Updated Three-Flame Modeling of Composite AP/HTPB Propellants

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1 Introduction

The Beckstead-Derr-Price (BDP) model for the steady-state burning of ammonium perchlorate composite propellants (APCP) [1-2] is based on multiple flames above the propellant surface and has been widely utilized for purposes of modeling the complicated, heterogeneous combustion of APCPs. However, APCP burning rate data that have been previously utilized to validate various versions of the BDP model have not spanned adequate propellant formulations (AP particle size and concentration) and combustion pressure. The authors have recently developed an experimental database of unimodal APCP burning rates that includes AP particle sizes of 20-500 μ m, AP mass concentrations of 70-87.5%, and combustion pressures up to 15.5 MPa (2250 psia). [3] In the current study, a BDP model framework is outlined and updated to built-in, variable flame temperatures and combustion product transport properties determined from combustion equilibrium analyses (CEA). Model parameters are initially taken from previous literature and are tuned to the burning rate data that have been recently published.

2 Model Formulation

The general flame structure of the BDP model is shown in Fig. 1, where the three flames encompass (1) a monopropellant combustion flame, (2) a primary diffusion flame, and (3) a final diffusion flame. Cohen [4] reviewed the various available APCP modeling approaches at that time and cited numerous deficiencies with all of them. Cohen and Strand [5] later made several updates to the BDP model to correct these deficiencies. The BDP model has also been extended to propellant formulations containing multimodal oxidizer distributions, alternative oxidizers, aluminum particles, and energetic binders. [5-6] In general, the updated Cohen and Strand model [5] has been utilized for APCP burning rate predictions herein, but several modifications have been made. The steady-state burning model is described in this section of the report. Original modeling notation has been retained herein for fidelity.



Figure 1. Schematic of a single AP particle in an APCP and the three flames: primary diffusion flame, oxidizer monopropellant flame, and final diffusion flame.

Mass continuity at the composite propellant surface can be written as:

$$m_T = \rho_T r_T = m_{ox} (S_{ox}/S_o) + m_f (S_f/S_o) \tag{1}$$

2.1 Oxidizer Monopropellant Flame

The oxidizer monopropellant model presented in the original BDP model did not contain pressuredependent heat release, so that it under predicted the overall burning rate at higher pressures where heat feedback from the AP flame becomes dominant. The Price-Boggs-Derr monopropellant model [7] was adopted by Cohen and Strand [5] to partially correct this deficiency. The mass flux at the oxidizer surface is given by an Arrhenius law:

$$m_{ox} = \rho_{ox} r_{ox} = A_{ox} exp(-E_{ox}/R_u T_{s,ox})$$
⁽²⁾

The fraction of oxidizer that reacts in the gas phase is given by:

$$\beta_P = 1 - A_s exp(-E_s/R_u T_{s,ox})/m_{ox}$$
(3)

The remaining fraction of oxidizer $(1 - \beta_P)$ reacts in the condensed phase. The total heat content of the adiabatic oxidizer monopropellant flame and the net heat release at the oxidizer surface are given, respectively, by:

$$Q_F = c_g (T_{AP} - T_{ref}) - c_s (T_0 - T_{ref}) + \Delta H_g$$
(4)

$$Q_L = \beta_P \left(\Delta H_{ev} - \Delta H_g \right) - (1 - \beta_P) Q_F \tag{5}$$

The net heat release in the oxidizer monopropellant flame, Q_{ox} , is the sum of these two components. The oxidizer flame standoff distance was approximated as a premixed laminar flame in the original BDP model, but was later implemented as a formal distributed reaction flame:

$$X_{ox}^{*} = m_{ox} \left[a + A_{AP} exp(-E_{AP}/R_{u}T_{AP})P^{\delta_{AP}} \right]^{-1}$$
(6)

This flame standoff can be non-dimensionalized by:

$$\xi_{ox} = \left(c_g / \lambda_g\right) m_{ox} X_{ox}^* \tag{7}$$

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An energy balance at the surface yields the oxidizer surface temperature:

$$T_{s,ox} = T_0 + (1/c_s)[Q_{ox}exp(-\xi_{ox}) - (Q_L + \Delta H_s)]$$
(8)

which is initially guessed and then iterated until convergence. The overall oxidizer regression rate is subsequently calculated according to Eq. (2).

2.3 Propellant Surface Geometry

To evaluate the surface area ratios which appear in the mass continuity equation, a geometrical relationship between the oxidizer and fuel is established. Beckstead et al. [1] have assumed that a protruding or recessed oxidizer crystal is spherical and always joins the planar fuel surface. The fractional distance that the oxidizer crystal protrudes above or is recessed below the surface can be written as:

$$\left(\frac{h}{D}\right)_{P,N} = \left(\frac{1}{2}\right) \left(1 \pm \frac{1}{\sqrt{3}}\right) \left(1 - \frac{r_{ox}}{r_f}\right) + r_{ox} \frac{t_{ign}}{D_{ox}} \tag{9}$$

The ignition delay time of the oxidizer crystal was correlated to experimental AP data by Shannon and Petersen [8] and was originally written as a function of the of the oxidizer particle size [1], but was later rewritten as a function of the oxidizer regression rate [6] so that it could be applied to oxidizers other than AP. The oxidizer ignition delay time is thus given by:

$$t_{ign} = K D_{ox}^n / r_{ox} \tag{10}$$

The surface area relations for the total, oxidizer, and fuel surface area are written, respectively, as:

$$S_o = 1 + 3\zeta_{ox}[(h/D)_P^2 + (h/D)_N^2]$$
(11)

$$S_{ox} = \zeta_{ox} + 3\zeta_{ox}[(h/D)_P^2 + (h/D)_N^2]$$
(12)

$$S_f = S_o - S_{ox} \tag{13}$$

The characteristic dimension, b, is the distance from the center of an oxidizer crystal to the center of the binder. The definition for the characteristic surface dimension herein was derived by Glick [4], is considered generally applicable outside of the oxidizer-rich regime [4-5], and is given by:

$$b = \left(\frac{D_{ox}}{\sqrt{6}}\right) \left[1 + \left(\frac{\rho_{ox}}{p_f}\right) \left(\frac{1 - \alpha_{ox}}{\alpha_{ox}}\right) \right]$$
(14)

