

PROPULSIVE PARAMETERS OF THERMALLY PERFECT GASES

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***Abstract.** Propulsive parameters of rockets are usually defined for perfect gases with constant properties. However propellants can reach high temperatures in the chamber and the specific heats of the exhaustion gases can vary significantly throughout the nozzle, especially if they contain polyatomic molecules. This paper derives equations for propulsion parameters of rockets, including specific impulse, characteristic velocity, critical mass flow constant and thrust coefficient, assuming isentropic one-dimensional flow of thermally perfect gases. Theoretical results for CO₂, H₂O and N₂ flows are obtained considering specific heats obeying NASA fourth order polynomials of temperature.*

***Keywords:** thermally perfect gases, specific impulse, characteristic velocity, thrust coefficient*

1. INTRODUCTION

Propulsive parameters are used to evaluate different performance aspects of rockets. Specific impulse is a parameter that relates instantaneous thrust and weight flow rate or, generally, relates the total impulse delivered with propellant weight spent during burning time. The characteristic velocity is a propulsive parameter which indicates the propellant performance and the motor design quality, whereas the thrust coefficient measures the nozzle design efficiency. The critical mass flow constant allows determining the mass flow rate from chamber stagnation conditions (Zucrow and Hoffmann, 1976).

The classical equations for propulsive parameters are generally derived assuming one-dimensional isentropic flow of perfect gases and considering constant properties along the nozzle (Shapiro, 1953). However, perfect gases usually are not calorically perfect, i.e., they present specific heats varying significantly with temperature. In the case of real gases the specific heats are dependent on temperature and pressure. Propellants in chemical, electrothermal, laser, microwave and nuclear rockets can reach up to temperatures above 3000 K in the chamber, and, consequently, temperature variations along the nozzle are important, thus affecting strongly the specific heats of the flowing gases.

Several authors have considered the one-dimensional isentropic flows of thermally perfect gases or real gases. Donaldson (1946) evaluated the effects of imperfect gases and the variation of specific heats of diatomic gases; Tsien (1947) described the flow properties of Van der Waals gases with specific heats varying with temperature; Eggers (1948) examined the flow of diatomic gases obeying the Berthelot equation of state with specific heats varying with temperature; Johnson (1965) determined effects of real gases on the critical nozzle mass flow constant and on thermodynamic properties of isentropic flows; and Witte and Tatum (1994) developed a computer code to determine the thermally ideal gas properties, using specific heats approximated as NASA fourth order polynomials of the temperature. Ding et al. (2014) described flow characteristics of hydrogen gas through a critical nozzle using equations of state based on Helmholtz energy and compared the theoretical results with experimental data and CFD simulations with different equations of state.

However, no reference was found describing equations for the propulsive parameters of rockets based on isentropic flow relations of thermally perfect gases or real gases. Therefore, this paper derives expressions for propulsive parameters of rockets, considering steady compressible one-dimensional isentropic flow of perfect and thermally perfect gases, i.e., with specific heats varying with temperature. Numerical results are obtained assuming a fourth degree polynomial variation of specific heats with temperature. The nozzle exit and throat conditions of thermally perfect gases are also compared to the values found for calorically perfect gases.

2. ONE-DIMENSIONAL ISENTROPIC FLOW OF A THERMALLY PERFECT GAS

An energy balance along a one-dimensional isentropic flow through a nozzle with variable cross section area, $A = A(x)$, where x is a longitudinal position along the nozzle, yields:

$$h_o = h_c + \frac{v_c^2}{2} = h + \frac{v^2}{2} \quad (1)$$

where h_o is the specific stagnation enthalpy, h_c is the specific enthalpy at the chamber exit, v_c is the chamber exit velocity, h is the specific enthalpy and v is the velocity at any position x along the nozzle. The stagnation enthalpy h_o

represents the flow enthalpy at a point where the kinetic energy was converted to thermal energy by an adiabatic reversible process.

The internal energy u and the enthalpy h of a fluid are, in general, functions of two other thermodynamic properties, e.g., $u = u(P,T)$ and $h = h(P,T)$, where P and T are pressure and temperature, respectively. Internal energy includes kinetic, vibrational, rotational and electronic energies from the molecules and the enthalpy is defined as $h = u + P/\rho$, where ρ is flow density.

