COBEM 2021 26th International Congress of Mechanical Engineering

ABCM Associação Brasileira de Engenharia e Ciências Mecânicas
November 22-26, 2021, Virtual Congress, Brazil

# COB-2021-0529
# HEAT TRANSFER ANALYSIS OF A SOLID-PROPELLANT ROCKET COMBUSTION CHAMBER

**José Felipe Alves Avelino**
**Daniel José Nahid Mansur Chalhub**
Group for Studies and Environmental Simulations in Reservoirs (GESAR), Rio de Janeiro State University (UERJ), Rua Fonseca Teles,121, 20940-903, Rio de Janeiro, RJ, Brazil
jfelipeavelino@hotmail.com, daniel.chalhub@eng.uerj.br

***Abstract.*** *The present work aims to obtain the temperature profile of a rocket combustion chamber with solid propulsion without the need of experimental data. The rocket engine consists of a cylindrical chamber containing its respective propellant grain inside, which is a homogeneous mixture of fuel and an oxidizer. For this purpose, the heat of combustion was estimated using a total enthalpy of the chemical reaction. Different portions of this value were considered to estimate the heat flow. It was also necessary to obtain the thermal properties of the propellant grain. Their values were approximated proportionally, depending on their composition. With these data, it was possible to determine the engine temperature profile. The method used was the Generalized Integral Transform Technique (GITT) for a moving boundary. The consumption of the propellant in the radial direction was considered in the mathematical model, causing the eigenvalues and eigenfunctions to vary over time. The temperature distributions were analyzed and it was observed that the propellant acts as a strong thermal insulator for the combustion chamber.*

***Keywords:*** *Integral Transforms, Moving Boundary Model, Rocket Propulsion,Heat Transfer, Combustion*

## 1. INTRODUCTION

For centuries, solving heat transfer problems involving combustion processes has been an enormous challenge for science. It should be noted that problems of this type are not fully understood, as they involve processes of convection and radiation, thus making them extremely complicated to be solved. It is worth mentioning that the study on rocket engines is an example of these cases. Although there are numerous studies targeting them, most are based on inverse problems, using experimental data to obtain the heat flux.

The rocket engine is a cylindrical chamber charged with fuel, which causes the combustion process to appear inside. Such a procedure causes an extreme increase in pressure, and, consequently, the accumulation of gases inside are expelled at high speed through the nozzle. According to Sutton and Biblarz (2010), about 5% of the heat generated is converted into thermal energy for the material, and the rest in kinetic energy in the nozzle. However, this small percentage can cause catastrophic failures in its structure. For this reason, the study of heat transfer is extremely important, in order to obtain the necessary temperature range for choosing the most efficient materials for the project.

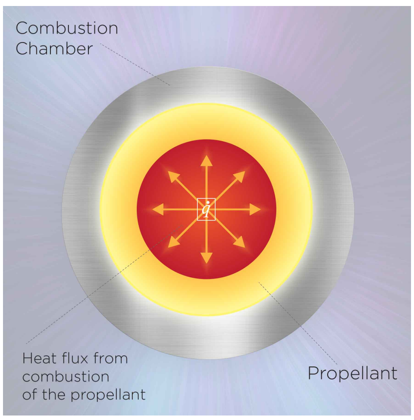


Figure 1. Heat transfer process in the combustion chamber

In this sense, the use of experimental data is an excellent alternative to obtain the heat flux. However, testing the engine to obtain these data can be much more expensive. This happens because some materials cannot be reused, such as fuel, as well as the engine itself. It is important to highlight that without knowledge of the temperature profile, it is possible to erroneously choose the material, which can result in catastrophic failures in the project. Thus, it is observed that this theme lacks a direct approach, in order to obtain the temperature profile of the engine instead of using experimental data.

The use of experimental temperature data to determine temperature profiles and estimate heat fluxes over time is called an inverse problem. For the study of heat transfer in rocket engines, numerous authors have relied on this approach for their calculations.

Mehta (1981) calculated the temperature distribution in a nozzle of a rocket by finite differences. Using Newton Raphston's method, the author used experimental data of the internal temperature to determine the heat flux and the temperature of the flue gases.

