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Estimating specific impulse by using adiabatic flame temperature: some empirical equations

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Abstract Considering the importance of the specific impulse (Is) in chemical propulsion, measuring or calculating this parameter is fundamental in propulsion research. The present work is dedicated to deriving empirical equations to estimate values of (Is) based on the adiabatic flame temperature (AFT). Four empirical equations were derived and applied to data in the literature, resulting in agreement.

Keywords: Chemical propulsion; Specific impulse; adiabatic flame temperature; empirical equations.

INTRODUCTION

As is well known, the specific impulse (I_s) is a key parameter in chemical propulsion, so much so that, for new propellants, two performance factors must be considered: specific impulse and density [1].

The specific impulse strictly defines the amount of useful energy that can be obtained from the combustion and expansion of a propellant. In addition to its thermodynamic significance, the specific impulse also has an inherent ballistic importance [2]. Therefore, measuring or calculating this parameter is of paramount importance in propulsion research.

Roughly speaking, the adiabatic flame temperature (AFT) can be defined as the maximum theoretical temperature that a combustion can reach, assuming that no energy is given to the environment. There are two types of AFT: constant pressure our constant volume, the latter being higher than the former, because in that case, no energy is used to do work (i.e., to produce changing on the systems volume).

In the literature, some empirical equations can be found to to calculate I_s, mainly based on the chemical composition of the propellants [3,4]. However, it could a real advantage to be able to estimate I_s based on just a few physical parameters. In this context, the present work is dedicated to deriving empirical equations that can be used to estimate I_s values based on the AFT.

METHODOLOGY

The empirical equations were derived using data from the literature [5], summarized in Table 1.

Table 1. Auxiliary data [5] used to derive the empirical equations.

Propellant	Adiabatic flame temperature/K	Average Molar mass/ kg $kmol^{-1}$ of combustion products	Is/s
Kerosene-Oxygen	3144	22	240
Hydrogen-Oxygen	3517	16	360
Hydrogen-Fluorine	4756	10	390

From Table 1 data, adiabatic flame temperature as a function of the average molar mass (kg/kmol) of combustion products gives a linear relation (r = 0.9551), providing the equation:

$$T = -134.33\ MM + 5955 \quad (1)$$

Where T is the adiabatic flame temperature and MM is the average molar mass (kg/kmol) of combustion products.

Specific impulse as a function of the average molar mass of combustion products gives also a linear curve (r = 0.9449) and the equation:

$$I_s = -12.5\ MM + 530 \quad (2)$$

Combining equations (1) and (2), and with the suitable algebraic manipulations, were have:

$$Is = [12.5\ T - 3242.6]/134.44 \quad (3)$$

Of course, we can simply use I_s and T values to obtain a liner curve (r = 0.8055) and the empirical equation:

$$Is = 0.076\ T + 41.662 \quad (4)$$

By using the same data (Table 1) the following empirical equations were also derived:

$$Is = [(R/10)\ T]/MM \quad \text{if } T > 3600\ K \quad (5)$$

$$Is = [(2R/10)\ T]/MM \quad \text{if } T < 3600\ K \quad (6)$$

Where R is the universal gas constant (8.314 $JK^{-1}mol^{-1}$)

It must be emphasized that all derived equations are "coherent" from a physical/thermodynamic point of view: higher T values are associated with higher I_s and lower MM values are also associated with higher I_s.

RESULTS AND DISCUSSION

First of all, it is necessary to verify the self-consistence of the derived equations. The obtained results are summarized in Table 2.

Table 2. Self-consistency test: specific impulse calculated by using several derived empirical equations.

Propellant	Is/s (ref.5)	Is/s (eq.3)	Is/s (eq.4)	Is/s (eq.5)	Is/s (eq.6)
Kerosene-Oxygen	240	268.2	280.6	_	237.6
Hydrogen-Oxygen	360	303.1	309.0	_	365.5
Hydrogen-Fluorine	390	418.4	403.1	395.4	

As can be verified, Eq. 5 and 6 (which includes de MM values) works really very well. On the other hand, Eq. 3 and 4, which uses only adiabatic flame temperature values exhibits a good, but not impressive agreement with the reference values [5]. It is worth noting that both (Eq. 3 and 4) works better to the propellant with highest T value (hydrogen-fluorine).

After the self-consistence test, it is necessary to apply the derived equations to another propellants/systems, in order to verity their reliability. Of course, only literature data for which MM and/or T, as well as I_s values were available, could be tested.

In a study focused on the combustion of liquid propellants used in engines for space propulsion applications [6] the T and MM values for a Space Shuttle Main Engine were 3664.52 K and 13.523 kg/kmol, respectively. The I_s value was 458.491 s. Applying Eq. 3, 4, 5 and 6 for such T and MM values, we calculate I_s as 316.6, 320.2, 225.3 and 450.6 s, respectively. As can be verified, Eq. 6 provides a really very good result. Since the T value is only a few degrees above 3600 K, Eq. 6 was the suitable one. Furthermore, can be verified that Eq. 3 and 4, with a single parameter (T) are the lesser reliable ones.

In the same study [6] to a upper stage Aestus engine, the T, MM and I_s values are, respectively: 3197.98 K, 22.008 kg/kmol and 325.79 s. Applying eq. 3,4 5 and 6 for such system, gives, for I_s: 273.2, 284.7, 120.8 and 241,7 s, respectively. Considering the reference value (325.79 s) Eq. 4 provides de better result, with a 12.6% difference.

However, for both data set taken from Ref. 6 must be emphasized that the I_s values are vacuum specific impulses which are, of course, higher than the "realistic" values.

Furthermore, taking into account all experimental values that can exert influence on Is values, ie. propellant composition, propellant flow injection, etc., the obtained results can be considered as acceptable.

To a 70% NH_4ClO_4, 16% aluminium and 14% binder and additives propellant [7] the obtained results are summarized in Table 3.

Table 3. Reference and calculated I_s values for a NH_4ClO_4/Al propellant (Ref. 7).

System	T/K (ref. 7)	Is/s (ref. 7)	Is/s (eq. 3)	Is/s (eq. 4)
First-Stage Minuteman I Missile Motor)	3472	254	298.7	305.5
Orbus-6 Inertial Upper-Stage Motor (vacuum)	3672	289.6	317.3	320.7
STARTM 27 Apogee Motor (vacuum)	3538	290.8	304.8	310.3

As a general result, can be stated that the calculated values by using Eq. 3 and 4 are in good agreement with the reference ones.

Hence, despite the fact that Eq. 3 and 4 where derived from liquid propellant data, they can work very well for solid rocket propellants too.

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