The specific heat at constant pressure, c_p , and the specific heat at constant volume, c_v , of a fluid are defined, respectively, by:

$$c_p = \left(\frac{\partial h}{\partial T} \right)_p ; \quad c_v = \left(\frac{\partial u}{\partial T} \right)_v \quad (2)$$

A perfect gas obeys the state equation $P = \rho RT$ where R is the gas constant. It can be demonstrated experimentally (Gay Lussac – Joule experiment) or theoretically (by using Maxwell relations) that the internal energy of a perfect gas depends only on temperature and, therefore, the partial derivatives in the specific heats' definitions become ordinary derivatives of temperature: $c_p = dh/dT$ and $c_v = du/dT$.

Since the specific enthalpy of a perfect gas is $h = u + RT$, then:

$$c_p - c_v = R \quad (3)$$

The specific heat ratio is defined by $\gamma = c_p / c_v$ that, combined with Eq. (3), yields:

$$\frac{c_p}{R} = \frac{\gamma}{\gamma-1} \quad \text{and} \quad \frac{c_v}{R} = \frac{1}{\gamma-1} \quad (4)$$

Sound speed

The momentum equation, $dP + \rho v dv = 0$ (Euler equation), combined to the energy equation in differential form, $dh + v dv = 0$, assuming a perfect gas, $\rho = P/RT$, with $dh = c_p dT$, yields:

$$\frac{dT}{T} = \frac{R}{c_p} \frac{dP}{P} \quad (5)$$

From the perfect gas equation it follows that $\frac{dP}{P} = \frac{d\rho}{\rho} + \frac{dT}{T}$. Substituting into (5), gives $\frac{dP}{d\rho} = \gamma \frac{P}{\rho} = \gamma RT$.

Therefore the sound speed of a thermally perfect gas is obtained:

$$v_{som} = \left(\frac{\partial P}{\partial \rho} \right)_s^{1/2} = \sqrt{\gamma RT} \quad (6)$$

where s is the specific gas entropy. This expression is similar to the one obtained for the sound speed in a calorically perfect gas, however in this case γ varies with temperature.

Energy equation

Replacing $dh = c_p dT$, $c_p = \gamma R / (\gamma - 1)$, $v_{som}^2 = \gamma RT$ and $M = v / v_{som}$ in the energy equation, $dh + v dv = 0$, yields:

$$\frac{dT}{T} + (\gamma - 1) M^2 \frac{dv}{v} = 0 \quad (7)$$

The mass flow rate through the nozzle is given by $\dot{m} = \rho v A$. Assuming steady state, and differentiating, then:

$$\frac{d\rho}{\rho} + \frac{dv}{v} + \frac{dA}{A} = 0 \quad (8)$$

Since $\frac{dT}{T} = \frac{R}{c_p} \frac{dP}{P}$, then $\frac{dT}{T} = \frac{\gamma-1}{\gamma} \frac{dP}{P}$ and once $\frac{d\rho}{\rho} = \frac{1}{\gamma} \frac{dP}{P}$ then $\frac{d\rho}{\rho} = \frac{1}{\gamma-1} \frac{dT}{T}$.

Replacing in (8) gives $\frac{1}{\gamma-1} \frac{dT}{T} + \frac{dv}{v} + \frac{dA}{A} = 0$ and, combining with (7), it follows that:

$$(1-M^2) \frac{dv}{v} + \frac{dA}{A} = 0 \quad (9)$$

Consequently, in a nozzle, if $dA = 0 \Rightarrow M = 1$, similarly to a calorically perfect gas.