Nunes (2017) increased the efficiency of the thermal protection of a hybrid engine with the increase in the burn time of the propellant. Through data obtained at external temperature, one author estimated the heat flow values by the method of Mehta (1981). With that, the author selects the temperature distribution curves (internal and external) with time, in two ways: analytically and by the finite element method. In the first one, she used the Hankel-Webber transformer and, in the second one, Nunes did a simulation with Ansys.

Vicentin *et al.* (2019) obtained the heat flux from a rocket combustion chamber to solid propulsion using the inverse method. With temperature data on the outer wall of the engine, the authors used the modified least squares method, developed by adding the zero-order Tikhonov term. This technique is effective for ill-posed problems, which often occurs in reverse problems. The sensitivity coefficients were obtained by Duhammel's theorem. The authors noted that, despite the experimental errors, their studies showed satisfactory results.

Often the method of separation of variables is not enough to obtain the solution of heat transfer problems in the transient regime. Thus, the integral transform technique is quite useful for transforming the problem into simpler equations to be solved.

Özisik and Murray (1974) noted that there were no effective analytical methods for the transient heat transfer solution. In their work, they presented the Integral Transformation method to solve a problem with position and time-dependent boundary conditions. The problem had non-transformable terms, even though the inversion formula was inserted. This resulted in an infinite coupled system of ordinary differential equations. Thus, they obtained an approximate solution considering only a finite number of equations. This was the starting point for the development of the Generalized Integral Transform Technique, in which it has an analytical-numerical nature

Chalhub (2011) solved several diffusion and comparison problems by comparing two approaches: the Generalized Integral Transformation Technique (GITT) and the Finite Volume Methods (FVM). In addition, the author proposed a mistaken approach, which used a combination of the hybrid method (GITT) and traditional discrete methods such as finite difference methods and the finite volume method itself. The main objective of this combination is that the advantages of these different methods are integrated, thus obtaining more effective solutions to diffusion problems.

Silva (2017) proposes a method to obtain and evaluate the Nusselt number distribution and the temperature profile in the axial flow duct of orthotropic material. With the dimensionless energy equation, the author applies the Generalized Integral Transform Technique. This approach resulted in a system of Ordinary Differential Equations, which were solved using a matrix analytical method. For validation, the results were compared with existing literature.

The present work aims to obtain the temperature profile of a combustion chamber made of 6063 T6 aluminum. The engine is loaded by its respective propellant grain, which, in this study, consists of a homogeneous mixture of Sorbitol (fuel) and Potassium Nitrate (oxidant). Its geometry is cylindrical with a hole in its center, which is extended until the grain is completely consumed. Therefore, its internal radius will vary with time.

## 2. MATHEMATICAL FORMULATION

### 2.1 Heat Equation

The combustion chamber and the propellant have cylindrical geometry. Thus, the problem will be described as a hollow cylinder with the inner and outer radial $R_a$ and $R_c$, respectively. For convenience, it will be considered that the problem has a single domain containing two layers: the propellant grain and the combustion chamber. A schematic of the problem can be seen in Figure 2. According to this, the specific heat $c$, thermal conduction $k$ and density $\rho$ will vary in the intersection radius ($R_b$). Considering only the variation in time ($t$), radial ($r$) and ruling out heat generation, the heat equation becomes:

$$\rho(r)c(r)\frac{\partial T}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(k(r)r\frac{\partial T}{\partial r}\right) \quad \text{for} \quad R_a(t) \le r \le R_c \quad \text{and} \quad t \ge 0 \tag{1}$$

where:

$$k(r) = \begin{cases} k_p, & R_a(t) < r \le R_b \\ k_c, & R_b < r \le R_c \end{cases} \tag{2}$$

$$\rho(r)c(r) = \begin{cases} \rho_p c_p, & R_a(t) < r \leq R_b \\ \rho_c c_c, & R_b < r \leq R_c \end{cases} \tag{3}$$

