Study of fluid flow of the combustion products for the determination of bipropellants performances

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Abstract:
This paper presents a study on the combustion and flow of the combustion products of popular liquid bipropellant used for space applications. Study of fluid flow inside 2D axisymmetric nozzle of the bipropellant engine is necessary in order to determine all the thermodynamic parameters (pressure, Temperature, Density and Velocity) of the gas mixture at the exit of the nozzle. The calculated parameters were used to evaluate the performances of the bipropellants in terms of vacuum specific impulse. The performances were determined and analysed as function of the mixture ratio-by-mass of oxidizer by fuel (O/F), and the pressure of the propellants. In this study, the combustion of hydrogen fuel with oxygen as oxidizer has been taken into consideration. Many results in terms of vacuum specific impulse were presented for different pressure conditions and mixture ratio-by-mass. Some results were presented and compared with results of previous researches based on 1D fluid flow assumption. The comparison shows a difference of less than 4 \%, however the current results can be considered as good improvement in the estimation of the performances of bipropellants.

Keywords: specific impulse, thrust, bipropellant, propulsion system

Nomenclature

g_0 = acceleration of gravity (g_0 = 9.807 m/s^2)
A_e = nozzle exit area [m^2]
A_t = nozzle throat area [m^2]
C_p = heat capacity at constant pressure [J/kg. K]
F = Thrust level [Newton]
Isp = specific impulse [s]
M = molar mass [Kg/Kmol]
M_i = molecular mass of the product (i) [Kg /Kmol]
m* = mass flow rate [kg /s]
m_{fuel} = fuel mass [kg]
m_{oxidizer} = oxidizer mass [kg]
\eta_{pi} = number of moles of the product (i) [ mol ]
P_0 = combustion pressure [ bar ]
P_a = ambient pressure [ bar ]
P_e = exit pressure [ bar ]
R = universal gas constant [J/Kmol. K ]
T = temperature [ K ]
T_0 = initial temperature [ K ]
T_c = combustion chamber temperature [ K ]
\gamma = specific heat ratio
e = internal energy mass [ Joule ]
\rho = density [ Kg/m^3 ]
u = axial velocity [ m/sec ]
As an important parameter to estimate the performance of the propulsion engine, the specific impulse is referred to the thrust produced by the engine per unit weight flow rate. The calculation of this parameter for bipropellant engine needs to study the combustion of the fuel with oxidizer inside the combustion chamber and the fluid flow through the nozzle. The study of the combustion is needed in order to determine the flame temperature and all the thermochemical parameters of the gas mixture. These parameters can be used to study the flow of the combustion products through the nozzle to give the distribution of the thermodynamic parameters in terms of velocity, Mach number, pressure, temperature and density.

The aim of this paper is to study the performance of the hydrogen/oxygen bipropellant as function of mixture ratio by mass at different values of pressure, and this by studying the flow of the combustion products inside 2D axisymmetric nozzle of the bipropellant engine.

\[ v = \text{radial velocity [m/sec]} \]

1 Introduction

**Combustion products and flame temperature**

To determine the thermochemical parameters of the combustion of the hydrogen fuel with oxygen oxidizer, it is necessary to solve two basic thermochemical problems [1]:

- Given the combustion chamber conditions (pressure \( P_0 \), temperature \( T_0 \)) at assumed temperature, we determine the chemical reaction products.
- Given the chemical reaction products, we determine the flame temperature which verifies the energy equation, then we determine all the other thermochemical parameters of the combustion.

The general energy equation of the chemical reactions is written by [1]:

\[
\Delta H^0_r + \sum_i n_{pi,reactants} \int_{298}^{T_a} C_{pi} dT = \sum_i n_{pi,products} \int_{298}^{T_c} C_{pi} dT
\]  

(1)

Where \( \Delta H^0_r \) is the energy difference between the reactants and products under standard conditions (kJ).

After determination of the flame temperature and number of moles of the products [1], the molecular mass (M) and isentropic parameter (\( \gamma \)) of the combustion products can be calculated by the following equations:

\[
M = \frac{\sum_i n_{pi}M_i}{\sum_i n_{pi}}
\]

(2)

\[
C_p = \frac{\sum_i n_{pi}C_{pi}}{\sum_i n_{pi}}
\]

(3)

\[
\gamma = \frac{C_p}{C_p - R}
\]

(4)

The mixture ratio by mass is calculated from the reactants of the chemical reactions as follows:
\[ \left( \frac{m_{\text{Oxidizer}}}{m_{\text{Fuel}}} \right) = \frac{(\text{molecular weight of oxidizer}) \times (\text{number of moles of oxidizer})}{(\text{molecular weight of fuel}) \times (\text{number of moles of fuel})} \]  

(5)

### 3 One dimensional (1D) fluid flow of the combustion products

In one dimensional study we supposed frozen flow approach, the equilibrium chemical reaction is assumed to occur very slowly, the products of combustion do not change in chemical composition while traversing the nozzle, so the thermochemical parameters (\( T_c, M, \gamma \)) do not change through the engine [2]. The following simplifying assumptions are made: isentropic flow, flow is in one dimension, products of combustion constitute a perfect gas, flow is frozen and steady. The specific impulse (Isp) can be calculated by the following equation [3, 4]:

\[ I_{sp} = \frac{A_r P_0 \gamma \left[ \frac{2}{\gamma - 1} \left( \frac{2}{\gamma + 1} \right)^{\frac{\gamma + 1}{\gamma - 1}} \left( 1 - \left( \frac{P_e}{P_0} \right)^{\frac{\gamma - 1}{\gamma}} \right) \right]^{\frac{1}{2}} + (P_e - P_a) A_e}{m \cdot g_0} \]  