Flow velocity

Neglecting the flow velocity in the chamber, the equation da energy for a control volume along the nozzle becomes $h_c = h + \frac{v^2}{2}$ and, consequently, the flow velocity is given by:

$$v = \sqrt{2 \int_T^{T_c} c_p dT} \quad (10)$$

where T_c is the chamber temperature. Replacing $M = \frac{v}{\sqrt{\gamma RT}}$, yields the flow Mach number:

$$M = \sqrt{\frac{2}{\gamma T} \int_T^{T_c} \frac{c_p}{R} dT} \quad (11)$$

Nozzle throat temperature

Flow velocity in the nozzle throat is obtained from Eq. (10): $v_g = \left(2 \int_{T_g}^{T_c} c_p dT \right)^{1/2}$ where the subscript “g” designates condition in the nozzle throat. Since $M = 1$ in the throat, $v_g^2 = v_{som}^2 = \gamma_g RT_g$, thus yielding:

$$T_g = \frac{2}{\gamma_g} \int_{T_g}^{T_c} \frac{c_p}{R} dT \quad (12)$$

which can be solved iteratively, once the function $c_p = c_p(T)$ is known.

Isentropic relations

Combining the Euler equation and energy equation, then $dh = dP/\rho$, or $c_p dT = dP/\rho$, giving, for a perfect gas:

$$c_p \frac{dT}{T} = R \frac{dP}{P} \quad (13)$$

Integrating between temperatures T_1 and T_2 and pressures P_1 and P_2 , yields:

$$\frac{P_2}{P_1} = \exp \left(\int_{T_1}^{T_2} \frac{c_p}{R} \frac{dT}{T} \right) \quad (14)$$

and, therefore, the ratio between the chamber and nozzle throat pressures is $\frac{P_c}{P_g} = \exp \left(\int_{T_g}^{T_c} \frac{c_p}{R} \frac{dT}{T} \right)$.

Using the perfect gas equation, it yields $\frac{\rho_2}{\rho_1} = \frac{P_2 T_1}{P_1 T_2} \Rightarrow \frac{\rho_2}{\rho_1} = \frac{T_1}{T_2} \exp\left(\int_{T_1}^{T_2} \frac{c_p}{R} \frac{dT}{T}\right)$.

Critical mass flow constant

The mass flow rate through the nozzle throat is $\dot{m} = \rho_g v_g A_g = \frac{P_g}{RT_g} \sqrt{\gamma_g RT_g} A_g$.

Since $P_g = P_c \exp\left(-\int_{T_g}^{T_c} \frac{c_p}{R} \frac{dT}{T}\right)$, it follows that:

$$\dot{m} = \Gamma_{TP} A_g \frac{P_c}{\sqrt{RT_c}} \quad (15)$$

where Γ_{TP} is the critical mass flow constant for a thermally perfect gas, given by:

$$\Gamma_{TP} = \sqrt{\gamma_g \frac{T_c}{T_g}} \exp\left(-\int_{T_g}^{T_c} \frac{c_p}{R} \frac{dT}{T}\right). \quad (16)$$

Γ_{TP} reduces to the critical mass flow constant of a calorically perfect gas, Γ_{CP} , by making $c_p = \text{constant}$ and $\gamma = \gamma_g = \text{constant}$:

$$\Gamma_{CP} = \sqrt{\gamma} \left(\frac{2}{\gamma+1}\right)^{\frac{1}{2} \left(\frac{\gamma+1}{\gamma-1}\right)}$$

In this case, the γ value in the chamber or an average γ along the nozzle can be adopted.

Characteristic velocity

The characteristic velocity is given by:

$$c^* = \frac{P_c A_g}{\dot{m}} \rightarrow c_{TP}^* = \frac{\sqrt{RT_c}}{\Gamma_{TP}} \quad (17)$$

Thrust coefficient

The thrust coefficient is defined by:

$$c_F = \frac{F}{P_c A_g} = \frac{\dot{m} v_e + (P_e - P_a) A_e}{P_c A_g} \quad (18)$$

where F is the thrust and the subscript “e” designates conditions at the nozzle exit section.

Replacing $\dot{m} = \Gamma_{TP} A_g \frac{P_c}{\sqrt{RT_c}}$ and $v_e = \sqrt{2 \int_{T_e}^{T_c} c_p dT}$, it follows that:

$$c_{F,TP} = \Gamma_{TP} \sqrt{\frac{2}{T_c} \int_{T_e}^{T_c} \frac{c_p}{R} dT} + \left(\frac{P_e}{P_c} - \frac{P_a}{P_c}\right) \frac{A_e}{A_g} \quad (19)$$

where $\frac{P_e}{P_c} = \exp\left(\int_{T_e}^{T_c} \frac{c_p}{R} \frac{dT}{T}\right)$.