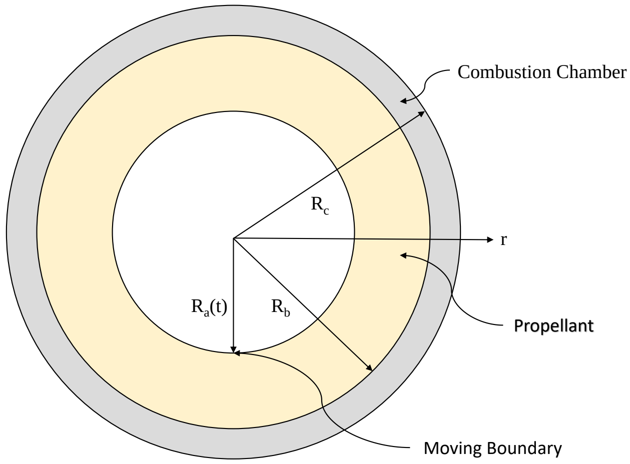


Figure 2. Schematic illustration of the problem

In addition, it is necessary to define the boundary and initial conditions. Internally it will be considered that there is a heat flux from the heat released by combustion. Externally, it will be considered an isolated boundary condition, as the heat flux in this boundary can be neglected in comparison with the former, in addition to low convection heat transfer for low altitudes. According to these settings the boundary and initial condition are as follows:

$$-k_p \frac{\partial T(R_a(t),t)}{\partial r} = \dot{q}''_a(t) \tag{4}$$

$$\frac{\partial T(R_c,t)}{\partial r} = 0 \tag{5}$$

$$T(r,0) = T_{env} \tag{6}$$

where $T_{env}$ is the ambient temperature and $\dot{q}''_a(t)$ is the heat flux from the combustion reaction.

## 3. Solution Methodology

### 3.1 Combustion

One of the fundamental steps for studying the heat transfer of an engine is to understand how the combustion process works, since it is responsible for the heat transfer that will occur through the engine structure.

The combustion process is constituted by an exothermic reaction, in which the oxidation of a fuel occurs. During burning, molecules break down and result in a certain amount of heat release. According to Turns (2011), considering complete combustion, the heat released is calculated by the difference in the enthalpy of the products and reactants.The combustion reaction below was obtained using the "PROPEP" software that determines the chemical equilibrium composition for the combustion of a solid or liquid rocket propellant.

$$14.6C_6H_12O_6 + 48.6KNO_3 \Rightarrow 27.6CO_2 + 36.4CO + 70.2H_2O + 31.2H_2 + 24.4N_2 + 23.6K_2CO_3 \tag{7}$$

To find the enthalpy of products and reagents, it is necessary to have the enthalpy of formation $(h_f)$ and the variation of sensible enthalpy $(\Delta h_s)$ of the molecules. The first is linked to the energy present in the chemical bonds, and the second is associated only with temperature. These enthalpies are associated with a reference temperature that is usually environmental temperature. For this reason, $\Delta h_s$ of the reactants equal to zero if considering the initial temperature as the reference one. Considering a chemical equation with $n_i$ moles of each reactant and $n_f$ moles of each product, the heat combustion equation becomes:

$$Q = \sum_{prod} n_f[h_f + \Delta h_s] - \sum_{reac} n_i[h_f + \Delta h_s] \tag{8}$$

### 3.2 Generalized Integral Transform (GITT)

The problem presented is a Partial Differential Equation (EDP) and one of the alternatives for its solution is the Generalized Integral Transform Method (GITT). The first step in solving the problem addressed would be to develop the appropriate eigenvalue problem for the moving boundary.The solution of the eigenvalue problem in cylindrical coordinates is quite complicated, as it involvse Bessel equations that are extremely complex to be solved. An alternative to avoid such difficulties would be to solve the Sturm-Lioville problem in Cartesian coordinates, despite the original problem being in cylindrical coordinates. In this way, the solution is extremely simplified, as it will result in trigonometric functions.

$$\frac{d^2\psi_n(r,t)}{d^2r} + \lambda^2\psi_n(r,t) = 0 \quad \text{for} \quad R_a(t) \leq r \leq R_c \quad \text{and} \quad t \geq 0 \tag{9a}$$

$$\frac{\partial\psi_n(r,t)}{\partial r} = 0 \quad \text{at} \quad r = R_a(t) \tag{9b}$$

$$\frac{\partial\psi_n(r,t)}{\partial r} = 0 \quad \text{at} \quad r = R_c \tag{9c}$$

