Propellant combustion, etc

Table 7.4: Ingredients of Double base (DB), composite (CP) and composite-modified double base (CMDB) propellants

Nature	For DB	For CP	For CMDB
"Fuel"	NC	PU, PBAN, PBAA CTPB, HTPB	NC + HMX or RDX
"Oxidiser" Stabiliser Plasticiser Burn rate modifier	NG EC, 2NDPA DEP, TA PbSa, LiF Pb2EH CuSt, PbSt	AP, AN - DOP, DOA, IDP IDP, Fe ₂ O ₃ nBF, CuCH DnBF, LiF	NG EC, 2NDPA DEP, TA Like for DB
Metal Fuel Curing agent Wetting agent Stability additive	Al, Mg - - Metal	Al, Mg, B TDI, MAPO, IPDI Lecithin Metal	Al, Mg - Lecithin Metal

PU = Polyurethane, PBAN = Poly Butyl Acrylo Nitrile, PBAA = Poly Butyl Acrylic Acid CTPB = Carboxy Terminated Poly Butadiene, HTPB = Hydroxy terminated Poly Butadiene, EC = Ethyl centralite, 2NDPA = 2 Nitro Di Phenyl Amine, AN = Ammonium Nitrate, DEP = Di Ethyl Phtalate, TA = Tri Acitin, DOP = Di Octyl Phtalate, DOA = Di Octyl Adipate, IDP = Iso Decyl Penargonate, PbSa = lead Salicilate, LiF = Lithium Fluoride, Pb2EH = Lead 2-Ethyl Hexoate, nBF = n-Butyl Ferrocene, CuCH = Copper Chromite, DnBF = Di-n-Butyl Ferrocene, TDI = Toulene-2, 4-Di-Isocyanate, MAPO = Tris (I-(2-Methyl) Aziridinyl) Phosphine Oxide, IDPI = Isophorone Di-Isocyanate

Table 7.5: Composition and properties of active ingredients, NC = NC (12.6 %N), ΔH_f = Heat of formation at 298.16 K

Ingredient	Chemical formula	F or Ox , %	State (300 K)	$ ho_p \ kg/m^3$	ΔH_f kJ/mole
NC	$C_6H_{7.55}O_5(NO_2)_{2.45}$	F, 12.9	Solid	1660	- 670.6
\mathbf{NG}	$C_3H_5O_3(NO_2)_3$	Ox, 0.04	Liquid	1660	- 400.6
AP	$\rm NH_4ClO_4$	Ox, 31.0	Solid	1950	-296.1
AN	$\rm NH_4NO_3$	Ox, 20.0	Solid	1730	-327.6
RDX	$C_3H_6N_3(NO_2)_3$	F, 20.0	Solid	1820	+61.5
HMX	$C_4H_8N_4(NO_2)_4$	F, 20.0	Solid	1900	+75.0

Species	NC	NG	AP	AN	RDX	HMX
T_c, \mathbf{K}	2590	3289	1405	1247	3286	3278
X_i						
O_2		0.069	0.287	0.143	-	-
H_2O	0.225	0.280	0.377	0.571	0.226	0.227
CO	0.417	0.107	-	-	0.246	0.246
CO_2	0.128	0.275	-	-	0.082	0.082
\mathbf{H}_2	0.116	0.014	-	-	0.089	0.089
N_2	0.111	0.181	0.119	0.286	0.326	0.326
HCl	-	-	0.197	-	-	-
Cl_2	-	-	0.020	-	-	-
OH	-	0.041	-	-	0.013	0.013
Η	-	-	-	-	0.013	0.012
NO	-	0.018	-	-	-	-
M , **	24.7	28.9	27.9	22.9	24.3	24.3
I_{sp} , *	2.30	2.44	1.57	1.61	2.66	2.66

Table 7.6: Equilibrium combustion features of active ingredients, X_i = Mole fraction, * = kN s/kg, \mathcal{M} = Average molecular weight of the gases, ** = g/mole