For optimum expansion in vacuum then $P_a = P_e = T_e = 0$, yielding

$$c_{F,TP,opt,vac} = \Gamma_{TP} \sqrt{\frac{2}{T_c} \int_0^{T_c} \frac{c_p}{R} dT} \quad (20)$$

Nozzle expansion rate

The mass flow rate through the exit section is $\dot{m} = \rho_e v_e A_e = \Gamma_{TP} A_g \frac{P_c}{\sqrt{RT_c}}$. Replacing $\rho_e = \frac{P_e}{RT_e}$ and

$$v_e = \sqrt{2 \int_{T_e}^{T_c} c_p dT}, \text{ yields:}$$

$$\frac{A_e}{A_g} = \frac{\Gamma_{TP}}{\sqrt{\frac{2}{T_e} \int_{T_e}^{T_c} \frac{c_p}{R} dT}} \sqrt{\frac{T_e}{T_c}} \exp\left(\int_{T_e}^{T_c} \frac{c_p}{R T} dT\right) \quad (21)$$

Therefore, T_e can be calculated if $c_p = c_p(T)$, R , T_c and A_e/A_g are given. Consequently, the temperature ratio T_e/T_c depends on the expansion ratio A_e/A_g and $c_{F,TP}$ depends basically on the nozzle geometry.

The thrust coefficient of a thermally perfect gas can be compared to the corresponding calorically perfect gas thrust coefficient:

$$c_{F,CP} = \Gamma_{CP} \sqrt{\frac{2\gamma}{\gamma-1} \left[1 - \left(\frac{P_e}{P_c}\right)^{\frac{\gamma-1}{\gamma}} \right]} + \left(\frac{P_e}{P_c} - \frac{P_a}{P_c}\right) \frac{A_e}{A_g} \quad (22)$$

Specific impulse

The specific impulse, assuming constant thrust F and constant mass flow rate, is given by:

$$Isp = \frac{F}{\dot{m} g_o} = \frac{c_F c^*}{g_o} \quad (23)$$

Considering optimum expansion of a thermally perfect gas in vacuum, it follows that:

$$Isp_{TP,opt,vac} = \frac{1}{g_o} \sqrt{2 \int_0^{T_c} c_p dT} \quad (24)$$

3. RESULTS

Simulations of isentropic one-dimensional flows of CO₂, H₂O and N₂ were performed, versus chamber temperature, and using specific heats obeying fourth order polynomials of temperature, as described in NASA TP-2002-211556:

$$\frac{c_p}{R} = a_1 T^{-2} + a_2 T^{-1} + a_3 + a_4 T + a_5 T^2 + a_6 T^3 + a_7 T^4 \quad (25)$$

The temperature coefficients $a_{i=1,\dots,7}$ in different temperature ranges are presented in Table 1.

Figures 1 to 6 show the calculated propulsive parameters, flow properties at throat and nozzle exit sections, and percent errors, comparing the vacuum expansion of thermally perfect gases and calorically perfect gases, along a nozzle with expansion rate equal to 100, for chamber temperatures varying from 1000 K to 4000K.

The percent error of $\phi = Isp, F$, etc is defined as:

$$error = 100 \frac{\phi_{CP} - \phi_{TP}}{\phi_{TP}} \quad (26)$$

It was assumed $\gamma = \gamma(T_c)$ in the case of calorically perfect gases, however other values, for example, $\gamma = \gamma(T_{av})$, where $T_{av} = (T_c + T_e)/2$, could be adopted.

Table 1 – Polynomial coefficients of specific heats. Source: NASA TP-2002-211556.