The solution of the eiegenfunction $\psi_n(r,t)$ and the eigenvalues $\lambda_n(t)$ terms are given respectively by

$$\psi_n(r,t) = \cos[\lambda_n(t)(r - R_a(t))] \tag{10}$$

$$\lambda_n(t) = \frac{n\pi}{R_c - R_a(t)} \tag{11}$$

The original problem of equation (1) does not have homogeneous boundary conditions like those of the eigenfunctions solved earlier. This is problematic as GITT's method will have difficulties in converging its solution. An alternative to get around this would be to apply a filter term in the original equation to make its boundary conditions homogeneous. The filtered equation with its respective boundary and initial conditions is:

$$\rho(r)c(r)\frac{\partial T^*}{\partial t} + \rho(r)c(r)\frac{\partial F(r,t)}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(k(r)r\frac{\partial T^*}{\partial r}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(k(r)r\frac{\partial F}{\partial r}\right) \tag{12}$$

$$\frac{\partial T^*(R_a(t),t)}{\partial r} = 0 \tag{13}$$

$$\frac{\partial T^*(R_c,t)}{\partial r} = 0 \tag{14}$$

$$T^*(r,0) = T_{env} - F(r,0) \tag{15}$$

where:

$$T(r,t) = T^*(r,t) + F(r,t) \tag{16}$$

$$F(r,t) = \frac{q''(t)r^2}{2k_p(R_a(t) - R_c)} + \frac{R_c q''(t)r}{(R_a(t) - R_c)k_p} \tag{17}$$

$$\dot{q}_a''(t) = \frac{Q_{comb}}{t_{comb}A_{sur}} \tag{18}$$

Solving the eigenvalue problem and applying the filter to the equation, the transformed pair is then defined:

$$\bar{T}^*(\lambda,t) = \int_{R_a(t)}^{R_c} \psi_n(r,t)T^*(r,t)\,dr \qquad \textit{Transform} \tag{19}$$

$$T^*(r,t) = \sum_{n=0}^{\infty} \frac{\psi_n(r,t)}{N_n(t)}\bar{T} \qquad \textit{Inverse} \tag{20}$$

The Norm ($N_n$) is defined by:

$$N_n(t) = \int_{R_a(t)}^{R_c} [\psi_n(r,t)]^2\,dr \tag{21}$$

First, we multiply both sides of equation(12) by $r\psi_n(r,t)$, integrating over the domain.

$$\int_{R_a(t)}^{R_c} \rho(r)c(r)r\psi_n(r,t)\frac{\partial}{\partial t}T^*\,dr + \int_{R_a(t)}^{R_c} \rho(r)c(r)\frac{\partial F(r,t)}{\partial t}\,dr = \int_{R_a(t)}^{R_c} r\psi_n(r,t)\frac{1}{r}\frac{\partial}{\partial r}(k(r)r\frac{\partial T^*}{\partial r})\,dr + \quad (22)$$

$$+\int_{R_a(t)}^{R_c} \frac{1}{r}\frac{\partial}{\partial r}(k(r)r\frac{\partial F}{\partial r}\,dr$$

The first integral on the right is evaluated by integrating by parts once. We usually integrate twice, however the conductivity therm doesn't allow us to do this. The first integral on the left hand side was developed by the product rule and then Leibniz's Rule was applied in one of the terms to simplify it. Applying the inverse of the resulting equation, we obtain the following system of differential equations :

$$\sum_{m=0}^{\infty}\bar{T'}_m A_{n,m}(t) + \sum_{m=0}^{\infty}\bar{T}_m A'_{n,m}(t) + \sum_{m=0}^{\infty}\bar{T}_m B_{n,m}(t) + \sum_{m=0}^{\infty}\bar{T}_m D_{n,m}(t) - \sum_{m=0}^{\infty}\bar{T}_m C_{n,m}(t) + E_n(t) = 0 \quad (23)$$

The initial condition becomes:

$$\bar{T^*}_n(0) = \int_{R_a(t)}^{R_c} \psi_n(r,0)r(T_{env} - F(r,0))\,dr \quad (24)$$

