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Rapid Estimation of Specific Impulse

V.K. Bhat, A.R. Kulkarni and Haridwar Singh

Explosives Research and Development Laboratory, Pune–411 021

ABSTRACT

Specific impulse (Isp) is one of the important criteria for propellant characterisation. In the present paper a semiempirical approach has been suggested to calculate Isp of composite modified doublebase (CMDB) propellant formulations by utilizing calorimetric value (Cal-Val) of the propellant composition. The Cal-Val of aluminium has been computed on the basis of oxygen balance of the propellant composition. The validity of the new approach has been demonstrated by comparing predicted values with actual results.

1. INTRODUCTION

Specific impulse (Isp) figure is an important criteria for the selection of propellants for any specific application. At present, there are few strict thermodynamic methods capable of predicting Isp accurately[1-3]. These methods are based on the assumption of water-gas reaction equilibrium, formation of metal oxides and other metallic products and dissociation species of propellant ingredients at the chamber temperature. However, in some cases, where gross assumptions have been made for the thermodynamic constants used or product gas composition, calculated performance is often inaccurate and sometimes misleading. This is very much true with highly aluminised propellants. Moreover these methods require a degree of familiarisation with rocket propellant computations. On the other hand practical evaluation of Isp is cumbersome, time consuming and requires handling and processing of large amount of explosives. In the early stage of development of energetic propellant system involving sensitive and hazardous materials, this poses a major handicap for a promising propellant formulation. To overcome these difficulties, several short methods have been proposed. Free, *et al.*[4] in their rapid estimation of Isp for liquid bipropellant system made use of a reference curve plotted for a hypothetical homologous series

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with ascending flame temperature and with assumed molecular weight of 25. Griffin, *et al.*[5] used ballistic bomb measurements of impetus to calculate characteristic velocity and Isp of liquid monopropellants. Landsbaum, *et al.*[6] analysed different efficiency factors affecting the Isp of aluminised compositions, assuming 100 per cent combustion efficiency for aluminium. Delivered Isp obtained was lower by 5–10 per cent of the theoretical value.

In the present paper, attempt has been made to predict Isp of CMDB propellant compositions from calorimetric value (Cal-Val) of the composition. Cal-Val of the propellant is the measure of its energy (heat release under constant volume without any contribution from atmospheric air). Cal-Val of propellant was calculated from the Cal-Val of the ingredients. Reported values have been used for Cal-Val of all ingredients[1,7] (Table 1) except aluminium. Cal-Val of aluminium was calculated for each composition from the oxygen balance of the propellant composition using a semiempirical equation.

Table 1. Oxygen balance and Cal-Val data on propellant ingredients[1,7]

Sl. No.	Compound	Oxygen balance (OB) (%)	Cal-Val (cal/g)
1.	Nitrocellulose (NC) (12.2% N2)	– 37.5	+897
2.	Nitroglycerine (NG)	+3.5	+1750
3.	Diethyl phthalate (DEP)	–194.1	–1765
4.	Dibutyl phthalate (DBP)	–216.4	–2070
5.	2-Nitrodiphenyl amine (2NDPA)	–201.8	–1813
6.	Carbamite	–256.4	–2440
7.	Resorcinol (Res)	–189.1	– 1388
8.	Ammonium perchlorate (AP)	+34.0	+1605
9.	Toluene diisocyanate (TDI)	–174.6	–1512
10.	Aluminium powder (Al)	– 88.9	Calculated from Eqn.(1)

