Numerical Simulation of Liquid Propellant Rocket Engines

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Abstract - The development of liquid propellant rocket engines requires tests and dynamical simulations of all its elements in a computer environment. With the advances of the numerical methodologies, particularly of the implicit schemes, the solution of flow problems which require real gas modeling became also feasible by the end of last century. Many research activities are devoted to the numerical simulation of combustion and particularly to flame modeling, being quite important for the development of low emission rocket engines. We present the first results of our developed code that simulates a liquid propellant engine. The code was developed in a modular structure, simulating structural elements such as the combustion chamber, injector, nozzle supersonic, valves and piping and pumping system. Each of these elements was modeled and numerically coded in C++. The elements can be chosen in such a way that many different engine configurations can be evaluated, with different combinations of propellant and oxidant. We present results for a green propellant combination, where alcohol (ethanol) was used together with liquid oxygen and hydrogen peroxide. As a result one can appreciate the evolution of fluxes, pressures, temperatures and other important variables as a function of time.

I. INTRODUCTION

During the middle years of the XX century, mostly the main development of rocket engines took place. Today, one can consider we achieved a mature stage in this subject. Actual rocket engines are the epitome of rocket design. While design and projects from the 1960s are still flying, the needs of the new century, mostly commercial, are pushing the development of rocket engines, which appear worldwide in significant numbers and concepts [1].

Included in the actual approach are the green concerns, and these preoccupations lead to choices of combustibles that contribute to lower levels of atmospheric pollution. One of the candidates is the hydrogen peroxide, whose catalytic decomposition is in agreement with our ecological interests.

The hydrogen peroxide presents some characteristics that lead to a very interesting choice for utilization in propulsive systems [2]. About this composite, the main points are: 1) versatility: the hydrogen peroxide can be used as monopropellant and as oxidant in pre-mixed bipropellant systems; 2) higher density when compared to the majority of propellants, leading to a smaller reservoir volume and consequently a higher mass for the payload; 3) smaller toxic potential (much less toxic than hydrazine or nitrogen tetra oxide); 4) higher oxidant/combustible ratio; 5) long time storage; 6) compatibility with low cost reservoir materials, as aluminum and stainless steel; 7) low cost when compared to other combustibles; 8) easily available in Brazil.

This work presents a model developed to simulate a thrust chamber based on the catalytic decomposition of the hydrogen peroxide. All physics and chemistry are included, like heat transfer, gaseous latent decomposition, and also the other rocket engine components, like pipes, valves and orifice injectors, each component with its own contribution to load loss.

II. THE MODEL

A. Ideal Catalytic Thrust Chamber

As presented by [3], the ideal thrust catalytic chamber design must be based on the following assumptions: 1) ideal gas; 2) the temperature inside the combustion chamber is uniform; 3) the thrust chamber is adiabatic; 4) the propellant is injected, gasified and decomposed instantly; 5) one-dimensional flow; 6) the decomposition reaction is an exclusive function of the catalytic; 7) the thermo chemical properties of gases decomposition are functions uniquely of the chemical compositions of the propellant and the catalytic; 8) the catalyst is incompressible.

It is worth noting that this engine’s combustion chamber is filled with a fixed catalytic bed and is not stagnant, there is a pressure gradient over the entire bed, so it is convenient to divide the chamber as sketched in the fig. 1.

The mean pressure rate, \( P_C \), as a function of time, \( t \), in the chamber for the monopropellant system is modeled...
by the expression [4]
\[
d\frac{\rho C}{dt} = \frac{RT_p}{ML^* A_T} \left( F_p \rho_p - \frac{P_2 A_T}{C^*} \right),
\]
where \( F_p \) is the propellant flow, \( \rho_p \) is the propellant density, \( T_p \) is the chamber temperature, \( M \) is the Mach speed, \( L^* \) is the characteristic length of the chamber, \( A_T \) is the throat area, \( P_2 \) is the stagnation pressure, \( R \) is the perfect gas constant and the characteristic speed, \( C^* \), is given by
\[
C^* = \sqrt{\frac{\gamma RT_p}{M}} \left( \frac{2}{\gamma (\gamma - 1)} \right)^\frac{\gamma + 1}{\gamma - 1},
\]
where \( \gamma \) is the ratio of specific heats, \( P_2 \) is related to the pressure at point 2 (see figure 1), \( P_2 \), by
\[
P_2 = P_1 \left[ 1 + \left( \frac{\gamma - 1}{2} \right) M_2^2 \right]^{\frac{1}{\gamma - 1}},
\]
where \( M_2 \) is the Mach speed in 2. At this point, it is important to remember that when \( M_2 < 1 \), it is valid
\[
M_2 = A_T \left( \frac{2}{\gamma + 1} \right)^{\frac{1}{\gamma - 1}},
\]
where \( A_T \) is the chamber section area. \( P_C \) is related to the loss of pressure due to the catalytic bed, \( \Delta P_C \) by
\[
P_C = P_1 - \frac{\Delta P_C}{2},
\]
where \( P_1 \) is the pressure in the entry of the thrust chamber. The decomposition gases thermo chemical properties are represented by functions dependents only on the propellant chemical composition and the oxidant/fuel mixture ratio (O/F) and the catalytic, or \( T = T_e (\text{propellant, O/F}) \). It is convenient to define a thrust coefficient, \( C_p \), as ([4])
\[
C_p = \sqrt{\frac{2 \gamma^2 (\gamma - 1)}{\gamma - 1}} \left[ 1 - \left( \frac{P_2}{P_1} \right)^\frac{\gamma - 1}{\gamma} \right] + \left( \frac{P_2 - P_1}{P_2} \right) \frac{A_T}{A_T},
\]
where \( P_1 \) is the pressure in the outlet section under optimal conditions and \( A_T \) is the output section area.

