Reaction Dynamics of Aluminum-Viton-Acetone Droplets

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ABSTRACT

The fluoroelastomer, Viton® A ($C_5H_{3.5}F_{6.5}$), is a binder used in energetic material composites which can be dissolved in acetone and mixed with solid metal fuel particles, such as aluminum (Al). The slurry can be molded into any configuration and the acetone is evaporated off leaving a solid homogeneous reactant mixture. Fundamentally understanding the reaction dynamics of acetone, Viton, and Al is useful for not only consolidating reactants but also for the potential to use nanometric (nm) Al particles in liquid combustion applications. The objective of this study is to examine acetone-Viton droplet burning as a function of Al particle size and concentration. A diagnostic was developed that suspends the multiphase 3 mm droplet on a fiber and enables droplet surface regression rates to be monitored with a high speed video camera. Results show that acetone combined with Viton (5%) and either 2.5% micron Al (10-14 μm) or nm Al (80 nm) burned with two distinct stages. But, acetone combined with Viton and more than 5% nm Al burned with a distinct 3-stage behavior. The three stages are described as evaporation, combustion, and burning of carbon residue. Addition of micron Al to Viton and acetone droplets decrease the droplet regression rate 82% when compared with Viton and acetone droplets with nm Al particles.

Introduction

Nanometric particle fuels such as aluminum (Al) demonstrate unique combustion behaviors over their micron scale counterparts. These combined with a metal oxide or organic or inorganic oxidizer show dramatically increased burn rates and reduced ignition times [1] over micron particle formulations. One motivation for this study is to engineer an approach to consolidating powders such that mechanical imperfections to the alumina shell are not introduced. The approach would require the introduction of a liquid to produce a slurry that could be molded into a shaped charge as opposed to pressed. Liquid can be evaporated leaving a consolidated solid particle matrix. In this way, consolidated mixtures could potentially react according to the melt dispersion mechanism such that heightened reactivity may be better exploited. Motivated by both the exploitation of the melt dispersion mechanism and MEM applications, the purpose of this study was to experimentally examine the fundamental reaction dynamics of a liquid droplet containing a reactive material formulation that includes nanometric Al particles (nm Al). This understanding is effectively a pre-cursor to future efforts devoted to engineering a consolidated reactive material created via a slurry and mold-cast into a shape charge. This fundamental understanding is especially useful in safety protocols where accidental ignition can occur during the consolidation of the reactive material. In this way, understanding the burning behavior of the multiphase and multi-component system better predicts the response for auto-ignition and accident scenarios associated with nEM consolidation.

Viton is a binder that has been used with Al [2] and was found to dissolve in acetone. Viton ($C_5H_{3.5}F_{6.5}$) is a fluoroelastomer in which fluorine acts as an oxidizer. The Viton-acetone liquid mixture can be combined with Al particles to effectively coat Al particles with Viton after the evaporation of acetone. Hence, in the liquid-solid state, this mixture can be molded into any configuration prior to acetone evaporation. Additionally, the study was conducted using an original droplet suspending apparatus that can suspend droplets of approximately 3 mm. The objectives of this study are to (1) create a diagnostic that can test single or multicomponent droplets: (2) examine the D^n-law applied to droplet evaporation and combustion of Viton-acetone solution combined with micron or nm Al particles.

Experimental Setup and Testing Procedure

Multicomponent droplet mixtures were prepared by mixing acetone with 5% mass Viton® A. Viton was cut into 5 mm pieces, measured to the appropriate mass and placed in acetone to dissolve. This mixture is fuel rich with an equivalence ratio of 2.3. The acetone-Viton were mixed with different Al particle sizes and for either 2.5 or 5.0 mass % Al concentration. Droplet evaporation and combustion were recorded with the *Phantom IV (Vision Research*, Wayne, NJ) high speed digital camera which captured images at 100 frames per second. A 1-mm quartz fiber droplet suspending apparatus was developed to suspend an average 3-mm droplet. In this study, only the D_{max} was measured and normalized based on the assumption that gravitational distortion affected all droplets in the same way.

Results

Viton® A (5% by mass) burns with three distinct stages in an acetone droplet. The three stages are evaporation, combustion, and burning of carbon residue. During the first stage, the droplet evaporates until it reaches an ignition threshold. The outer surface regression during evaporation is represented by a gentle slope. These first two stages are also representative of those observed when Al particles are added to the droplet. The second stage begins with bubble formation inside the droplet and transitions to combustion. Combustion appears uniform throughout the droplet and has a faster regression rate compared to the first stage: evaporation. Viton-acetone droplets also demonstrate a third stage which may correspond to combustion of remaining carbon with a distinct flame. The third stage is not observed when Al particles are added. The bubble formation from within the liquid droplet and subsequent combustion can be described as *disruptive burning* and was observed to occur for the Viton-acetone droplets with and without the addition of Al particles. During disruptive burning (Stage 2), the rate of evaporation is negligible compared to the rate of combustion and thus ignored. For the Viton-acetone droplets Viton decomposes at 457 ℃ and acetone boils at 56 ℃ suggesting that initial disruptive burning may be triggered by boiling of acetone. When Al particles are introduced

