Integration of Fuels Types and Chemical Properties with the Design of the Rocket Engine's Bell Exhaust Nozzle and Combustion Chamber

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The chemical properties of the fuels are crucial for obtaining the numerical accuracy during the design and performance analysis in case of liquid fuel propelled rocket engines, as well as the trajectory optimization. In this paper, the research was primarily focused on optimizing the numerical accuracy for non-linear two-dimensional approximation the Fuel Combustion Charts; secondarily, the investigation was carried on the design of the bell-nozzle of a liquid propelled rocket engine, taking into account the variation of the coefficients which are significant for expressing the fuels chemical properties. From the Fuel Combustion Charts, the authors selected a the LOX - Kerosene combination for propelling the rocket engine, due to the most convenient matching with the technology and material specifications, safety and environmental friendly requirements; from the LOX-Kerosene Charts, the authors have originally developed a method to obtain the expression of a non-linear approximation function of two variables. The design of the bell shaped nozzle and combustion chamber for a liquid propelled rocket engine was included, in purpose to illustrate the link between the LPRE design and the fuels types and chemical properties.

Keywords: fuel combustion charts, liquid propelled rocket engines, combustion chambers

The design and performance analysis of jet engines and rocket engines require appropriate mathematical modeling for complex intricate phenomena; the main goal is the obtaining of the best numerical accuracy. The algorithms and input data can be validated in experiment and comparison with available data from state of art survey.

Relevant to this topic, can be approached investigations for complex and intricate phenomena, such as: propellant atomization, mixing, evaporation, chemical reaction, gas expansion, as well as effects (e.g. chemical reaction rates, and boundary-layer and streamline and velocity-vector divergence in the converging and diverging nozzles) intended to a more accurate description of real phenomena.

As potential fuels for liquid-propelled rocket engines can be considered the following: Liquid Oxygen-LOX as oxidizer and Kerosene (n-Dodecane, $C_{12}H_{26}$), LOX-Liquid Hydrogen, Liquid Methane CH_4 and Ethyl Alcohol CH_3CH_2OH, LOX–UDMH (1,1 - dimethylhydrazine), Red-Fuming Nitric Acid - Kerosene, Red - Fuming Nitric Acid – MMH (Monomethylhydrazine, $CH_3N_2H_3$), Red-Fuming Nitric Acid – UDMH (1,1 - dimethylhydrazine), Nitrogen Tetroxide – MMH (Monomethylhydrazine, $CH_3N_2H_3$), Nitrogen Tetroxide-Aerozine 50, Hydrogen Peroxide-Kerosene.

Taking into account significant design criteria, such as: minimizing costs, enhancing operational safety, more environmental friendly, from all the above mentioned combinations, there are best fit: Liquid Oxygen - LOX as oxidizer and Kerosene $C_{12}H_{26}$, Liquid Methane CH_4 and Ethyl Alcohol CH_3CH_2OH.

Experimental part

The experimental data obtained by Aerojet Rocketdyne (which was previously known as Pratt & Whitney Rocketdyne, during 2005-2013, and before that, as Rocketdyne Division) were concluded such as to express the performances of rocket propellant combinations, [Huzel].

The JANNAF Rocket Engine Perormance Prediction and Evaluation Manual [JANNAF], gives thorough information regarding the mathematical algorithms customized for numerical simulations of all types of jet propelled engines. Relevant to this topic, can be approached investigations for complex and intricate phenomena, such as:

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propellant atomization, mixing, evaporation, chemical reaction, gas expansion, as well as effects (e.g. chemical reaction rates, and boundary-layer and streamline and velocity-vector divergence in the converging and diverging nozzles) intended to a more accurate description of real phenomena.