CO₂	a_1	a_2	a_3	a_4
200	4.943650540D+04	-6.264116010D+02	5.301725240D+00	2.503813816D-03
$\leq T < 1000$	a_5	a_6	a_7	
	-2.127308728D-07	-7.689988780D-10	2.849677801D-13	
1000	a_1	a_2	a_3	a_4
$\leq T < 6000$	1.176962419D+05	-1.788791477D+03	8.291523190D+00	-9.223156780D-05
	a_5	a_6	a_7	
	4.863676880D-09	-1.891053312D-12	6.330036590D-16	
H₂O	a_1	a_2	a_3	a_4
200	-3.947960830D+04	5.755731020D+02	9.317826530D-01	7.222712860D-03
$\leq T < 1000$	a_5	a_6	a_7	
	-7.342557370D-06	4.955043490D-09	-1.336933246D-12	
1000	a_1	a_2	a_3	a_4
$\leq T < 6000$	1.034972096D+06	-2.412698562D+03	4.646110780D+00	2.291998307D-03
	a_5	a_6	a_7	
	-6.836830480D-07	9.426468930D-11	-4.822380530D-15	
N₂	a_1	a_2	a_3	a_4
200	2.210371497D+04	-3.818461820D+02	6.082738360D+00	-8.530914410D-03
$\leq T < 1000$	a_5	a_6	a_7	
	1.384646189D-05	-9.625793620D-09	2.519705809D-12	
1000	a_1	a_2	a_3	a_4
$\leq T < 6000$	5.877124060D+05	-2.239249073D+03	6.066949220D+00	-6.139685500D-04
	a_5	a_6	a_7	
	1.491806679D-07	-1.923105485D-11	1.061954386D-15	

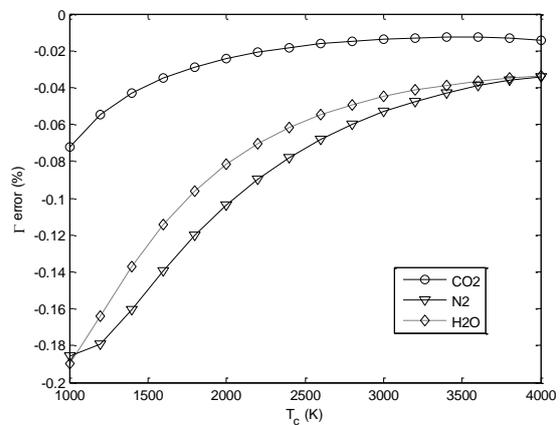
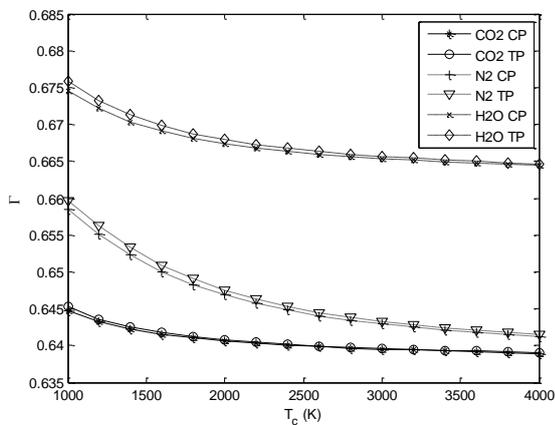


Figure 1. Critical mass flow constant and percent error: $100(\Gamma_{CP} - \Gamma_{TP}) / \Gamma_{TP}$.

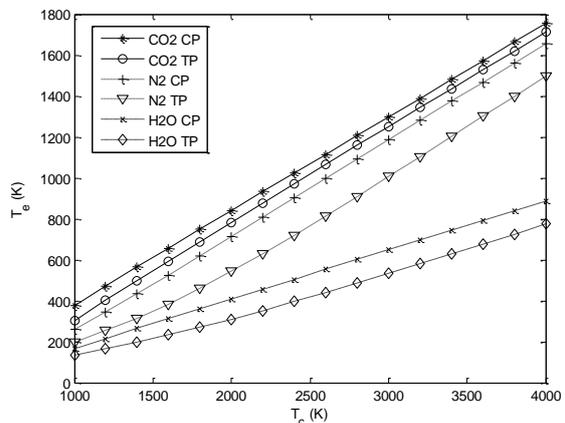
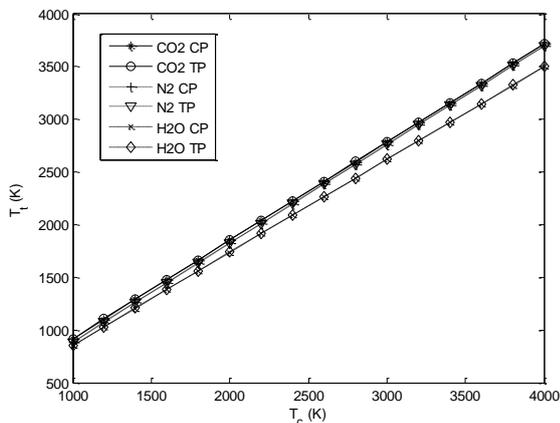


Figure 2. Throat and exit temperatures.