Table 7.8: Performance of solid propellants as in Table 7.7, optimum expansion from 70 atm to 1 atm, X_i = Mole fraction, 1*, 2*, 3* = CMDB1, CMDB2, CMDB3, LAlOx* = Liquid Al₂O₃, \mathcal{M} in g/mole, $I_{sp,e}$ and $I_{sp,f}$ are the specific impulse values for equilibrium and frozen conditions in kN.s/kg

Species	DB1	DB2	DB3	CP1	CP2	CP3	1^{*}	2^*	3*
T_c, \mathbf{K}	2602	3009	2500	1785	3403	3005	3091	2835	3623
X_i									
СО	0.424	0.342	0.446	0.382	0.249	0.074	0.229	0.372	0.350
H_2O	0.210	0.267	0.195	0.003	0.088	0.336	0.315	0.219	0.151
H_2	0.139	0.074	0.158	0.360	0.320	0.012	0.054	0.122	0.163
CO_2	0.100	0.169	0.090	0.001	0.009	0.289	0.181	0.095	0.039
N_2	0.124	0.133	0.109	0.191	0.078	0.159	0.130	0.185	0.111
HCl	-	-	-	-	0.126	0.067	0.063	-	0.041
Cl	-	-	-	-	0.008	0.008	-	-	0.006
OH	0.001	0.006	-	-	0.004	0.020	0.012	0.002	0.017
Н	0.002	0.005	0.001	-	0.030	0.002	0.006	0.004	0.036
NO	-	-	-	-	-	0.008	0.002	-	0.002
CH_4	-	-	-	0.008	-	-	-	-	-
C (s)	-	-	-	0.052	-	-	-	-	-
LAlOx*	-	-	-	-	0.079	-	-	-	0.075
AlCl	-	-	-	-	0.007	-	-	-	0.001
$AlCl_2$	-	-	-	-	0.002	-	-	-	-
М	23.8	25.9	23.4	18.7	27.7	29.4	26.6	24.0	30.1
$I_{sp,e}$	2.29	2.41	2.26	2.16	2.59	2.38	2.44	2.39	2.58
$I_{sp,f}$	2.28	2.38	2.24	2.06	2.45	2.27	2.39	2.37	2.46

Table 7.11: Effects of chamber pressure on the mixture properties at the chamber and exit, temperature, ratio of specific heats, γ , average molecular weight of gases, \mathcal{M}

p_c atm.	T_c K	$T_e \\ \mathbf{K}$	γ_c	γ_e	\mathcal{M}_c g/mole	${\mathscr M}_e$ g/mole
30.0	3336	2327	1.134	0.998	27.6	28.5
50.0	3378	2252	1.137	1.177	27.7	28.5
70.0	3403	2142	1.138	1.185	27.8	28.6
100.0	3429	2024	1.140	1.192	27.9	28.6

Burn rate behavior.

Adiabatic flame temperature is an equilibrium property

Burn behavior is a rate process



Table 7.7: Propellant compositions (wt. %)

Propellant	NC	NG	DEP	\mathbf{EC}	AP	Al	HTPB	HMX
DB1	44.0	43.0	11.0	2.0				
DB2	55.6	40.4	4.0					
DB3	50.4	36.6	13.0					
CP1					80.0		20.0	
CP2					68.0	18.0	14.0	
CP3							20.0	80.0
CMDB1	30.8	30.1	7.7	1.4	30.0			
CMDB2	30.8	30.1	7.7	1.4				30.0
CMDB3	26.0	30.0	8.0		21.0	15.0		

	Material	a_{70}	n	σ_T
		mm /s $(atm)^n$	-	% / K
1	AP	7.9	0.77	0.20
2	HMX	10.0	0.93	0.20
3	DB1 (44NC + 43NG + 11DEP + 2EC)	7.0	0.72	0.56
4	DB2 (56NC + 40NG + 4DEP)	10.0	0.58	0.34
5	$\mathrm{DB3}\left(50\mathrm{NC}+37\mathrm{NG}+13\mathrm{DEP}\right)$	7.3	0.82	0.62
6	CP1 (80AP + 20HTPB)	7.5	0.38	0.25
7	CP2 (68AP + 18 Al + 14 HTPB)	6.7	0.42	0.32
8	CP2 + 0.25 IO -0.25 AP	8.3	0.49	0.34
9	CP2 + 0.50 IO -0.50 AP	8.9	0.51	0.36
10	CP2 + 1.00 IO -1.00 AP	9.8	0.54	0.37
11	CP2 + 2.00 IO -2.00 AP	10.3	0.55	0.38
12	CP2 + 0.25 CC -0.25 AP	12.0	0.43	0.26
13	CP2 + 3.00 CC -3.00 AP (CP2')	15.0	0.44	0.28
14	CP3 (80HMX + 29HTPB)	1.9	0.64	0.55
15	CMDB1 (DB1 with 30AP)	15.0	0.40	0.54
16	CMDB2 (DB1 with 30HMX)	6.5	0.83	0.54

Table 7.14: Burn rate behavior with pressure and initial temperature of solid propellants, $\dot{r} = a_{70} [p_{c,s}/70]^n$, IO = Fe_2O_3 , CC = $CuCr_2O_4$, 44NC = 44 % NC

Material	Burn rate law, rdot, mm/s	E/R in surface pyrolysis law, K
NG	33 (p/70) ^{0.77}	
AP	8 (p/70) ^{0.75}	5314
RDX	15(p/70) ^{0.82}	
AN		6840
НМХ		5923
DB		5314



From Chen and Strand, An improved model for the combustion of AP Composite propellants, AIAA J, p 1739, Dec 1982

Burn rate (mm/s) vs. pressure, atm



TABLE 1

AP _c ^c	Binder ^d
41	18
41	18
41	18
41	18
	^b AP _c ^c 41 41 41 41 41 41

⁶5 μm.

^b25 µm ammonium perchlorate.

^c200 µm ammonium perchlorate.

^dHTPB (hydroxyterminated polybutadiene).



Fig. 1. Burning rate of aluminized propellants.

rdot = 8.0 (p/70)^{0.476} (0%Al), = 8.7 (p/70)^{0.476} (10%Al), = 10 (p/70)^{0.476}, (20 % Al)

From Ishihara, Brewster, Sheridan and Krier, The influence of radiative heat feedback on burning rate in aluminized propellants, Combustion and Flame, v. 84, pp 141 – 153, 1991

$$r = \frac{q_c + q_r}{\rho_s [C_s (T_s - T_0) - Q_s]} \,. \tag{18}$$

The radiation data can be simply correlated by $q''(kW/m^2) = 450 - 492 \exp(-3.2 p/70)$ for AI = 0%, $q''(kW/m^2) = 1400 - 1500 \exp(-2.25 p/70) = 10\%$, $q''(kW/m^2) = 4000 - 4385 \exp(-3.04 p/70) = 20\%$, p = atm







Pressure P, MPe Fig. 17. Radiative heat feedback from gas phase.

Since T_s , r, q_c , and q_r were all measured in this study, the condensed phase heat release Q_s could be calculated from Eq. 18. Substituting values for ρ_s , and C_s from Table 2 into Eq. 18 gave values for Q_s at 1 MPa of 312 kJ/kg for A-0 propellant, 308 kJ/kg for A-10, and 215 kJ/kg for A-20. These results indicate that the heat of condensed phase reaction per unit mass of propellant decreases with increasing aluminum loading at this pressure.



From Beckstead – Recent Progress in modeling solid propellant combustion

Material	Burn rate law, rdot, mm/s	E/R in surface pyrolysis law, K
NG	33 (p/70) ^{0.75}	
AP	8 (p/70) ^{0.75}	5314
RDX	15(p/70) ^{0.82}	
AN		6840
HMX		5923
DB		5314



Fig. 3. Comparison of calculated surface temperature and data.

Effect of particle size distribution

Miller, R. R., "Effects of Particle Size on Reduced Smoke Propellant Ballistic Propu*lsion Conference* AIAA Paper 82-1096, *AIAA/SAE/ASME 18th Joint Propulsion conference,* June 21-23, 1982.



Figure 2-12: Effect of pressure and fine AP particle size on AP/HTPB burning rates (200-micron coarse AP).



Gross and Beckstead, JPP, Jan 2009

Fig. 2 Predicted particle-size dependence of AP burning rate at 68 atm [7].

Size and Shape of Ammonium Perchlorate and their Influence on Properties of Composite Propellant

Sunil Jain, Mehilal, S. Nandagopal, P.P. Singh, K.K. Radhakrishnan, and B. Bhattacharya High Energy Materials Research Laboratory, Pune-411 021



PCL - AP

APEP

The data reveal that due to more spherical nature of particles of PCL AP, EOM viscosity of propellant slurry was less compared to APEP AP. However, propellant compositions having PCL AP gave less burn rate compared to propellant compositions containing APEP AP. This is due to the fact that burn rate is affected by surface area of AP particles. As the shape factor of particles increases, the particles become more spherical. Thus, surface area of particles decreases. The decrease in surface area is responsible for decrease in burn rate of propellant which is shown by PCL AP as it has less surface area.

Let us analyze the statement....

We must compare the surface area for the same total solid loading. Let us see how it does that.

B.S.S	PCL Ammonium perchlorate per cent	APEP Ammonium perchlorate per cent	
+30	1.45	1.0	
+44	22.60	24.95	
+52	24.80	15.40	
+60	37.4	34.45	
+85	9.35	16.90	
+100	2.35	5.55	
-100	2.05	2.20	
Average Particle size	313.72 µm	309.72 µm	

Table 1. Particle size distribution of AP (PCL & APEP)

 $+30 = 500 \ \mu\text{m}, + 44 = 354 \ \mu\text{m}, + 52 = 297 \ \mu\text{m}, + 60 = 251 \ \mu\text{m}, + 72 = ? + 85 = 178 \ \mu\text{m}, + 100 = 152 \ \mu\text{m}$

Same solid loading implies

 $n_1 \pi d_s^3/6 = n_2 \pi d_c^2 L/4$,

 $n_1 = No.$ spherical particles, $n_2 = No.$ cylindrical particles, $d_s = dia of spherical particle, d_c and L = dia and length of cylindrical particle.$ $Therefore, <math>n_1/n_2 = (3/2) (L/d_s) (d_c/d_s)^2$

The surface area ratio between spherical and cylindrical particles is

SAR_{sc} =
$$n_1 \pi d_s^2 / n_2 (2 \pi d_c^2 / 4 + \pi d_c L) = (3/2) (d_c / d_s) / (1 + d_c / 2L)$$

= 1.0 (for $d_c / d_s = 1$ and $d_c / L = 1$)
= 1.2 (for $d_c / d_s = 1$ and $d_c / L = 0.5$)

Will this make a substantial difference? ... Remember the particle size effect actually observed? It is indeed significant. Hence to truly extract the shape effect, we must separate the size effect, Is it not?













Figure 2.1: Section of a simulated propellant with Al, solid loading = 85%.





Plots on a single axis will reveal features that you cannot otherwise see

Firing no	Charge no	Mass	tb	Dt	C*	Pc avg
16403	2541	1.869	3.49	13.44	1567.69	53.72
16404	2541	1.87		12.2	1478	65.2
16405	2541	1.877		11.52	1433	72.52

Notice the significant variation in c* in Seemingly same class of BEM studies Does this bother you? Should it bother you?