Thrust evaluation or thrust prediction at different flight regimes, as well as the analysis of flight dynamics, trajectory optimization are important tasks for both the design and performance analysis of liquid propelled rocket engines; in such context, of crucial interest are the Propellant Combustion Charts, Braeunig, 2005 [1], which provide graphically the correlations between the chamber pressure p_c, exit pressure conditions p_e (i.e. burned gas expelled at ambient pressure or in vacuum) and mixture ratio r (which expresses the ratio of Oxygen to Fuel O/F), adiabatic flame temperature T_c (also referred as the Chamber Temperature), gas molecular weight M_w and specific heat ratio γ, (also referred as the adiabatic power coefficient), for different types and combinations of fuel and oxidizer, Braeunig [1].

The research presented in this paper is focused on the LOX - Kerosene combination, with the consideration of the LOX - Kerosene Charts (Liquid Oxygen and Kerosene (n-Dodecane, $C_{12}H_{26}$)), which are shown in Fig. 1 ÷ Fig. 4; [1].

The importance of the Propellant Combustion Charts consists in the fact that enables the realistic and accurate prediction of the rocket engines global on- and off-design performances.

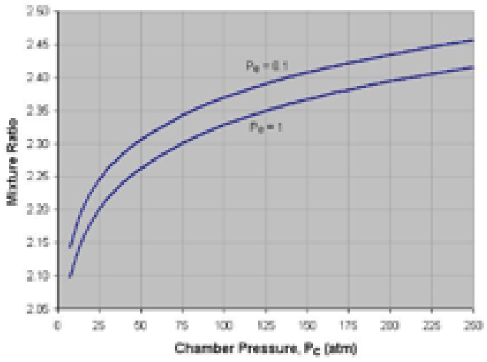

Fig. 1.Optimum mixture ratio, LOX-K, [1]

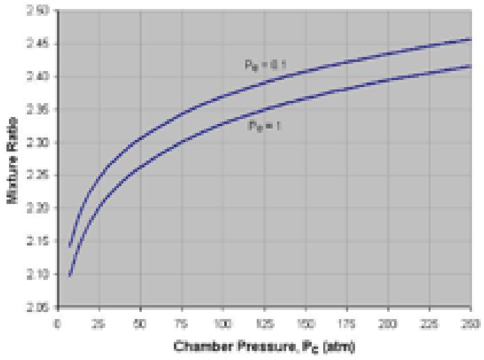

Fig. 2. Adiabatic flame temperature, LOX-K, [1]

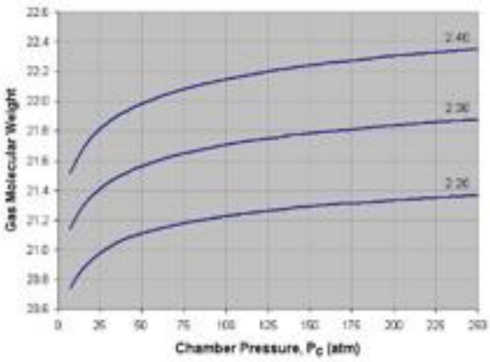

Fig. 3. Gas Molecular Weight, LOX-K, [1]

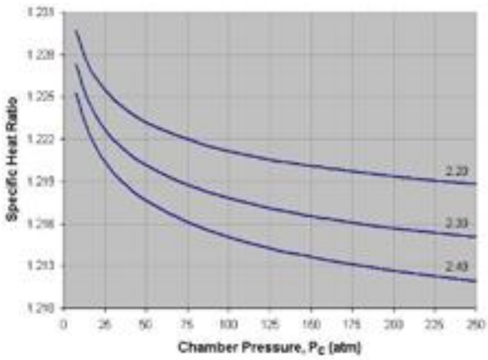

Fig. 4.Secific Heat Ratio, LOX-K, [1]

Results and discussions

For the development of efficient codes and their optimization, the Fuel Combustion Charts must be frequently called. For processing a large amount of data, a significant reduction of the computation time can be obtained by replacing the nodal read input sequnces with the call of an unique two-dimensional non-linear approximation function.

In this paper is presented an original approach Andrei I. [4] in order to determine a 2D non-linear approximation function, of two variables: the chamber pressure and the nozzle exit pressure ratio.

