

Simplified Burn-Rate Model for CMDB Propellants

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ABSTRACT

A single model has been proposed to predict the burning rates of bimodal AP, RDX and aluminium containing CMDB propellants. This is done in terms of the respective physical constants on the basis of a recently developed model of combustion of CMDB propellants. The study has been carried out to examine the effects of changes in propellants composition, AP particle size and pressures on burning rate. Computer programs were developed for this purpose and the results obtained for typical sets of input data have been presented and compared with the actual results.

NOMENCLATURE

C	specific heat, cal/g °K
d	diameter of oxidiser
E	activation energy, cal/mole
P	pressure, kg/cm ²
Q	energy of reaction per unit mass, cal/g
R	gas constant
	burning rate, cm/s
T	temperature, °K
T_0	initial propellant temperature, °K
Z	pre-exponential factor
ϵ	mass fraction
λ	thermal conductivity, cal/cm s °K
ρ	density, g/cm ³
ϕ	weight fraction

Subscripts

<i>g</i>	gas phase
<i>p</i>	condensed phase
<i>s</i>	burning surface
<i>m</i>	matrix
<i>N</i>	RDX
<i>AP1 & AP2</i>	ammonium perchlorate with varying particle size
<i>Al</i>	aluminium
<i>DB</i>	double-base

1. INTRODUCTION

Composite modified double base (CMDB) propellants are relatively new class of propellants and are increasingly being used in various applications because of its flexibility of burn-rate, high performance, superior mechanical properties and non-smoky exhaust. The improved performance is achieved by incorporating various high energy materials in double-base (DB) matrix. Inclusion of these materials affect the combustion characteristics of DB matrix and a few modelling attempts have been made in the past to predict burn-rate of CMDB propellants. Kubota *et al.*¹ in their study of flame structure of CMDB propellants propose a model based essentially on the assumption that the propellant burns with two different rates, one as DB matrix and other as AP for AP-based CMDB propellants. They have described an elegant method for the calculation of volume fraction of ammonium perchlorate (AP) portion and overall burn-rate is calculated as fractionally weighed sum of the two rates. However, with HMX no change is observed in DB matrix combustion pattern and equation for DB burn-rate is utilised modifying heat release terms to account for HMX heat release. Beckstead² proposed a model for DB propellant with an intention of applying it to CMDB and cross-linked DB (XLDB) propellant systems. This is basically an adaptation of BDP model³ applicable to composite propellant (CP). Surface heat release terms are related to binder heat of explosion by an empirical equation in this BDP model applicable to DB propellant and burn-rate is determined by iterative solution of equations related to surface kinetics, energy balance at the surface and gas phase kinetics.

These models attempt to predict burn-rate for compositions containing either monomodal AP or nitramines. However, CMDB formulations as reported in literature⁴⁻⁶ contain various combinations of differing partial size AP with nitramine and aluminium. The burn-rate prediction of such combinations of ingredients in DB matrix is not available. In the present paper a simplified approach for burn-rate prediction has been proposed based essentially on Kubota's model for CMDB propellants containing AP, RDX and *Al*. Predicted results by present approach and Kubota model have been examined and compared with the experimental burn-rate results.

2. APPROACH TO THE PROBLEM

2.1 Propellant Density

The densities of the ingredients have been considered to calculate the density of the propellant using the following equations.

$$\rho_m = \frac{\rho_{Al}\rho_N\rho_{DB}(1 - \phi_{AP1} - \phi_{AP2})}{\rho_N\rho_{DB}\phi_{Al} + \rho_{Al}\rho_{DB}\phi_N + \rho_{Al}\rho_N(1 - \phi_{AP1} - \phi_{AP2} - \phi_{Al} - \phi_N)} \quad (1)$$

$$\rho_p = \frac{\rho_{AP}\rho_m}{\rho_m(\phi_{AP1} + \phi_{AP2}) + \rho_{AP}(1 - \phi_{AP1} - \phi_{AP2})} \quad (2)$$

The following conditions are imposed for Eqns. (1) and (2)

$$\begin{array}{llll} \text{If } & \phi_{AP1} + \phi_{AP2} = 0 & \text{then } & \rho_{AP} = \\ & \phi_N = 0 & \text{then } & \rho_N = \\ \text{If } & \phi_{Al} = 0 & \text{then } & \rho_{Al} = \end{array}$$

