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Modeling of combustion and ignition of solid-propellant ingredients

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Abstract

Techniques for modeling energetic-material combustion and ignition have evolved tremendously in the last two decades and have been successfully applied to various solid-propellant ingredients. There has been a paradigm shift in the predictive capability of solid-propellant combustion models as the field has advanced from a simple and global-kinetics approach to a detailed approach that employs elementary reaction mechanisms in the gas phase, and accommodates thermal decomposition and subsequent reactions in the condensed phase. The detailed models not only allow calculation of propellant burning-rate characteristics, such as pressure and temperature sensitivities, but also of the surface conditions and entire combustion-wave structure, including the spatial variations in temperature and species concentrations.

This paper provides a comprehensive review of recent advances in the modeling and simulation of various solid-propellant ingredients over a wide range of ambient conditions. The specific materials of concern include nitramines (RDX, HMX), azides (GAP), nitrate esters (NG, BTTN, TMETN), ADN, and AP monopropellants, as well as homogeneous mixtures representing binary (RDX/GAP, HMX/GAP, and AP/HTPB) and ternary (RDX/GAP/BTTN) pseudo-propellants. Emphasis is placed on the steady-state combustion and laser-induced ignition of nitramines. The capabilities and deficiencies of existing approaches are addressed. In general, the detailed gas-phase reaction mechanisms developed so far represent the chemistry of monopropellants and associated mixtures consistently well, and help understand the intricate processes of solid-propellant combustion. The reaction mechanisms in the condensed phase, however, still pose an important challenge. Furthermore, the current knowledge of the initial decomposition of molecules emerging from the propellant surface is insufficient to render the models fully predictive. Modeling is thus not yet a predictive tool, but it is a useful guide. In the near future, it is likely that detailed combustion models can assist in the formulation of advanced solid propellants meeting various performance and emission requirements.

Keywords: Combustion and ignition of solid propellants; Energetic materials; Combustion modeling

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1. Introduction

A solid propellant consists of several chemical ingredients such as oxidizer, fuel, binder, plasticizer, curing agent, stabilizer, and cross-linking agent. The specific chemical composition depends on the desired combustion characteristics for a particular application. Two main types of propellants (homogeneous and heterogeneous) are distinguished by the condition in which their constituent ingredients are interconnected. In a homogeneous propellant, the ingredients are linked chemically and the resulting physical structure is homogeneous throughout. Typical examples of homogeneous propellants are single-base (NC nitrocellulose) or double-base (NC and NG nitroglycerine) propellants. In a heterogeneous or composite propellant, the ingredients are physically mixed, leading to a heterogeneous physical structure. It is composed of crystalline particles acting as oxidizer and organic plastic fuels acting as binder to adhere oxidizer particles together [1]. The ingredients often used as oxidizers are ammonium perchlorate (AP), ammonium nitrate (AN), ammonium dintramide (ADN), cyclotrimethylenetrinitramine (RDX), and cyclotetramethylenetetranitramine (HMX). The most commonly employed binders are either inert (typically HTPB, hydroxyl-terminated polybutadiene, with various plasticizers, ballistic modifiers, and cross-linking agents), or active (NG and NC, polyether polymer, and azide polymer such as GAP glycidyl azide polymer, BAMO bis-azidomethyl oxetane, and AMMO 3-azidomethyl-3-methyl oxetane) [1,2].

The quest for more energetic propellants with reduced pollutant emissions has resulted in the use of several non-AP ingredients in solid propellants. The ingredients belong to a wide spectrum of chemical families, but mostly fall into one of four categories: