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Three-dimensional simulations of ignition of composite solid propellants

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ABSTRACT

This paper reports three-dimensional direct numerical simulations of ignition of a composite AP (ammonium perchlorate)–HTPB (hydroxyl-terminated polybutadiene) propellant subjected to a constant flux ϕ. The model includes solid heat transfer, gas-phase combustion with global kinetics and explicit description of propellant microstructure. Simulations show that ignition starts from AP particles because of primary AP/binder flame. Go/no-go computations reveal an unreported intermediate regime between go and no-go with apparent quenching followed by a delayed ignition. This delay is linked to a slow flame spreading from localized scattered hot spots on surface. In accordance with experiments, ignition delays deviate from classical ϕ^{-2} scaling for high flux and low pressure conditions. For intense flux levels, simulations attest deradiation extinction upon flux termination meaning that there is a critical flux above which ignition is no longer possible. The role of AP particle shape and size distribution on ignition delay is studied and predicted to be limited. The effect of propellant surface conditions is also investigated and can lead to substantial effects on ignition delay. Finally, semi-transparent propellants are also considered and low absorption materials result in longer ignition times, reduced ϕ-dependence, and absence of deradiation extinction. This work eventually highlights the importance of microstructure-based details in the physics of composite propellant ignition and opens the way towards better understanding of the role of AP particles.

1. Introduction

Rapid pressurization of a solid rocket chamber during ignition transients leads to a promptly changing flowfield and structural loadings that can result in motor failures [1]. Ignition transient is usually defined as the time lag between ignition signal and steady-state operating conditions. Following d'Agostino et al. [2], it is composed of three distinct phases: first, the induction period for a first local ignition of solid propellant; second, the flame spreading over the propellant grain; third, the chamber filling. In the frame of this study, only the first step is investigated – namely, solid propellant ignition – which includes all the transient phenomena eventually leading to propellant steady-state combustion. This work specifically focuses on AP (ammonium perchlorate)–HTPB (hydroxyl-terminated polybutadiene) composite propellants.

Ignition of composite propellants is a complex process encompassing many physical and chemical features such as unsteady heat conduction, radiative in-depth absorption, surface chemistry and gas-phase combustion. Basically, the external heat supply first increases propellant surface temperature by subsurface conduction. This temperature rise may strongly depend on propellant optical characteristics (in-depth absorption, reflectivity, emissivity). When the temperature in the subsurface region is high enough, significant chemical reactions take place both at the surface and in the gas phase due to oxidizer decomposition and binder pyrolysis. This eventually leads to the flame formation. If external energy is supplied during a sufficient amount of time, the flame heat feedback can sustain propellant decomposition. In that case, combustion is self-sustained and continues even though external flux has been turned off.

Figure 1 presents a typical ignition map adapted from the works by DeLuca et al. [3]. For a fixed radiant flux – the vertical line in the figure – it delineates the different regimes observed during propellant ignition. For short heating times, surface temperature is too low to induce significant reactions. A first event, at time $t = L_{1a}$, is the propellant gasification denoting intense chemical process in the condensed phase. This boundary L_{1a} is pressure-independent and approximately follows a -2 slope in a flux–time log–log plot. A second time L_{1b} indicates a domain of measurable infrared (IR) signal that substantiates the onset of exothermic re-

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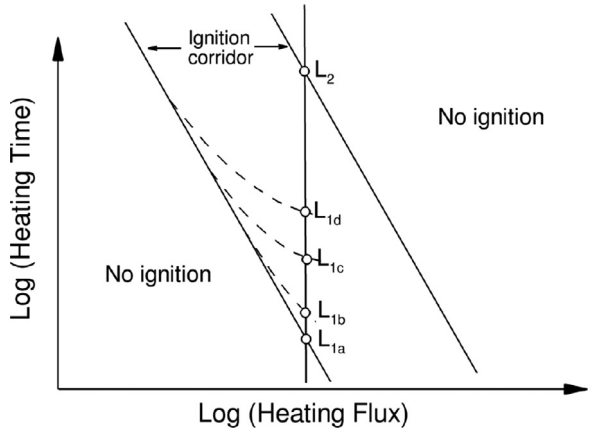

Fig. 1. Ignition map adapted from DeLuca et al. [3]. See the text for the definition of L_1 delays.

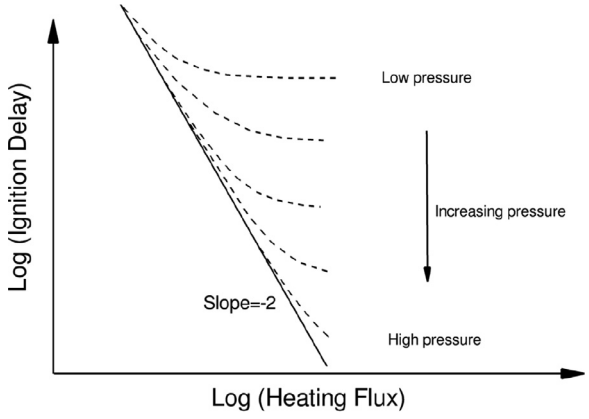

Fig. 2. Typical evolution of experimental ignition delays L_{1d} for AP-based propellants (adapted from [15]).

actions. The boundary L_{1c} is characterized by a substantial flame development and large increase in IR intensity. The limit L_{1d} defines the onset of self-sustained combustion and can be measured unambiguously considering go/no-go tests. In many studies, L_{1d} is the last limit noted and longer heating times result in combustion. However, other experiments [4] suggest that in some conditions, there exists an extinction due to rapid deradiation. This upper limit – referred to as L_2 – depends on pressure. Combustion in that case is overdriven: upon an abrupt termination of the radiative flux, the surface layer burns off without establishing a sufficiently deep preheated layer in the solid and the propellant is quenched. This consequently defines a so-called ignition corridor between $t = L_{1a}$ and $t = L_2$. For certain conditions and propellants, L_{1a} and L_{1d} boundaries collapse, which seems to be the case for AP-based propellants [3]. Likewise, L_2 may not always exist and may depend on the deradiation rate. Various studies [3,5,6] showed that for flux levels below a certain critical threshold ϕ^{cr}_{min}, there were no L_2 limits, i.e. no upper limit on the ignition corridor. On the opposite, they also found a maximum critical flux ϕ^{cr}_{max} above which L_{1d} and L_2 collapse. This means that a flux above this upper limit results in no ignition.

For AP-based propellants, studies report that ignition is mostly controlled by AP decomposition and that the effect of binder or additives is negligible [7–9]. As an exception, ignition at subatmospheric pressures is affected by the binder [10]. The role of propellant formulation or AP size on ignition delays seems moderate [10]. For high pressures, the measured ignition delay t_{ign} (somewhere between L_{1b} and L_{1d} depending on the exact experimental interpretation) for flux level ϕ scales as $t_{ign} \propto \phi^{-2}$, in accordance with inert heating to a constant ignition temperature, and is therefore independent of pressure. This is however no longer the case for low pressures and/or high flux levels where the exponent becomes more positive than -2 and the ignition delay may depend upon pressure as well. Figure 2 presents some go/no-go experiments schematically and a -2 slope is noticed only if pressure is high enough or flux level is low. At a given pressure, ignition delays level off for high flux suggesting a finite pressure-dependent time to reach self-sustained combustion. This high flux limit increases with pressure. Note that this behavior has been confirmed by most experiments [1,3,10–14]. Basically, the -2 slope is only noticed for first gasification (L_{1a}) or first light event (L_{1c}) but go/no-go limit (L_{1d}) is affected by pressure predominantly at high flux levels or low pressures. This means that first light event, on its own, is not always an accurate indication of ignition.

Radiant ignition of solid propellants is known to be strongly affected by material optical properties. Some studies [3,5] show that increasing propellant opacity (by adding carbon black) leads to earlier ignition and alters the L_2 limit. This might however depend on the spectral content of the radiant flux since other experiments on fine AP/HTPB mixtures report minor effects when carbon black content was varied between 0 and 1.4 % [12]. When propellant is not completely opaque, the ignition delay scales as ϕ^{β} with β in the range -1.0 to -1.7, significant less than the expected -2 slope [6,12].

This literature survey mostly reports on radiative ignition because lab-scale studies on ignition are often conducted with lasers. Actual motors, however, are ignited by hot gas flows generated by a pyrotechnic igniter, i.e. convective heat flux. The exact nature of the flux seems negligible and only the flux level and duration are relevant [7–9]. This means that the phenomenological description presented above is expected to be relevant irrespective of the ignition source.

As pointed out by some authors [12,16], the fundamental physics and chemistry are complex so that comprehensive understanding and reliable models are still lacking. An extensive review of available theoretical ignition models is proposed by Hermance and Summerfield [16]. The simplest zero-dimensional models are useful, at least to provide a preliminary flavor of ignition physics. The most basic zero-dimensional model considers inert material heating subjected to constant flux ϕ. Solving the heat equation gives the surface temperature $T_s(t)$ as

$$T_s(t) = T_i + \frac{2\phi}{b\sqrt{\pi}}\sqrt{t} \tag{1}$$

where T_i is the initial temperature and b the material thermal effusivity. Assuming a constant ignition surface temperature T_{ign} (typically in the range 600–800 K), Eq. (1) gives the ignition delay t_{ign} as

$$t_{ign} = \frac{\pi b^2 (T_{ign} - T_i)^2}{4\phi^2} \tag{2}$$

This yields the expected scaling $t_{ign} \propto \phi^{-2}$, at least in the pressure-independent regime since Eq. (2) does not explicitly account for pressure. Experiments suggest that ignition temperature is however not constant and slightly increases with flux level [8,9]. Works by Baer and Ryan [9] proposed a power-law $T_{ign} - T_i \propto \phi^{0.08}$ which seems to be supported by measurements [8]. Other models [8,17] consider the one-dimensional heat equation with an additional exothermic Arrhenius-like source term and correlate correctly experimental data on ignition temperature and ignition delay. A refined model proposed by Bizot [18] similarly solves the one-dimensional unsteady heat equation and investigates different quasi-steady flame models. Results essentially show that the gas-phase flame structure does not significantly affect ignition delay