2.2 Effect of Aluminium

Aluminium is reported to melt inside a sack of aluminium oxide during initial stages of burning. Renie and Oshron⁸ in their model assume that aluminium acts as a heat sink at the propellant surface to the extent that it melts and absorbs its heat of fusion as well as a heat source in the gas to the extent that it ignites and burns sufficiently close to the propellant to affect the heat feed-back. Cohen and Flanigan⁹ observe that heat sink effect may be predominant with finer AP and heat source affect with coarser AP. Aluminium on complete combustion gives out a large amount of heat (7400 cal/g) and in the present approach a small positive surface heat liberation is assumed which appears realistic considering the energetic nature of the binder which decompose at an early stage. Aluminium heat release at surface and at gas phase is included in the Kubota model to account for the effect of aluminium on DB burn-rate. Secondly as thermal conductivity of aluminised propellants is comparatively higher than that of DB propellants, thermal conductivity values in the Kubota model are modified and allowed to vary with the concentration of aluminium in the composition using the following equation :

$$\lambda_g = 0.001 \phi_{Al} + 0.0002$$

2.3 AP Heat Release Terms

In Kubota model, AP particle regression rate is calculated by an empirical equation responding to pressure and particle size of AP. This is based on their experimental findings with AP crystals embedded in DB matrix. This AP burn-rate is combined with DB regression rate to get overall burn-rate of CMDB propellant. In BDP model applicable to CP, the diffusion flame heights are related to AP crystal diameter and surface temperature increases with AP concentration and diffusional distance decreases with decrease in AP particle size. In their¹ analysis of the model, they calculated that

half of the AP heat release (405 cal/g) was liberated in the liquid surface layer. Jovic *et al.*¹⁰ use an approximate expression for surface heat release in their study of erosive burning. AP heat release assumed by them is about 250 cal/g. In the present approach AP heat release terms as reported by Beckstead *et al.*³ are included in the DB burn-rate expression of Kubota¹. This is a simplification from the Kubota model and may not correspond to the actual flame situation as depicted by Kubota. Pressure dependency term is also incorporated in AP heat release equations as done by King¹¹ for DB matrix and the assumed values correspond to that of Kubota *et al.*¹².

The equations are

$$Q_{s,AP} = 33.3 \left(\frac{P}{P_0} \right)^{0.7} \log P_p(d+1)^3$$

$$Q_{s,AP} = 404 \left(\frac{P}{P_0} \right)^{0.1} Q_g \quad (4)$$

where P_0 equals 35 kg/cm² pressure. The Q_s value reaches a maximum of 404 cal/g and Q_g tends to zero with very fine AP particles (d tending to zero) and with very coarse particles ($d \approx 1$ cm) Q_s value tends to zero and Q_g to a limiting value of 404 cal/g at 35 kg/cm² pressure.

2.4. Burn-Rate Model

The heat release terms of all the ingredients are summed up to get the propellant heat release values as follows :

$$Q_s = \phi_{AP1} Q_{s,AP1} + \phi_{AP2} Q_{s,AP2} + \phi_{DB} Q_{s,DB} + \phi_{Al} Q_{s,Al} + \phi_N Q_{s,N} \quad (5)$$

$$Q_g = \phi_{AP1} Q_{g,AP1} + \phi_{AP2} Q_{g,AP2} + \phi_{DB} Q_{g,DB} + \phi_{Al} Q_{g,Al} + \phi_N Q_{g,N} \quad (6)$$

However, in the present approach $Q_{s,DB}$ and $Q_{s,N}$ values are slightly different from that assumed by Kubota. The following burn-rate equations proposed by Kubota¹ are used as such without any modifications. Fizz zone temperature computed for $C_p = C_g$ as

$$T_g = T_0 + \frac{Q_s}{C_p} + \frac{Q_g}{C_p} \quad (7)$$

Surface regression rate of propellant as

$$\gamma = P \left[\frac{\lambda_g Q_s \epsilon^2 Z_g \exp(-E_g/RT_g)^2}{\rho_p^2 C_p C_g (T_g - T_0 - (Q_s/C_p))(RT_g)^2} \right] \quad (8)$$

Regression rate of surface to be one-step Arrhenius-type equation as

$$\gamma = Z_s \exp(-E_s/RT_g) \quad (9)$$

Simultaneous solution of Eqns. (1) to (9) gives the burning rates at different pressures. Computer programmes were made and change in particle size of AP and

variations in formulation of CMDB propellant are studied for burn-rate and surface temperature prediction. The values used in the calculations are given in Table 1.

Table 1 Physical constants and parameters

Parameter	Magnitude
C	0.37 cal/g ^o K
	0.37 cal/g ^o K
	1.54 g/cm ³
	14 × 10 ³ cal/mole
Z	3.6 × 10 ⁴ cal/s
E	17 × 10 ³ cal/mole
	1.4 × 10 ⁸ cm ³ /g/s
Q _{s,Al}	-50 cal/g
Q _{s,N}	50 cal/g
Q _{s,DB}	100 cal/g

3. RESULTS AND DISCUSSIONS

Predicted burn-rate results alongwith realised burn-rate at 70 kg/cm² pressure for various CMDB formulations are given in Table 2. Predicted burn-rate of DB varied from 5 mm/s at 35 kg/cm² pressure to 10.9 mm/s at 140 kg/cm² pressure. The realised and predicted burn-rate at 70 kg/cm² are 7.5 and 7.1 mm/s. As expected predicted burn-rate increases from 10 to 11.9 mm/s at 70 kg/cm² pressure with increase in solid loading. Realised burn-rate for the same composition, at the same pressure varied from 9.5 to 13 mm/s. With the incorporation of aluminium in DB matrix predicted burn-rate remained more or less same at low pressure. However, a slight increase in burn-rate was observed at higher pressure. Realised burn-rate more or less matches with the predicted results at 70 kg/cm² pressure. Other results listed in Table 2 from AP- and RDX-based CMDB formulations also show expected trends.

Comparative data on the surface temperature and burn-rate, predicted by the Kubota model and present approach are listed in Table 3. Similar trends in burn-rate are exhibited by both the approaches with respect to particle size of AP and RDX incorporation. However, results from the present approach are consistently higher than that of Kubota for similar compositions. This may be because of the higher assumed values of Q_{s,DB} and Q_{s,N} compared to Kubota's model which resulted in prediction of higher surface temperature and thus higher burning rate. Surface temperature increase with respect to pressure is also observed in both the models. However, dependence of surface temperature on AP concentration and AP particle size is not clear in Kubota model as calculations are carried out for DB matrix temperature. In the present approach surface temperature increases with increase in AP concentration and decrease in AP particle size. This observation is consistent with the reported steep fizz zone temperature gradient for fine AP by Kubota¹ and also

Table 2. Predicted burn-rate results for CMDB formulations

Propellant composition (by parts)						Particle size (μ)		Burning rate (mm/s) at pressure kg/cm ²				
DNC	CL	AP1	AP2	AI	RDX	AP1	AP2	35	50	70*	90	120
60	40	-	-	-				5.0	5.9	7.1 (7.5)	8.2	
40	35	10.5	4.5	10		150	15	7.0	8.3	10.0 (9.5)	11.7	
35	35	12.6	5.4	12		150	15	7.3	8.8	10.6 (10.9)	12.4	
30	35	14.7	6.3	14		150	15	7.8	9.2	11.3 (11.7)	13.2	
25	35	16.8	7.2	16		150	15	8.1	9.8	11.9 (13.0)	14.0	
55	40	-	-	5				5.1	6.1	7.5 (7.9)	8.8	
50	40	-	-	10	-			5.2	6.3	7.9 (7.7)	9.4	
50	40	10	-	-	-	150		6.0	6.9	8.3 (8.1)	9.4	
30	40	30	-	-	-	150		9.3	10.3	12.2 (12.2)	13.5	
30	40	30		10	-	150		7.8	9.2	10.3 (9.3)	13.0	
50	40	-	-	-	10			4.2	5.1	6.8 (7.3)	7.2	
	40	-	-	-	30			3.0	3.8	5.9 (6.3)	5.7	

DNC—Dense nitrocellulose containing nitrocellulose 88.89 per cent, (12.2 per cent N₂), nitroglycerine 7.11 per cent, carbamate 2.67 percent and dibutylphthalate 1.33 per cent; CL—Casting liquid containing nitroglycerine 80 per cent, Diethylphthalate 18 per cent and 2-nitrodiphenylamine 2 per cent.

* Results in brackets are realised burning rates at 70 kg/cm² pressure generated in ERDL, Pune.

Table 3. Comparison of predicted and realised data from Kubota model and present approach

Propellant composition (by parts)				AP particle size (μ)	Parameters	Pressure (kg/cm ²)					
DNC	CL	AP	RDX			Kubota model			Present approach		
						35	70	140	35	70	140
60	40				T_s (°K)	606	631	663	630	649	
					r (mm/s)	3.2	5.1	8.7	5.0	7.1	
50	40	10		150	T_s	606	631	663	640	658	
					r	3.4	5.4	9.2	6.0	8.1	
30	40	30		150	T_s	606	631	663	666	683	
					r	4.3	6.5	11.0	9.3	11.8	
30	40	30		100	T_s	606	631	663	679	695	
					r	4.5	6.7	10.5	11.3	14.3	
30	40	30		50	T_s	606	631	663	702	717	
					r	5.1	7.5	12.9	15.5	19.5	
30	40	30		20	T_s	606	631	663	732	749	
					r	9.0	12.9	19.2	24.0	29.4	
30	40	30		10	T_s	606	631	663	755	773	
					r	15.7	16.9	27.8	31.8	39.4	
30	40		30		T_s	589	613	633	599	625	
					r	2.4	3.9	5.7	3.0	5.9	

DNC—Dense nitrocellulose containing nitrocellulose 88.89 per cent (12.2 per cent N₂); nitroglycerine 7.11 per cent, carbamate 2.67 per cent dibutyl phthalate 1.33 per cent; CL—Casting liquid containing nitroglycerine 80 per cent, diethylphthalate 18 per cent and 2-nitrodiphenylamine 2 per cent.

with the assumption of decrease in diffusion/mono-propellant flame heights by BDP³. The present approach is thus simple, applicable to various combinations of CMDB formulations and validated by close match with the realised results.

4. CONCLUSION

A detailed examination of the burning rate characteristic has been carried out for AP- and RDX-based CMDB and AP-based nitramine propellants, formulating a simplified model based on Kubota model for CMDB propellant combustion. This single model is useful for prediction of burning rates for variety of CMDB class of propellants, including bimodal category. This model is of interest in getting a useful burning rate data for diverse CMDB formulations incorporating nitramine, AP and Al, particularly in view of the excellent agreement between the experimented parameters and the values suggested by this model.

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