(6)

### 4 Two dimensional (2D) axisymmetric fluid flow of the combustion products

In this part, Fluent code was used to analyse and simulate the two dimensional (2D) axisymmetric fluid flow inside the nozzle. The thermochemical parameters of the gas mixture obtained from the combustion of hydrogen/oxygen at defined mixture ratio by mass have been taken as input of this analysis. The equations which are based this code for steady inviscid fluid flow are written in vector form in the following system equations.

\[ \frac{\partial W}{\partial t} + \text{div}(\phi(W)) = 0 \quad \text{With: } \quad W = \begin{bmatrix} \rho \\ \rho u \\ \rho v \\ \rho e \end{bmatrix}, \quad \phi = F.i + G.j + H.k \]  

(7)

Where the vectors \( F, G, H \) are defined as:

\[ F = \begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ (\rho e + p)u \end{bmatrix}, \quad G = \begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ (\rho e + p)v \end{bmatrix}, \quad H = \begin{bmatrix} 0 \\ 0 \\ 2p \\ 0 \end{bmatrix} \]  

(8)

The specific impulse (Isp) for 2D axisymmetric fluid flow was calculated using the thermodynamic properties of the gas at the exit section of the nozzle and the following equation :

\[ I_{sp} = \frac{F}{m \cdot g_0} \]  

(9)
5 Results and discussion
In this study bell nozzle geometry has been selected with chamber diameter of 1m, throat diameter of 0.2 m and an expansion ratio of 200. We consider a rectangular mesh composes of 456 nodes along the axis and 20 nodes along the radius (456 x 20). Figure 1 shows the geometry and the mesh of the bell nozzle.

![Geometry and mesh of the nozzle (456 x 20).](image)

Figure 2 shows the values of pressure and temperature through the nozzle for two hypothesis of fluid flow:
- One dimensional fluid flow.
- Two dimensional axisymmetric nozzle fluid flow.

These results are obtained by taking the combustion of hydrogen/oxygen with mixture ratio by mass equal to 8 (mass oxidizer/ mass fuel = 8) and pressure of 200 bar. The thermochemical parameters of the gas mixture after the combustion are:
• $C_p = 3205.362 \text{ J/kg.K}$.
• $M = 16.189 \text{ g/mol}$.
• $T_c = 3776.4 \text{ K}$.
• $\gamma = 1.1908$.

It is clear that the nozzle converts the thermal energy of the gas into dynamic energy for this why the figure 2 shows a decrease of temperature and pressure along the nozzle. A small difference can be observed between the results obtained using one dimensional and two dimensional fluid flow hypothesis.

Figure 3 presents the variation of specific impulse as function of mixture ratio by mass for different values of pressure inside the nozzle for the combustion of hydrogen and oxygen propellants combination. In this figure, the two hypothesis of fluid flow were taken into account (one dimensional fluid flow, two dimensional axisymmetric nozzle fluid flow). The comparison of the results with 1D fluid flow assumption shows a difference of less than 4%, however the results obtained using fluid flow through 2D axisymmetric nozzle can be considered as good amelioration in the estimation of the performances of bipropellants. In general, one dimensional hypothesis is taken for preliminary estimation of the performance of propulsion engines. However, two dimensional axisymmetric is used for the detailed analysis and design of the engines.

The curves of figure 3 show an increase of the specific impulse to a maximum and then it decreases. To explain that, we must remember that the temperature of combustion increase with mixture ratio by mass until a maximum value (maximum combustion temperature at stoichiometric coefficient), then this temperature drops. A higher temperature gas means higher thermal energy of the gas and this gives a higher specific impulse for the bipropellant engine. In other hand this figure illustrates the effect of the pressure on the specific impulse. It is clear that the specific impulse increases as the pressure increases. For this reason, in actual hydrogen/ oxygen bipropellant engines the propellants are stored at high pressures (more than 200 bars) to give high performance. As an example, in the space shuttle main engine (SSME) the propellants are stored at around 220 bars which gives a specific impulse of 454 seconds.

![FIG. 3 – Effect of the pressure and mixture ratio by mass on the specific impulse.](image-url)
6 Conclusion

The combustion of hydrogen fuel with oxygen as oxidizer (H2/O2) has been used in this paper to determine the flame temperature and all the thermochemical parameters of the gas mixture. Then, the study of the fluid flow of the combustion products was presented. Indeed we have chosen the hydrogen fuel with oxygen which is one of the most popular bipropellant combination. So this study of the fluid flow of the combustion products through 2D axisymmetric nozzle is very important in order to calculate all the thermodynamic parameters (pressure, temperature, density…) along the nozzle then this last parameters were used to evaluate the performances of the bipropellant engine in terms of specific impulse. The thermodynamic parameters along the nozzle were obtained and compared with 1D fluid flow assumption, as well the performances were calculated and analyzed as function of mixture ratio-by-mass and at different pressures. The comparison with 1D fluid flow assumption shows a difference of less than 4 %, however the results obtained can be considered as good amelioration in the estimation of the performances of bipropellants.

References