The numerical algorithm based on this two variable approximation function is more efficient due to its simplicity, capability to providing numerical accuracy and prospects for increased convergence rate of the optimization codes.

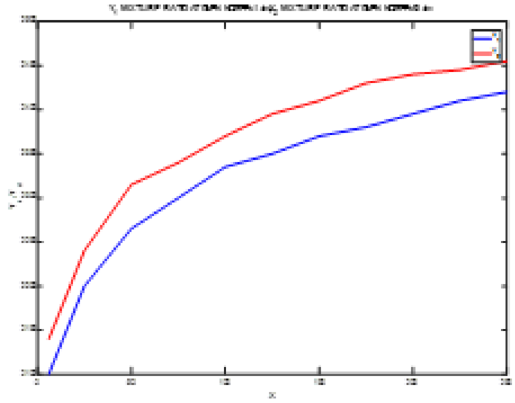

Fig. 5. Mixture ratio versus pressure chamber, for given pressure exit: a) 1 [atm], b) 0.1 [atm]

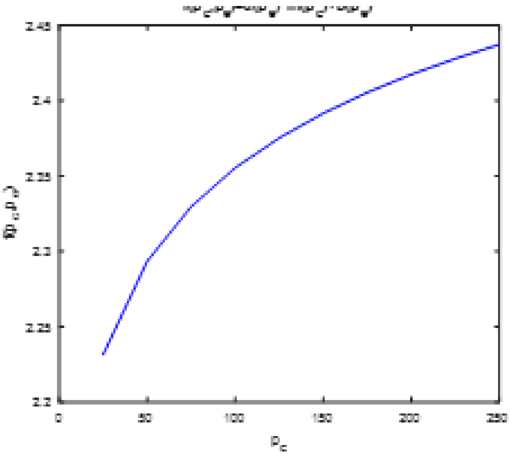

Fig. 6. 2D non-linear approximation function for mixture ratio versus pressure chamber, and nozzle pressure exit: a) 1 [atm], b) 0.1 [atm]

The first step of the proposed methodology, Andrei I. [4] is completed by the determination of the non-linear single variable approximation functions, Berbente [8], Hure & Pelat [9], Jedrzejewsky [10], Chapra [11], Press, Teukolsky, Vetterking & Flannery [12], Chasnov [13], which are verified and shown graphically in Fig. 5; in blue contour is the non-linear approximation determined for the nozzle exit pressure = 1 [atm], and in red contour is the one corresponding to the nozzle exit pressure = 0.1 [atm].

Basically, for determining the non-linear single variable approximation functions, Andrei I. [4], has been used a non-linear curve fitting instead of linear regression, Andrei I. [13-14], thus being provided an improved numerical accuracy for the least squares approximation method, Andrei I. [4, 13-14].

The nozzle exit pressure is considered as given constant, while the chamber pressure is an input variable.

The second step consists in determining the non-linear two-variable approximation function (1), Andrei I. [4], as shown in Fig. 6 and its verification. In this case, both nozzle exit pressure and chamber pressure are input variables.

$$f(p_c, p_e) = a(p_e)\ln(p_c) + b(p_e) \qquad (1)$$

The new function (1), Andrei I. [4] can generate all the values for the mixture ratio, for all combinations of the two variables: chamber pressure and nozzle exit pressure. The most important advantage provided by the new expression for the 2D non-linear approximation function (1) consists in the fact that it can be used in a very simple manner for all the variations ilustrated in Fig. 1-Fig. 4, for all types of propellants, which are presented in the Propellant Combustion Charts [1].

From practical use, errors in reading input data from given graphics (e.g. Fig. 1-Fig.4), can occur, Fig. 5. But, another important advantage of the new function (1) consists in smoothing the errors introduced when reading input data from given graphics, thus the numerical accuracy being successfully improved.

