Applied Thermal Engineering 130 (2018) 492–500

Contents lists available at ScienceDirect

Applied Thermal Engineering

journal homepage: www.elsevier.com/locate/apthermeng

Research Paper

A reduced order model for prediction of the burning rates of multicomponent pyrotechnic propellants

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HIGHLIGHTS

- Reduced order analytical model for burning rate of pyrotechnic compositions.
- Linear burning rate of multi-component granular porous pyrotechnics predicted.
- Conductive combustion regime with primary reactions occurring on the surface.
- Technique accounts for the propellant conductivity, heat of reaction, and porosity.
- Case study predictions for $KClO_4$ and KNO_3 based pyrotechnics reasonably accurate.

ARTICLE INFO

Article history:
Received 19 July 2017
Revised 29 September 2017
Accepted 1 November 2017

ABSTRACT

This study reports a reduced order model for the prediction of the burning rate of pyrotechnic compositions. The combustion process of most pyrotechnics is primarily driven by condensed phase reactions. A priory estimation of the burning rate of pyrotechnics with multiple components may not be possible using the established methods. The study provides a simplified approach based on integral analysis of a proposed combustion wave structure for estimating the burning rate when the pyrotechnic composition, pure component thermo-physical properties, and thermo-kinetics parameter are known. The proposed combustion wave assumes a staged combustion process where the oxidizer undergoes decomposition in a broad reactive zone while fuel combustion occurs in a thin surface region. This approach takes account of the effective thermal conductivity as well as porosity of the pyrotechnic matrix. The pyrotechnic compositions studied here are expected to burn conductively at atmospheric pressure with little or no overpressure. The phenomenology of the combustion process of energetic materials is elucidated, and the reduced order model is validated through a case study.

1. Introduction

Pyrotechnics are a particular class of fuel-rich energetic compositions that are distinct yet closely related with other energetic materials such as explosives and propellants. While, the word “pyrotechnic” is a literal Greek translation of the word “fireworks”, military pyrotechnics are considered separate from fireworks, which symbolize recreational purposes. Through the process of combustion, pyrotechnics may act as a source of gas, heat, light, smoke, sound, or any combination of thereof along with significant amount of solid phase combustion products. Typical pyrotechnics compositions consist of fine powders of oxidizer, fuel, as well as various additives, which are thoroughly mixed and compressed to form a porous solid charge. The additives may act as binders, stabilizers, catalysts, coloring agents, smoke dyes, and so on depending on the intended application. These granular heterogeneous porous composite energetic materials find utility in a range of applications such as chemical oxygen generators, pyrotechnic fasteners, automotive airbag inflators, thermites, material synthesis through solid-solid reactions, and fireworks.

The burning rate or the rate at which the combustion front progresses through the pyrotechnic material is an important characteristic that determines their performance and safety characteristics. Generally, the combustion of solid energetic materials is classified in four regimes [1] based on the burning rate viz. conductive burning, convective burning, compressive burning, and detonation. A large number of pyrotechnic applications such as illuminating flares, display pyrotechnics, gas generators, and delay fuses operate in a conductive burning regime. The factors that determine the burning rate of pyrotechnics have been discussed in detail in the literature [2]. However, a change in any of these factors controls one or more of the three fundamental aspects viz. the

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https://doi.org/10.1016/j.applthermaleng.2017.11.008
1359-4311/

Nomenclature

Latin alphabet

A	frequency factor (1/s)
C_p	specific heat (J/kg K)
Ea	activation energy (kJ/mol)
$g(n)$	a weak function of the reaction order that varies between 1 and 2
h_f^0	enthalpy of formation (kJ/mol)
Δh_R	heat of reaction (J/kg)
k	thermal conductivity (W/m K)
L_m	latent heat of melting (J/kg)
$\dot{m}''$	mass flux (kg/m^2 s)
$\dot{m}'''$	mass consumption rate (kg/m^3 s)
$\overline{\dot{m}'''}$	average mass consumption rate (kg/m^3 s)
Ru	universal gas constant (kJ/mol)
$\dot{r}$	burning rate (m/s)
T	temperature (K)
$\overline{T}$	average temperature (K)
Y	mass fraction