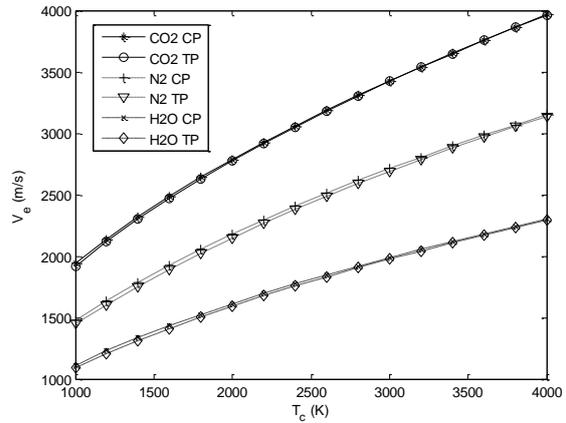
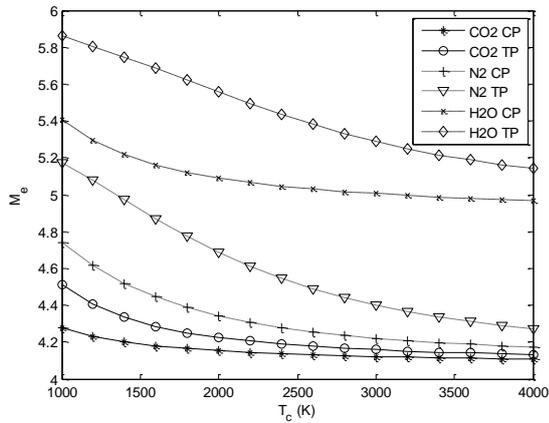


Figure 3. Mach number and flow velocity at nozzle exit with $\varepsilon = 100$.

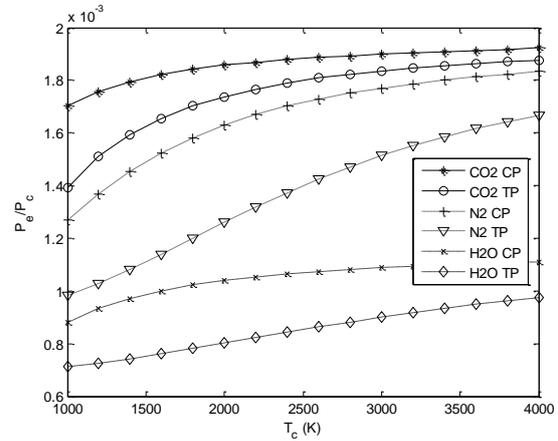
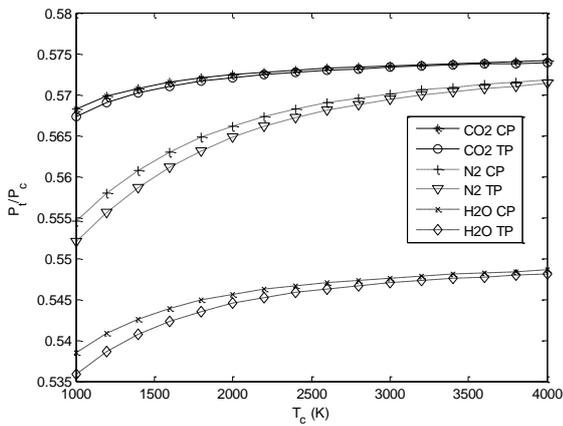


Figure 4. Throat and exit pressure ratios, with $\varepsilon = 100$.

