for the lack of agreement between simplified theory and the calculated results is a direct result of significant deviation between the vapor partial pressure from the equilibrium condition at the front of the droplet where the boundary layer is very thin. This indicates that the rate limiting process of a large vaporizing or burning Al droplet may transition from how fast vapor can be carried away from the surface to how fast it can be generated in high-speed flows. The computed results also show that the rear portion of the droplet may be vaporizing by diffusion-controlled mechanisms while the front portion of the same droplet may transition to kinetic-controlled mechanisms. Thus, the transition from diffusion- to kinetic-limited burning regimes may not only be a function of aluminum particle size, but also the flow condition and location on the droplet surface.

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