**B. Pressure losses in the catalytic bed**

The catalytic bed is made of particles of generic geometry (like dust), with well known sizes, packed in the thrust chamber interior. As can be seen in fig. 1, the catalytic bed is composed by two layers. The first one (formally represented by index 1) is made of particles with smaller effective diameter and the second (index 2) is made by particles with greater effective diameter. Then, the pressure loss due to the bed, following [5], can be represented by
\[
\Delta P_C = \Delta P_C + \Delta P_C = \frac{f_1 L_1 \rho v_b (1 - \varepsilon) \rho C}{D_1 \varepsilon^3} + \frac{f_2 L_2 \rho v_b (1 - \varepsilon) \rho C}{D_2 \varepsilon^3},
\]
where \( v_b \), the superficial speed, is given by \( v_b = F_p \rho / A_{CL} \rho C \), and the particle effective diameter is defined by \( D = 6 \varepsilon S \). Other important parameters, \( \varepsilon \), the porosity of the bed, \( f_1 \) the friction losses factor, \( f_2 \) the bed length, and \( S \), the specific surface of a representative particle, are all known parameters.

**C. Catalytic thrust chamber with mass transport effect**

The monopropellant injected in the chamber do not decomposes instantly. Initially as a liquid, it goes to gaseous through two basic mass transfer processes: vaporization and diffusion. The propellant decomposes after assuming the gaseous form. The diffusion is a result of the concentration gradient from the liquid monopropellant and the medium, composed by decomposition gases.

On the other hand, the vaporization occurs as a consequence of the heat change between the liquid propellant and the decomposition gases and the catalytic bed. To model these phenomena it is necessary to apply the energy conservation principle, based on the following hypotheses: 1) there is only convective heat transfer; 2) the heat flux is one-dimensional; 3) the gases resulting from catalytic decomposition are stagned; 4) the chamber is adiabatic; 5) the monopropellant specific heat is constant; 6) there is no temperature gradient inside the catalytic; 7) the contact surfaces gas/catalytic and gas/liquid are equivalent. With these assumptions, one can obtain an expression for the mass transfer rate from liquid to gas:
\[
\frac{dm}{dt} = F_p \rho - \left( \frac{dm}{dt} + \frac{dm}{dt} \right),
\]
where \( m_v \) is vapor mass, \( m_0 \) is the mass from the decomposition and \( \rho_0 \) is the density of propellant. The liquid temperature is given by
\[
\frac{dT}{dt} = \frac{F_p \rho_e c_p (T_p - T_1)}{m_{pl} c_p} + \frac{\eta_s (T_e - T_1)}{m_{pl} c_p} + \frac{m_v}{m_{pl} c_p} \left( c_v T_v - H_v \right) + c_v T_v \frac{dm_v}{dt},
\]
where $c_H$ is the propellant specific heat, $T_F$ is the temperature the propellant is injected in the chamber, $T_C$ is the instantaneous chamber temperature and $H_t$ is the vapor heat.

D. Monopropellant diffusion

The liquid monopropellant is injected in the catalytic chamber and involves the catalyst grains. The combustion occurs in a gaseous thin layer between the two reactants. This phenomenon is modeled by applying the mass conservation principle under the following hypotheses ([15]) 1) the gases resulting from catalytic decomposition are stagnant; 2) the chamber is adiabatic; 3) the contact surfaces gas/catalyst and gas/liquid are equivalent; 4) the liquid properties are constant; 5) the pipe systems offer no resistance to the flow. These assumptions lead to an expression of the volume flow through the pipes and other duct accessories.

$$\frac{dm_D}{dt} = (k_{p1}S_1 A_L + k_{p2}S_2 A_L - \xi \Delta P) \frac{P_M}{RT}$$

where $k_{p1}$ and $k_{p2}$ are coefficients of mass transfer by diffusion for each kind of particle, $S_1$ and $S_2$ are the specific surfaces of each catalyst grain, $L_1$ and $L_2$ are the length of each catalyst bed, $P_c$ is the pressure in the catalytic bed, $P_M$ is the initial liquid mass in the chamber, and $T_3$ is the temperature at the surface of the catalyst.