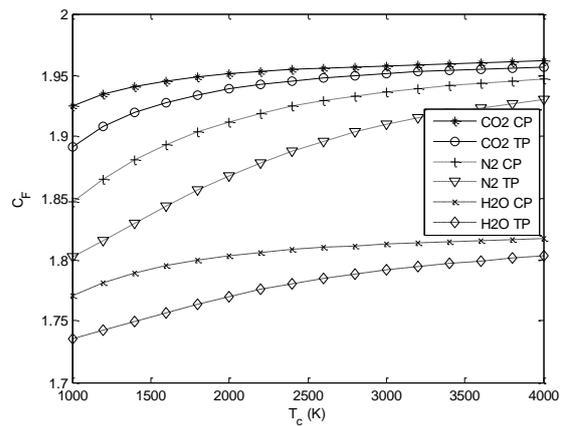
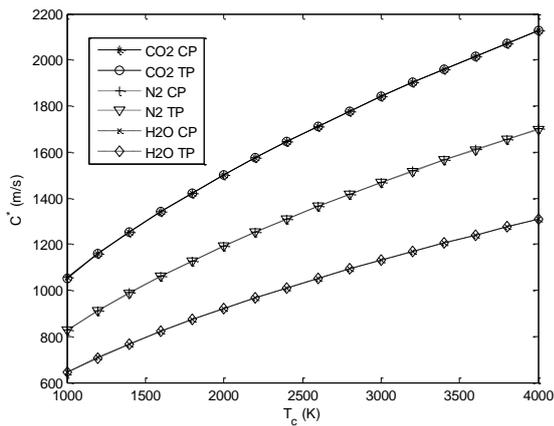


Figure 5. Characteristic velocity and thrust coefficient in vacuum, with $\varepsilon = 100$.

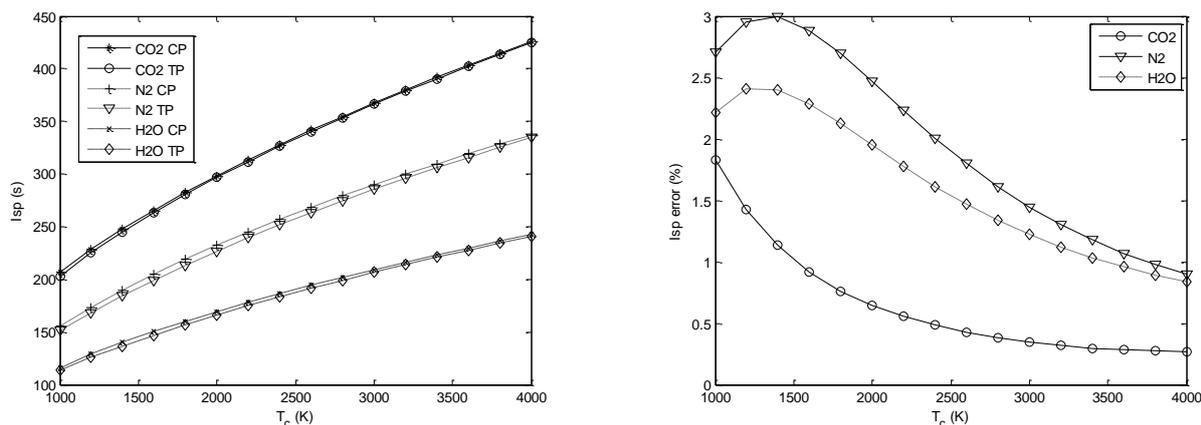


Figure 6. Vacuum specific impulse and percent error, $100(I_{sp_{CP}} - I_{sp_{TP}}) / I_{sp_{TP}}$, for $\varepsilon = 100$.

3. CONCLUSIONS

The propulsive parameters of rockets and nozzle flow properties were determined for the isentropic one-dimensional flow of thermally perfect gases. Calculations were performed for three different gases (CO_2 , H_2O and N_2) considering specific heats varying according to NASA fourth degree polynomials of temperature. For the assumed conditions, the thrust coefficients, vacuum specific impulses, exit Mach number, critical mass flow constant and exit pressures presented significant variations, whereas characteristic velocities, exit temperatures and exit velocities of thermally perfect gases have not presented significant variations as compared to calorically perfect gases. Further investigation can be made considering real gases or calorically perfect gases with specific heat ratios at an average temperature along the nozzle.

4. ACKNOWLEDGEMENTS

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