Since the liquid propelled rocket engine LPRE is a very complex product, its adequate design requires succesive iterations and further optimization. The most important is the aero-thermodynamic analysis, with a focus on sizing the exhaust nozzle and the combustion chamber.

Next, the aero-thermodynamic analysis will continue on two basic directions:

1)- determining the performances (i.e. engine thrust) for the liquid propelled rocket engine LPRE for the design regime and for all off-design regimes, Huzel & Huang [2], Sutton & Biblarz [3];

2)- engine control and throttleability, Sutton & Biblarz [3], Casiano, Hulka & Yang [7].

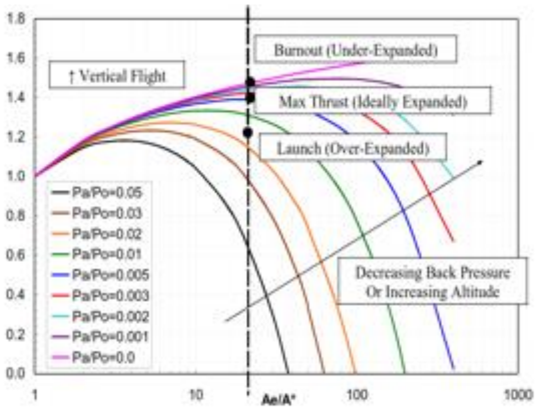

Fig. 7. Correlations between geometrical parameters of LPRE with Bell nozzle and operational conditions of the flight and aero-thermodynamical parameters

From the standpoint of LP rocket engine control, the controllable physical parameters of the rocket engine are, Huzel & Huang [2], Sutton & Biblarz [3], Casiano, Hulka & Yang [7]:

- Propellant flow rates,
- Propellant types, composition and the chemical properties,
- Nozzle exit area,
- Nozzle throat area.

The Throttling Critical Issues are:

- Combustion and system instabilities
- Performance degradation
- Excessive heat transfer
- Pump dynamics.

The geometrical solution following the iterative design of the liquid propelled rocket engine LPRE is successively improved Huzel & Huang [2], Sutton & Biblarz [3], after investigating operational conditions of the flight, in correlation with the vehicle flight dynamics, Balesdent [5-6].

Fig.ure7 illustrates the correlation between the ratio of nozzle exit area A_e to throat area A^* and ratio of ambient pressure to nozzle exit pressure.

The liquid propelled rocket engine LPRE can be designed Huzel & Huang [2], Sutton & Biblarz [3], with different types of nozzles; the most used are the conical nozzle (due to its simplicity construction, technology solution, manufacturing and maintenance) and the Bell shaped nozzle (which can be further optimized for a better adaptability to the operational conditions, with minimal pressure losses, due to shock wave interaction, boundary layer separation and/ or re-attachment.

In Figure 8 are detailed the geometrical parameters of the Bell nozzle.

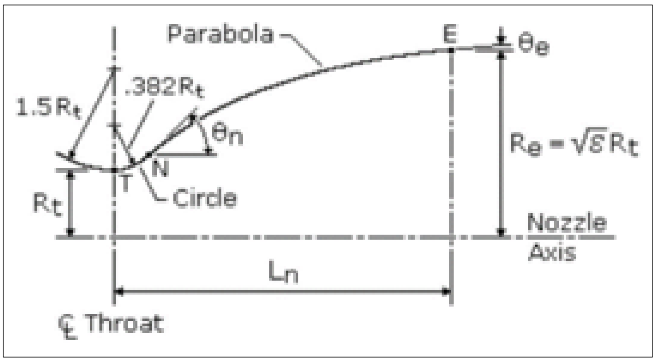

Fig. 8.Geometrical parameters of Bell nozzle [2]

The design of the main parts of the liquid propelled rocket engine LPRE, i.e. the combustion chamber and the nozzle is influenced in great extent by the fluid types considered to cross the engine, which involve different values in sizing the length of both the chamber and the nozzle.