E. Pipes, injectors and other duct accessories

The liquid propellant is conducted from its reservoir to the thrust chamber through specific pipes, and other devices like valves, sensors and joints (the duct accessories), all of fundamental importance for the proper operation of the engine [6]. The main accessories are the valves, responsible for flow control, and the orifice plates, that give the fine adjust of the flow. The hypotheses used to model the pipes system and accessories are: 1) the liquid propellant is incompressible; 2) the flow is one-dimensional; 3) the pipes and accessories are adiabatic; 4) the propellant properties are constant; 5) the pipes offer no resistance to the flow. These assumptions lead to an expression of the volume flow through the pipes and accessories:

$$\frac{dF}{dt} = [P_F + P_{HP} - \Delta P_{HP} - (P_1 + \Delta P_1) \frac{A_0}{\rho_1 L}]$$

where $P_F$ is the pressure due to the pressurizing gas, $P_{HP}$ is the propellant hydrostatic pressure, and $\Delta P_{HP}$ is the load loss in the propellant reservoir. $P_1$ is the pressure on point 1 (see figure 1) and the input of the chamber. $\Delta P_1$ is the load loss due to accessories, obtained by each component characteristic, $f_a$ represents the friction forces in all the pipe system, $\rho_1$ is the density of the liquid propellant, $L$ is the length of the pipes and $A_0$ is the area of one injector orifice. $\Delta P_1$ is the load loss in the propellant injector, given by

$$\Delta P_1 = \frac{\rho_F^2}{2C_D^2(\sum A_{ni})^2}, \quad \text{(11)}$$

where $\Sigma A_{ni}$ is the total area of the injector orifices and $C_D$, the discharge coefficient, is chosen according to tab. 1.

### III. NUMERICAL TECHNIQUES

The mathematical model presented in section 2 is mostly based on first order ordinary differential equations that compose a differential equation system, being time the main integration parameter. The code considers all variables with SI units.

We choose the 4th order Runge-Kutta method to integrate the system, due to its robustness, speed and simplicity to code. The algorithm was written in C++ language and the time step management is done dynamically, such as the integration of the physical equations is done properly [7].

Many coding details are beyond the scope of this work. Anyway, [8] provides useful information and techniques that were used in the code, and we suggest a deep lecture to the reader interested in going by this way.

### IV. RESULTS

The method looks for the values of the main control parameters as a function of time, like thrust, pressure in the chamber, propellant mass flow and load loss in the catalytic bed providing a solution for the model equations that reproduces the behavior of our rocket engine. We made simulations for a 10.5 N thrust engine and the initial values of the parameters are those that should be observed in quiescent state at normal atmosphere and normal pressure. Figs 2 to 5 present the behavior of these parameters since the ignition until the first tenth of second.

As can be seen, the model coded simulates the initial transients, going to a stabilized (or quiescent) regime after 0.015 s. It can be observed a propellant peak flow of about 13.5 g/s in t~0.002 s. This is due to the high speed when opening the propellant feed valve and also results in an increase of pressure in the thrust chamber.

<table>
<thead>
<tr>
<th>Geometry of injector orifice</th>
<th>Diameter (mm)</th>
<th>Discharge coefficient $C_p$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Conic output</td>
<td>&gt; 2.50</td>
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</tr>
<tr>
<td></td>
<td>&lt; 2.50</td>
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<td></td>
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<td>0.90</td>
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<tr>
<td>Short tube with spiral effect</td>
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<td>0.20</td>
</tr>
<tr>
<td></td>
<td>6.4</td>
<td>0.55</td>
</tr>
</tbody>
</table>

TABLE I. DISCHARGE COEFFICIENT FOR VARIOUS INJECTOR ORIFICES AND SIZES
The catalytic bed plays a very important role in smoothing the initial oscillations in pressure and flow, enabling a steady regime in about 0.015 s. Tab. 2 summarizes our results.

V. CONCLUSION

We presented a model that simulates a thrust chamber based on the catalytic decomposition of the hydrogen peroxide. The model is complete in the sense that all physics and chemistry were included and also important rocket engine components, like pipes, valves and orifice injectors.

The simulation results are in concordance with what is expected from the engine design, and show that the model is well defined, and can model the engine under a great number of conditions. The pre-mixed hydrogen peroxide use as a monopropellant simplifies greatly the engine design and also the mathematical model, simplifying the code.

This engine model was applied in an actual project with results that coincide in many details with these simulations.

ACKNOWLEDGMENTS

The authors want to thank AEB – Agência Espacial Brasileira / Programa UNIESPAÇO and CNPq – Conselho Nacional de Desenvolvimento Científico e Tecnológico.
REFERENCES