2. APPROACH TO THE PROBLEM

2.1 Cal-Val of Aluminium

Aluminium (Al) on complete combustion to its trioxide (Al_2O_3) gives out heat of 7400 cal/g. However, propellant combustion takes place in an oxygen deficient environment with several competing reactions and assumption of complete heat release by aluminium combustion may not be realistic[8]. Hence, experimentally determined Cal-Val data of various CMDB propellants containing aluminium were used for arriving at Cal-Val of Al. CMDB propellant samples were prepared using dense nitrocellulose (DNC), nitroglycerine (NG), diethyl phthalate (DEP), resorcinol (Res), 2-nitrodiphenyl amine (2-NDPA), ammonium perchlorate (AP) and aluminium (Al). AP and Al proportions were varied in the propellant formulations and Cal-Val values were determined by Julius-Peter apparatus at a loading density of 0.016 g/cc. The difference between the experimental Cal-Val of propellant and the sum of the calculated Cal-Val of ingredients, excluding Al was assumed to be the Cal-Val contribution by the Al combustion (Table 2). Oxygen balance (OB) of the composition was calculated from the reported OB for the ingredients[7]. It was of interest to note that the Cal-Val of Al thus calculated decreased with decrease in OB of the propellant composition.

A simple third order equation was obtained assuming complete combustion of Al (i.e. Cal-Val of Al as 7400 cal/g) at zero OB, and by using calculated Al Cal-Val values and OB of compositions from Table 2. A graphical relation of Cal-Val of Al and OB of composition is shown in Fig. 1. The dots indicating the experimentally determined values. Thus Cal-Val of Al can be given by the relationship.

$$\text{Cal-Val of Al (cal/g)} = 7400 + 58.8x - 1.78x^2 - 0.014x^3 \tag{1}$$

where, x is the oxygen balance of the composition. Eqn. (1) obtained above was used to calculate values of Cal-Val of aluminium.

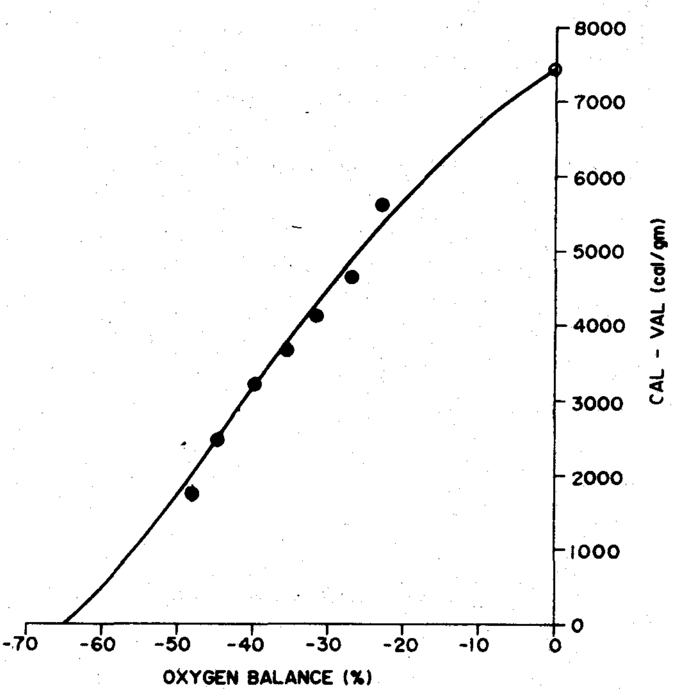

Figure 1. Variation of Cal-Val of *Al* with oxygen balance of the propellant composition.

2.2 Specific Impulse (Isp) Prediction

Specific impulse is defined as the unit mass flow rate of propellant during combustion and can be written as[8]

$$\text{Isp} = \frac{Ve}{g} = \frac{1}{g}\sqrt{2J\Delta H} \tag{2}$$

where V_e – exit velocity in cm/sec, g – gravitational constant in cm/sec^2, J – mechanical equivalent of heat in ergs/cal, and ΔH – heat release during gas expansion in cal/g.

Assuming isentropic expansion of the gases and also incorporating motor efficiency factor the equation can be written as

$$\text{Isp} = \frac{\phi}{g}\sqrt{2J\Delta H_c\left[1-\left(\frac{P_e}{P_c}\right)^{\gamma-1/\gamma}\right]} \tag{3}$$

where, ΔH_c – heat release in chamber, γ – ratio of specific heats, ϕ – motor efficiency factor, P_e and P_c – exit and chamber pressures respectively.