Following a current state of art, it was highlighted significant variation of the combustion chamber characteristic length, Huzel & Huang [2] with the consideration of the propellant combination, as listed in Table 1.

Table 1
CORRELATION BETWEEN LIQUID PROPELLED ROCKET ENGINE FUELS TYPESAND THE CHAMBER CHARACTERISTIC LENGTH, HUZEL & HUANG [2]

Propellant combination	L* [cm]
Nitric acid/ hydrazine-base fuel	76-89
Nitrogen tetroxide / hydrazine-base fuel	76-89
Hydrogen peroxide / RP-1 (including catalyst bed)	152-178
Liquid oxygen / RP -1	102-127
Liquid oxygen / ammonia	76-102
Liquid oxygen / Liquid hydrogen (GH_2 injection)	56-71
Liquid oxygen / Liquid hydrogen (LH_2 injection)	76-102
Liquid fluorine / Liquid hydrogen (GH_2 injection)	56-66
Liquid fluorine / Liquid hydrogen (LH_2 injection)	64-76
Liquid fluorine / hydrazine	61-71
Chlorine trifluoride / hydrazine-base fuel	51-89

A relevant example considered to support this study is the application consisting in the design of a Bell exhaust nozzle for a liquid propelled rocket engine LPRE, with the propellant combination Liquid oxygen / RP -1, intended to develop at design regime the thrust (2), (2.1) and the ratio (3) of exhaust nozzle area to throat area being (3.1):

$$F_T = \dot{m}v_e + (p_e - p_a)A_e \quad (2)$$

$$F_T = 2000\ [N] \quad (2.1)$$

$$\varepsilon = \frac{A_e}{A^*} \quad (3)$$

$$\varepsilon = 20 \quad (3.1)$$

Other input data are: the propellant flow rate $q = 0.615\ [kg/s]$, the chamber pressure $p_c = 25[bar]$, exit velocity $V_e = 3.251[km/s]$ at operating altitude $H = 20\ [km]$.

The engine considered for this study is of type pressure-fed cycle, because this architecture represents the system with simplest construction, since it does not have pumps or turbines, but instead relies on tank pressure to feed the propellants into the main chamber. In practice, the cycle is limited to relatively low chamber pressures because higher pressures make the vehicle tanks too heavy. The cycle can be reliable, given its reduced part count and complexity compared with other systems.

The optimization of engine thrust (2) is carried on according to the balance the nozzle exit pressure p_e and the ambient pressure p_a; the altitude ranges from 0 up to 20 [km], where the ambient pressure is low, $p_a = 0.0432\ [bar]$.

The Bell shape nozzle is functionally efficient, due to the fact that allows to minimize or to avoid the boundary layer separation; the Bell nozzles can be further improved by shortening their length to 80%, thus reducing the weight and global dimensions, without the damaging the aerodynamic properties of the LPRE.

From the Propellant Combustion Charts [1], for the propellant type: Liquid Oxygene (LOX) and kerosene (RP-1), resulted the following: combustion temperature $T_c = 3470\ [K]$, which ranges from 2500 up to 3600 [K], molecular weight for the oxygene = 21.4 [kg/kmol], specific heat ratio k = 1.221, and chamber pressure p_c, usually ranging from 7 up to 250 [bar], but restricted up to 50 [bar], in case of pressure-fed cycle LPRE.

Nozzle sizing satisfyies the condition (4) for thrust (2) optimization at operating altitude, meaning that the nozzle exit pressure p_e should match the ambient pressure p_a. Other situations are the underexpanded nozzle, specified by the condition (5) and the overexpanded nozzle, given by condition (6):

$$p_e = p_a \quad (4)$$

$$p_e < p_a \quad (5)$$

$$p_e > p_a \tag{6}$$

The thrust optimization supposes the determination of the optimal values of the chamber pressure, which results from the calculations performed for different values considered for the chamber pressure:

$$p_c \in \{7,10,20,30,40,50\} \text{ [bar]}.$$

Other connecting results:

The controlling pressure ratio:

$$\frac{p_e}{p_c} = \frac{p_a}{p_c} = \frac{0.00432}{20} = 0.00216 \tag{7}$$

The ratio of throat area to exit area:

$$\frac{A_t}{A_e} = \left(\frac{k+1}{2}\right)^{\frac{1}{k-1}} \cdot \left(\frac{p_e}{p_c}\right)^{\frac{1}{k}} \cdot \sqrt{\left[\frac{k+1}{k-1}\right] \cdot \left[1 - \frac{p_e}{p_c}\right]^{\left[\frac{k+1}{k}\right]}} \tag{8}$$

$$\frac{A_t}{A_e} = 0.03209 \tag{9}$$

Throat temperature $T_t = 3154.5\ [K]$

$$T_t = \left[\frac{2}{k+1}\right] T_c \tag{10}$$

Throat pressure $p_t = 11.289479\ [bar]$

$$p_t = p_t \cdot \left[\frac{k+1}{2}\right]^{\left[-\left[\frac{k}{k-1}\right]\right]} \tag{11}$$

Ideal exit velocity $V_e = 3218.944 \cong 3219\ \left[\frac{m}{s}\right] = 3.219\ \left[\frac{km}{s}\right]$

$$V_e = \sqrt{2 \cdot \left[\frac{k}{k-1}\right] \cdot R \cdot T_c \left[1 - \frac{p_e}{p_c}\right]^{\left[\frac{k-1}{k}\right]}} \tag{12}$$

where:

- $\mathcal{R} = 8314.4621\ [J/kmolK]$ is the universal gas constant
- R (13) is the gas constant for the fuel: RP-1 (kerosene)
- $\mathcal{M} = 388.5\ [kg/kmol]$ is the molecular weight for kerosene;

$$R = \frac{\mathcal{R}}{\mathcal{M}} \tag{13}$$

Equivalent velocity: c [m/s], $c = V_e$.

Specific impulse: I_{sp} [s]:

$$I_{sp} = \frac{c}{g_0} \tag{14}$$

$$I_{sp} = 328.41\ [s] \tag{14.1}$$

The gravitational acceleration is (15):

$$g_0 = 9.80665\ [m/s^2] \qquad (15)$$

Rate of mass ejected q [kg/s] (16)

$$q = \frac{F_T}{c} \qquad (16)$$

$$q = \frac{F_T}{c} = \frac{2000}{3219} = 0.621311 \qquad (16.1)$$

Throat area $A_t [m^2]$ (17)

$$A_t = \left(\frac{q}{p_c \cdot 10^5}\right) \cdot \sqrt{\frac{(R \cdot T_c)}{\left[k \cdot \left[\frac{2}{k+1}\right]^{\left[\frac{k+1}{k-1}\right]}\right]}} \qquad (17)$$

Exit area $A_e [m^2]$ (18) is obtained from the throat to nozzle exit area ratio ε and the throat area A_t:

$$A_e = \frac{A_t}{\varepsilon} \qquad (18)$$

Throat diameter (19) and nozzle exit diameter (20):

$$d_t = \sqrt{\frac{4 \cdot A_t}{\pi}} \qquad (19)$$

$$d_e = \sqrt{\frac{4 \cdot A_e}{\pi}} \qquad (20)$$

As a verification, the ratio ε (21) is the square of exit radius to throat radius ratio, (21); then, the iterative process is resumed, from a recalculating the pressure chamber.

$$\varepsilon = \left(\frac{d_e}{d_t}\right)^2 \qquad (21)$$

The results of the calculations are concluded by the design of the bell shaped nozzle and combustion chamber, illustrated in Figure 9.