the reaction dynamics are affected. With the 2.5 mass % additions of micron or nm-Al particles, the reaction dynamics take on only a two stage. There was no burning of the excess carbon residue observed for these droplets. To investigate this phenomenon further the second stage final diameter for each sample was measured. The Viton-acetone droplet contains more carbon residue after the second stage compared to the nm-Al-Viton-acetone droplet. This second stage final droplet diameter may be related to the ignition of the third stage burning such that the third stage may be the result of unburned excess carbon from Viton. The regression rate does not appreciably change with the addition of nm-Al, but substantially reduces when micron-Al particles are introduced. While there is not a significant regression rate deviation with addition of nm-Al to the Viton®-acetone droplets, there is a distinct change in burning behavior. Viton-acetone shows a three stage burn behavior, whereas, nm-Al-Viton-acetone only show a two-stage behavior. As a baseline for comparison, pure acetone droplets were also observed and compared to the multicomponent droplets. The addition of Viton and nm-Al particles increases the regression rate of acetone. A 3rd stage was not observed for the acetone droplets implying that the carbon residue that may be responsible for the 3rd stage combustion observed with the Viton-acetone droplets results from the excess carbon associated with Viton.

Discussion

One of the most interesting observations is the elimination of the 3rd-Stage (burning of carbon residue) by the addition of Al to Viton-acetone droplets. The 2nd stage final droplet diameter for Viton-acetone droplets was observed to be double the 2nd stage droplet diameter for nm-Al-Viton-acetone droplet. This implies that the presence of Al may facilitate localized reaction sites that produce temperatures high enough to consume carbon from decomposing Viton. The fluorine from Viton may be attracted to Al particles and similarly catalyze the decomposition of Viton. The aluminum fluorination reaction (i.e., $Al+3F \rightarrow AlF_3$) has an adiabatic flame temperature of 4352 K (computed using the thermal equilibrium program REAL). The localized hot spots resulting from this reaction could also consume carbon thereby reducing the amount of carbon residue available for 3rd-stage reaction. This effect is observed to be independent of Al particle size. However, the reduction in regression rate for micron-Al particles is seen. The characteristic time for thermal diffusion through an nm-Al particle was calculated to be τ_{diff} is 8×10^{-11} s and for the micron-Al particles τ_{diff} is 1×10^{-6} s. This estimate shows that heat diffuses through the smaller particles roughly 5 orders of magnitude faster than larger particles. Also, the characteristic time for the limiting reaction of acetone + air is estimated based on the kinetic model for acetone oxidation [3]. Based on these characteristic times, for the nanoparticles $\tau_{diff} < \tau_{rxn}$ such that nm-Al particles are likely to more fully react to completion during acetone combustion while the micron-Al particles may act as a heat sink because $\tau_{diff} > \tau_{rxn}$. For the micron-Al particles this implies that the acetone reaction occurs faster than heat can fully diffuse through the larger particles such that only the surface of the micron-Al particles may be participating in the combustion. The thermal lag associated with the micron Al particles may explain the significantly reduced regression rates measured.

As a comparison to the experimental values, a droplet combustion model was examined for the Viton-acetone droplets. The following assumptions were made: spherically symmetric geometry; transport properties independent of droplet radius; thermal inertial of the droplet is negligible; and, the adiabatic flame temperature is used as the flame temperature. The calculations were made for 95% acetone with 5% Viton in air. The calculated transfer number, $B_{o,q}$, is 0.73 and the using rate constant, K, is 1.05 mm^2/s. Coupled with the theoretical burn rate constant, K, the experimental values for D, D_o and t, 'n' was determined to be approximately 1.

Conclusions

The reaction dynamics of multicomponent droplets were investigated. The droplets of acetone with the fluoroelastomer (Viton® A) and either micron or nm-Al (2.5%) demonstrate a two stage combustion behavior. Droplets with only Viton® A and acetone demonstrate a three stage behavior. The three stages are evaporation, combustion, and burning of excess carbon. When the droplets contain Al particles, localized hot spots generated from Al reaction may consume excess carbon thereby eliminating the 3rd stage. It was also determined that the regression rate for droplets with micron-Al decreases 86% when compared to droplets with nm-Al. The larger Al particles may act as a heat sink because their characteristic diffusion times exceed the rate limiting acetone reaction time. Probabilistic analysis was conducted to determine the probability of observing the third stage. The study predicted that Viton® and Acetone has a high probability of demonstrating a third stage and nm-Al, Viton® and acetone show a very low probability of showing a three stage behavior, consistent with experimental observations. Dissolving Viton® A in acetone and adding Al is a technique that can be used to coat Al particles with a fluoroelastomer. Examining the combustion of the acetone-Viton®-Al system has implications toward the safe handling of this energetic material synthesis technique.

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