From elaborate theoretical calculations it is observed that specific heat ratio (γ) for most of the aluminised propellant compositions[9] lies between 1.15 to 1.20 and also Cal-Val calculated for constant volume conditions may be approximated to constant pressure heat release (ΔH_c) as done by Griffin[5]. Stephen, *et al.*[9] reported 2.2 per cent heat loss due to motor and nozzle in a 30 kg motor firing. In the present study heat loss was assumed to be about 4 per cent of the heat release (ΔH_c) as the motor size is comparatively smaller (2 kg) motor. Motor efficiency (ϕ) corresponds to the heat loss in the chamber and works out to be 0.98 in the present case. Best fit values of Isp were obtained by assuming γ as 1.18. Using these values for ϕ and γ, and values for J = 4.18 × 10^7 ergs/cal, P_c = 70 kg/cm^2, P_e = 1.003 kg/cm^2 and g = 981 cm/sec^2 in Eqn. (3) and equating ΔH_c to Cal-Val of propellant composition, specific impulse of the propellant can be written as

$$\text{Isp} = 6.3\sqrt{\text{Cal-Val}} \tag{4}$$

3. RESULTS AND DISCUSSION

Calculated and experimental results of Cal-Val for various aluminized compositions are given in Table 2. It is seen from the results that the predicted values are very close to the experimentally determined values. The variation of Cal-Val lies in the range of ±10 cal/g in most of the cases.

Table 2. Results of aluminium Cal-Val and oxygen balance of CMDB compositions

Composition : NC (12.2% N_2)–26.7, NG–30.1, DEP–6.3, DBP–0.4, Carbamite–0.8, 2NDPA–0.7, AP and Al–35.0 (percentage of AP and Al varying)

Sl. No.	AP-Al in propellant (%) AP	Al *a*	Propellant Cal-Val (experimental) (cal/g) *b*	Calculated results: Propellant Cal-Val excluding Al $\frac{1}{100}\Sigma$(% x Cal-Val ingredient) *c*	Cal-Val contribution of Al in the composition *(b–c)* *d*	Cal-Val of Al $\frac{100d}{a}$ (cal/g) *e*	OB of the composition (%) $\frac{1}{100}\Sigma$(% x OB ingredient *x*
1.	28.0	7.0	1457	1062	395	5643	–22.2
2.	24.5	10.5	1493	1005	488	4648	–26.5
3.	21.0	14.0	1537	949	588	4200	–30.8
4.	17.5	17.5	1549	893	656	3749	–35.1
5.	14.0	21.0	1517	837	680	3238	–39.4
6.	10.5	24.5	1401	781	620	2531	–43.7
7.	7.0	28.0	1231	725	506	1808	–48.0

Ingredient Cal-Val and OB are obtained from ref. 1 and 7.

Table 3. Comparative results of experimental and predicted Cal-Val of various aluminised CMDB compositions

Sl. No.	Composition								OB	Cal-Val of Al (from Eqn 1)	Predicted Cal-Val (cal/g)			Experimental Cal-Val
	DNC	NG	DEP	AP	Al	Res	2NDPA	TDI	(%)	(cal/g)	Without Al	Due to Al	Total	(cal/g)
1.	40.0	28.0	6.3	15.0	10.0	–	0.7	–	–33.6	3945	936.5	394.5	1331	1324
2.	35.0	28.0	6.3	18.0	12.0	–	0.7	–	–32.2	4128	943.6	495.4	1439	1439
3.	32.5	28.0	6.3	19.5	13.0	–	0.7	–	–31.5	4219	946.5	548.5	1495	1471
4.	30.0	28.0	6.3	21.0	14.0	–	0.7	–	–30.8	4309	949.7	603.3	1553	1544
5.	25.0	28.0	6.3	24.0	16.0	–	0.7	–	–29.4	4488	955.9	718.1	1674	1689
6.	40.0	28.0	6.3	14.3	10.0	0.7	0.7	3.6	–38.7	3270	853.4	315.6	1169	1162
7.	35.0	28.0	6.3	17.1	12.0	0.9	0.7	2.8	–37.0	3496	866.0	408.0	1274	1293
8.	32.5	28.0	6.3	18.6	13.0	0.9	0.7	2.5	–36.9	3510	856.8	445.2	1302	1327
9.	30.0	28.0	6.3	20.0	14.0	1.0	0.7	2.8	–36.0	3630	870.7	494.3	1365	1364