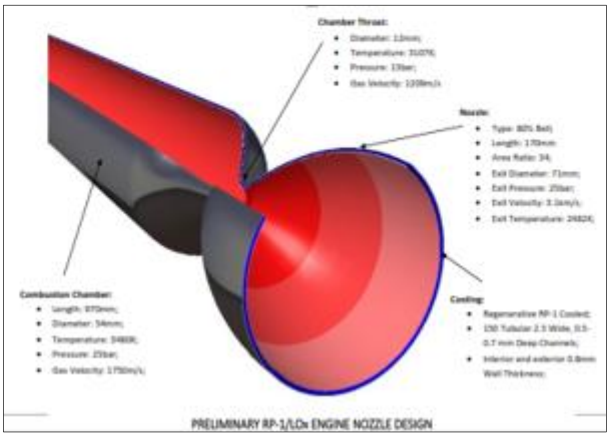

Fig. 9. Geometrical parameters of Bell nozzle [2]

An example of liquid propellant rocket engine LPRE design is summarized in Tables 2, 3 and 4.

Table 2
RESULTS FROM THE DESIGN OF A LIQUID PROPELLED ROCKET ENGINE LPRE

Parameter	Units IS	Value
Thrust	N	2000
Time of burning	s	302
Operational altitude	km	20
Velocity at operational altitude	Km/s	3.252
Propellant	Kerosene (RP-1)	
Oxidizer	Liquid Oxygene (LOX)	
Combustion chamber pressure	Bar	25
Mixture ratio	---	2.35
Combustion chamber Temperature	K	3470
Specific Impulse	s	331.6
Propellant Mass Flow	Kg/s	0.184
Oxidizer Mass Flow	Kg/s	0.431

Table 3
RESULTS FROM THE DESIGN OF THE LPRE EXHAUST NOZZLE (NOZZLE SHAPE = 80% BELL NOZZLE)

Parameter	Units IS	Value
Area ratio	---	37.5
Chamber throat diameter	mm	24
Nozzle exit diameter	mm	145
Nozzle length	mm	170
Nozzle exit temperature	K	2482
Nozzle exit pressure	Bar	0.05
Exhaust velocity	Km/s	3.252

Table 4
RESULTS FROM THE DESIGN OF THE LPRE COMBUSTION CHAMBER

Parameter	Units IS	Value
Combustion chamber diameter	mm	24
Chamber length	mm	970
Throat temperature	K	3155
Throat fluid pressure	Bar	13
Throat fluid velocity	Km/s	1.2

Conclusions

The fuels types and chemical properties have been integrated in the design LPRE, by the means of the following:

-Propellant Combustion Charts, where the molecular weight, ratio of specific heats, mixture ratio, adiabatic flame temperature, have been specified in correlation with the pressure chamber and nozzle exit pressure;

-The new determined function (1) can replace the Propellant Combustion Chart, for all types of fuels and their chemical properties; the major advantage resides in significant reduction of computer time, by calling one two-dimensional non-linear function, instead of reading vectors of nodes and calculating at each iteration new spline function;

-For an adequate design and further its optimization, it is necessary to investigate state of art and to use knowledge and databases which present correlations of geometrical parameters, sizes of LPRE parts and types of fuels and their chemical properties, which have been obtained from experiment and previous LPRE design history.

-Further, the integration of fuel types and chemical properties is very important and relevant in determining the thrust and the remaining performances of the LPRE, at the design regime and all off-design regimes; and also, for LPRE control and throttleability, Casiano, Hulka & Yang [7].

-From the standpoint of LP rocket engine control, from the list of the controllable physical parameters of the liquid propelled rocket engine LPRE, aside the fuel types and chemical properties, the propellant chemical composition plays a major part.

-The integration of fuel types, chemical properties and composition are very important and their appropriate consideration in monitoring LPRE throttle critical issues, influences the numerical accuracy in large extent.

The shape of the new function can be successfully used to generate all the values for fuel properties, for all the combinations of the two variables, meaning the chamber pressure and nozzle exit pressure. An other significant advantage of the new function consists in the ability to smoothen the errors introduced when reading input data from given graphics, thus the numerical accuracy being improved in a highly extent.

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