2.4 Flame Heights

The diffusion flame height in the original BDP model was modeled as the 'short flame' approximation of the Burke-Schumann diffusion analysis [9], as presented by Williams [10]. However, various approaches have since been utilized to model the flame phenomena, as discussed by Cohen [4]. The approximation utilized herein is given by:

$$X_D = A_{fh} b\left(\frac{1-\alpha_{ox}}{\alpha_{ox}}\right) \phi_1 \tag{15}$$

and was implemented in later versions of the BDP model by Beckstead as a simpler 'short flame' approximation which retained similar accuracy as the more computationally intensive approach that was originally employed. The diffusional flame height over the oxidizer and binder are given by constant multipliers:

$$X_{D,ox}^* = A_{fh} X_D \tag{16}$$

$$X_{D,f}^* = \beta_{fh} X_D \tag{17}$$

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where the implemented value of β_{fh} has generally been $A_{fh}/8$. Beckstead [6] later developed correlations that relate the diffusional flame height over the oxidizer and binder to the stoichiometric O/F ratio and the actual O/F ratio, so that intensive computations of X_D were not necessary within the combustion model. Similar to the oxidizer flame height, the primary flame height is given by:

$$X_{PF}^{*} = m_{T} \left[A_{PF} exp(-E_{PF}/R_{u}T_{PF})P^{\delta_{PF}} \right]^{-1}$$
(18)

It is worth noting that the temperature of the primary flame (T_F) and the primary diffusion flame (T_{PF}) are taken as equivalent and equal to the adiabatic flame temperature of the propellant formulation. The primary diffusion flame height is given by the summation of the primary flame height and the diffusion flame height over the fuel:

$$X_{PDF}^* = X_{PF}^* + X_{D,f}^* \tag{19}$$

The primary flame heights over the oxidizer and fuel are non-dimensionalized as before:

$$\xi_{PF,ox} = \left(\frac{c_g}{\lambda_g}\right) m_T \left(X_{ox}^* + X_{D,ox}^*\right) \tag{20}$$

$$\xi_{PF,f} = \left(\frac{c_g}{\lambda_g}\right) m_T \left(X_{PF}^* + X_{D,f}^*\right) \tag{21}$$

2.5 Separate Surface Energy Balances

The original model included a simplifying assumption that the surface temperature of the oxidizer and fuel were equal [1]. This assumption has been generally discredited through experimental observations [4] and is resolved by implementation of a separate mass flux relation for the fuel. Additionally, implementation of separate surface temperatures for the oxidizer and fuel also aids in improving the high-pressure prediction capabilities of the model [4]. The mass flux at the fuel surface is defined independent of the oxidizer mass flux herein, but in a manner similar to that at the oxidizer surface, by an Arrhenius law:

$$m_f = \rho_f r_f = A_f exp(-E_f/R_u T_{s,f})$$
(22)

The heat release in the primary diffusion flame is given by:

$$Q_{PF} = c_g (T_F - T_0) + \alpha_{ox} Q_L + (1 - \alpha_{ox}) Q_f$$
(23)

The partition of energy associated with the final flame to the monopropellant and primary flames through a projection of the flame areas on a planar surface [4] is given by:

$$\beta_F = \left(\frac{X_{ox}^* + X_{PF}^*}{X_{PDF}^*}\right) A_{fh} \tag{24}$$

The energy balances at the fuel and oxidizer surface, respectively, can thus be written as:

$$m_f S_f [c_s (T_{s,f} - T_0) + Q_f] = (1 - \beta_{ox}) (m_{ox} S_{ox} + m_f S_f) Q_{PF} exp(-\xi_{PF,f})$$
(25)
$$m_{ox} S_{ox} [c_s (T_{s,ox} - T_0) + \Delta H_s + Q_L] =$$

$$\beta_{ox}\beta_F (m_{ox}S_{ox} + m_f S_f)Q_{ox}exp(-\xi_{PF}) + \beta_{ox}(1-\beta_F)m_{ox}S_{ox}Q_{ox}exp(-\xi_{ox})$$
(26)

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2.6 Computational Approach

The computational approach adapted herein utilizes three separate iteration loops, as shown in Fig. 2. The combustion conditions $(S_{ox}/S_f, T_{s,f}, T_{s,ox})$ are initially estimated and iteratively solved for in that respective order according to a convergence criteria.



Figure 2. Generalized computational approach for the updated BDP burning rate model.

3 Discussion

The updated BDP model described within has been built and utilized to predict the burning rates of APCPs with varying AP concentration and size. Model and propellant parameter inputs, such as kinetics prefactors, activation energies, flame reaction orders, etc., have been taken from the literature and utilized as a first approximation. Some modeling parameters, such as the Arrhenius parameters for AP, have been updated according to more recent data available within the literature. AP monopropellant flame temperatures and combustion product transport properties (specific heat and thermal conductivity) have been refined according to CEA computations, and functional versions of these parameters are included within the model. Finally, model parameters which were uncertain were tuned to the available burning rate data to yield a higher degree of accuracy. The improved model is capable of accurately predicting the burning rates of APCPs over a wide range of propellant formulations (AP concentration and particle size) and operating conditions.

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