DNC–Dense nitrocellulose, containing at Sl.Nos. 1, 2, 3, 4, 5 and 8, NC (12.2% N2)–88.89, NG–7.11, Carbamite–2.67, DBP–1.33 and at Sl.Nos. 6, 7, 9, NC(12.2% N2)–88.89, NG–8.44, Carbamite–2.67
TDI–Toluene diisocyanate (added in parts per 100 parts of basic composition)

Table 4. Comparative results of specific impulse (Isp) (predicted and motor firing)

Sl. No.	Composition (%)								Predicted Cal-Val (cal/g)	Specific Impulse (Isp) (sec)	
	DNC	NG	DEP	AP	Al	Res	2NDPA	TDI		Predicted from Eqn. (4)	Delivered
1.	40.0	28.0	6.3	15.0	10.0	–	0.7	–	1331	230	227
2.	30.0	28.0	6.3	21.0	14.0	–	0.7	–	1553	248	246
3.	25.0	28.0	6.3	24.0	16.0	–	0.7	–	1674	258	257
4.	32.5	28.0	6.3	18.6	13.0	0.9	0.7	2.5	1302	227	227
5.	30.0	28.0	6.3	20.6	14.0	0.4	0.7	1.5	1444	239	234

DNC–Dense nitrocellulose, contains NC (12.2% N_2)–88.89, NG–7.11, Carbamite–2.67, DBP–1.33
TDI–Toluene diisocyanate (added in parts per 100 parts of basic composition)

Table 5. Few predicted results of Cal-Val and Isp for useful CMDB formulations

Sl. No	Composition (%)							Oxygen balance	Cal-Val of Al from Eqn. (1)	Predicted results	
	DNC	NG	DEP	AP	Al	2NDPA	TDI	(%)	(cal/g)	Cal-Val (cal/g)	Isp from Eqn. (4) (sec)
1.	20.0	28.0	6.3	27.0	18.0	0.7	–	–28.14	4648	1802	267
2.	20.0	28.0	6.3	27.0	18.0	0.7	3	–32.50	4090	1608	253
3.	15.0	28.0	6.3	30.0	20.0	0.7	–	–26.75	4821	1936	277
4.	15.0	28.0	6.3	30.0	20.0	0.7	3	–31.05	4277	1730	262
5.	10.0	28.0	6.3	33.0	22.0	0.7	–	–25.38	4990	2076	287
6.	10.0	28.0	6.3	33.0	22.0	0.7	3	–29.70	4447	1856	271
7.	40.0	28.0	6.3	15.0	10.0	0.7	–	–33.61	3945	1331	230
8.	40.0	28.0	6.3	15.0	10.0	0.7	1	–35.09	3750	1285	226
9.	40.0	28.0	6.3	15.0	10.0	0.7	2	–36.48	3566	1240	221
10.	40.0	28.0	6.3	15.0	10.0	0.7	3	–37.76	3395	1196	218
11.	40.0	28.0	6.3	15.0	10.0	0.7	4	–39.13	3212	1153	214
12.	40.0	28.0	6.3	15.0	10.0	0.7	5	–40.14	3037	1111	210

DNC–Dense nitrocellulose, contains NC (12.2% N2)–88.89, NG–7.11, Carbamite–2.67 and DBP–1.33

TDI–Toluene diisocyanate (added in parts per 100 parts of basic composition)

The results of predicted specific impulse values obtained by using Eqn. (4) and the actual values (experimental) with 2 kg motor firings are given in Table 4. A comparison of results indicate an error of ±1 per cent, suggesting the accuracy of the approach. This method was applied to calculate Cal-Val and Isp of a wide range of aluminised CMDB compositions. Predicted results for both these parameters are given in Table 5. These results can be further confirmed by conducting static evaluation of both the cross-linked and uncross-linked compositions.

4. CONCLUSION

A simple method based on the prior determination of Cal-Val of aluminium is suggested for Isp prediction of AP and Al containing CMDB propellants.

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