Greek letters

α	thermal diffusivity (m^2/s)
δ	reactive zone thickness (m)
ϕ	volume fraction
γ	fuel to oxidizer mass ratio
η	catalyst factor
ρ	density (kg/m^3)

Subscripts

0	ambient conditions
actual	measured value
c	combustion zone
eff	effective value
F	fuel
f	Flame
i	ith species
$KClO_4$	potassium perchlorate
max	maximum theoretical value
Ox	oxidizer
s	propellant surface

chemical activation energy, heat of reaction, and the fraction of the generated heat that reaches the unreacted propellant. Any technique for prediction of the burning rate must account for these three parameters with respect to the particular composition and configuration under consideration.

Certain pyrotechnic materials are designed to undergo unconfined combustion at atmospheric pressure with little or no pressure difference (overpressure) between the gaseous combustion products and the gases inside the pores of the unburned pyrotechnic matrix. Various theoretical and experimental studies regarding the burning rate of gasless pyrotechnics [3–5], confined deflagration of porous nitramine propellants [6,7], and combustion of metal-halocarbon pyrolants [8,9] have been conducted in the past. However, other than certain reviews [10–12] and experimental measurements [13,14] very few studies addressing the estimation of the unconfined burning rates of a granular multicomponent pyrotechnic material can be found in the literature.

The methods for the approximate solution of the governing equations of the theory of combustion of homogeneous gasless systems, which were intensively investigated during at least the last 50 years, are well-known and have been described in various journal articles as well as books [15,16].

Classically, the burning rate of solid materials have been expressed as a function of the material properties through theories proposed by Zeldovich [17] as well as Khaikin and Merzhanov [18]. The Zeldovich expression given in Eq. (1) while relationship proposed by Khaikin and Merzhanov is shown in Eq. (2).

$$\dot{m}'' = \sqrt{\frac{2\rho k \Delta h_R}{C_p^2 (T_s - T_0 + L_m/C_p)^2} \left(\frac{RuT_s^2}{Ea}\right) A e^{-Ea/RuT_s}} \tag{1}$$

$$\dot{r} = \sqrt{\frac{kARuT_c^2}{\rho Ea \Delta h_R g(n)} e^{-Ea/RuT_c}} \tag{2}$$

Waesche and Wenograd [19] report on calculation of solid propellant burning rates from condensed-phase decomposition kinetics. They conducted pressurized DSC and TGA experiments in order to evaluate chemical kinetic parameters, which were in turn utilized to determine the prevalent surface temperature at the operating pressure. They suggest a correlation for the mass burning rate in flameless regime based on the Zeldovich method.

Sinditskii et al. [20] have demonstrated the utility of the Zeldovich expression for predicting the mass burning rate of compositions based on ammonium nitrate. Similarly, Eq. (2) was utilized by Swanepoel et al. [5] who studied the use of manganese as a fuel for slow-burning gasless delay compositions. In each of these methods, the knowledge of the chemical kinetic parameters particular to the given composition is necessary. These parameters may be measured directly through a calorimetric study or inferred from measured burning rates. As the proportions of the constituents would affect the chemical kinetics of a given multicomponent pyrotechnic composition, accurate estimation of the burning rate would require repeated measurement of chemical kinetic parameters or burning rates for each new formulation. This may prove to be cumbersome and resource intensive.

However, the thermo-kinetic parameters for pure components have been well characterized and a method utilizing these characteristics for predicting the burning rate or the effective apparent kinetic parameters would prove to be useful. In addition to such an analytical method, the burning rate of pyrotechnics can also be investigated through numerical simulations. However, analytical approach has the advantage of providing a relatively quick estimation. Furthermore, the analytical technique enables an improved understanding of the phenomenon and the dominant processes involved in each case.

The current study proposes a reduced order model for the prediction of the burning rate of the porous heterogeneous pyrotechnics undergoing unconfined combustion. This simplified technique relies on finding a homogeneous analogue for the composite pyrotechnic. Subsequently, an expression obtained through analysis akin to the one classically applied for laminar flame speed in gaseous media was utilized to obtain the burning rates. The proposed method utilizes pure component thermo-physical and chemical kinetic properties along with the composition to estimate the burning rate. This is proposed as a distinct advantage compared to previously reported techniques where application of the