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Heterogeneous Combustion of AP / HTPB / RDX with Detailed Kinetics

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Abstract
Composite propellants are typically composed of a binder, transformed into combustible gases by pyrolysis, and particulate components which generate oxidizing gases or enhance energy release. Ammonium perchlorate (AP) is a widely used ingredient for solid propellants together with a polymeric binder such as hydroxyl-terminated polybutadiene (HTPB). This kind of solid composite propellant finds applications in civilian and military rocket systems. The combustion process is controlled by the modal distribution of AP particles within the propellant. The composite propellant can hence be tailored to meet specific requirements using a suitable AP particles loading. Owing to its prevalence in the rocket industry, the so-called AP / HTPB composite propellants have been extensively studied in the past. Next generation propellants may include nitramine (RDX or HMX) particles as a partial replacement for AP for some specific purposes. In particular, a decrease in the overall AP mass loading within the propellant reduces the amount of hydrochloric acid (HCl) produced by the combustion, hence resulting in an engine exhaust plume with reduced smoke signature [1].
In this study, we first present a detailed kinetic model for combustion of AP / HTPB / RDX composite propellants. It is shown that the model reproduces the main combustion characteristics (surface temperature, regression rate, temperature sensitivity) of pure PA, pure RDX, and homogenized AP / HTPB binder. Sub-mechanisms of interest for the considered ingredients are further validated with respect to fundamental experiments, such as HCl oxidation, NO_x conversion or C_1 chemistry. These latter validation cases were poorly reproduced by the reference model by Gross et al. [2] for AP / HTPB combustion.
We then present the µSCOP (Microscale Simulation of COmposite Propellants) code, dedicated to the simulation of heterogeneous combustion of solid propellants. It is a 2D Direct Numerical Simulation (DNS) solver based on the low Mach number approximation. Transport phenomena and chemical kinetics are modeled in detail. The flowfield is solved in a segregated approach, and the pressure-velocity coupling is treated by the projection method. Numerical methods are efficiently parallelized using the PETSc library [3]. The heterogeneities related to the ingredients are represented using appropriate models for flame / solid interactions.
Employing the above-mentioned detailed kinetic model with the µSCOP code, a 2D flame above an AP / HTPB / RDX composite propellant is simulated. The considered 2D axisymmetric configuration represents a RDX particle surrounded with a homogenized binder composed of fine AP particles and HTPB. To the knowledge of the authors, this is the first simulation of such a flame in the literature. A study on the effect of pressure and RDX particle diameter is conducted. We show that for each RDX particle size, there exists a pressure limit below which the RDX particle does not ignite. This phenomenon is caused mainly by the high dilution level induced by the presence of the binder gases, slowing down important chain-branching reactions in the RDX kinetic mechanism. This ignition pressure limit increases as RDX particles get finer. Reducing the RDX particle diameter hence decreases the overall regression rate. This behavior is opposed to the one observed with conventional AP / HTPB propellants.

References

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