Where the coefficients A, B C, D and E are given by:

$$A_{n,m}(t) = \frac{1}{N_m(t)}\int_{R_a(t)}^{R_c} \rho(r)c(r)r\psi_n(r,t)\psi_m,(r,t)\,dr \quad (25)$$

$$B_{n,m}(t) = \frac{R_a(t)\psi_n(R_a(t),t)\psi_m(R_a(t),t)R'_a(t)}{N_m} \quad (26)$$

$$C_{n,m}(t) = \frac{1}{N_m(t)}\int_{R_a(t)}^{R_c} \rho(r)c(r)r\psi_m(r,t)\frac{\partial}{\partial t}(\psi_n(r,t))\,dr \quad (27)$$

$$D_{n,m}(t) = \frac{1}{N_m(t)}\int_{R_a(t)}^{R_c} k(r)r\frac{\partial\psi_n(r,t)}{\partial r}\frac{\partial\psi_m(r,t)}{\partial r}\,dr \quad (28)$$

$$E_{n,m}(t) = \int_{R_a(t)}^{R_c} \rho(r)c(r)r\psi_n(r,t)\frac{\partial F(r,t)}{\partial t} - \int_{R_a(t)}^{R_c} \psi_n(r,t)\frac{\partial}{\partial r}\left(k(r)r\frac{\partial F}{\partial r}\right) \quad (29)$$

## 4. RESULTS

The results were obtained using the *Wolfram Mathematica* Software (Wolfram, 2003). This software can work with different mathematical expressions quickly and efficiently. In order to solve the system of differential equations (23), the **NDSolve** routine was used (Wolfram, 2003). Furthermore, it is important to highlight that the results were calculated for a hypothetical problem. The problem consists of a 1 meter long cylindrical tube of Aluminum 6063 T6 containing a propellant of the same shape inside. The combustion reaction will take place in approximately 4 seconds. The physical properties of the Propellant and Combustion Chamber are listed in Table 1 and 2, respectively. $H_{reac}$ corresponds to the total enthalpy of the reactants and will be used to estimate the heat transferred to the combustion chamber. As mentioned above, the propelling properties were estimated according to the physical properties of the fuel (Sorbitol) and the oxidant (Potassium nitrate).

Table 1. Physical properties of the Propellant

| Propellant | |
|---|---|
| Fuel | Sorbitol |
| Oxidant | Potassium Nitrate |
| Heat Conductivity (W/m.K) | 8 |
| Density(kg/m$^3$) | 1890 |
| Specific Heat (J/Kg.K) | 1076 |
| $H_{reac}(kJ)$ | -43804.4 |
| $R_a(t)(mm)$ | 20+6.75t |

Table 2. Physical properties of the Combustion Chamber

| Combustion Chamber | |
|---|---|
| Material | Alluminium 6063 t6 |
| Heat Conductivity (W/m.K) | 218 |
| Density(kg/m$^3$) | 2070 |
| Specific Heat (J/Kg.K) | 900 |
| R$_b(mm)$ | 47 |
| R$_c(mm)$ | 50 |

Table 3 shows the heat "Q" released from the combustion in kilojoules (kJ) for different temperatures obtained through equation (8). The enthalpy of formation and sensible data were acquired through the NIST-JANAF Thermochemical Tables((Chase, 1998)) of each element of equation (7). Note that, for the temperature of 1600 Kelvin, it is approximately the adiabatic temperature of the flame, as the released heat approaches zero. For the heat transfer process, different portions of $H_{reac}$ from Table 1 will be used.

Table 3. Heat Combustion

| T(K) | Q(kJ) |
|---|---|
| 2300 | -9458.20 |
| 2200 | -8109.68 |
| 2100 | -6743.20 |
| 2000 | -5383.57 |
| 1900 | -4525.98 |
| 1800 | -2687.67 |
| 1700 | -1352.76 |
| 1600 | -27.5776 |
| 1500 | 1286.84 |
| 1400 | 2589.69 |
| 1300 | 3905.29 |

Figures 3, 4 and 5 show the distribution of propellant/chamber temperature with radius for different time ranges. Firstly, it is observed that the propellant acts as an excellent insulator, as its low thermal conductivity prevents the arrival of heat in the chamber. Even considering a high amount of heat, the propellant protects the chamber most of the time. The truncation used was $n_{max} = 100$ of the expansion of the eigenfunctions in equation (20).

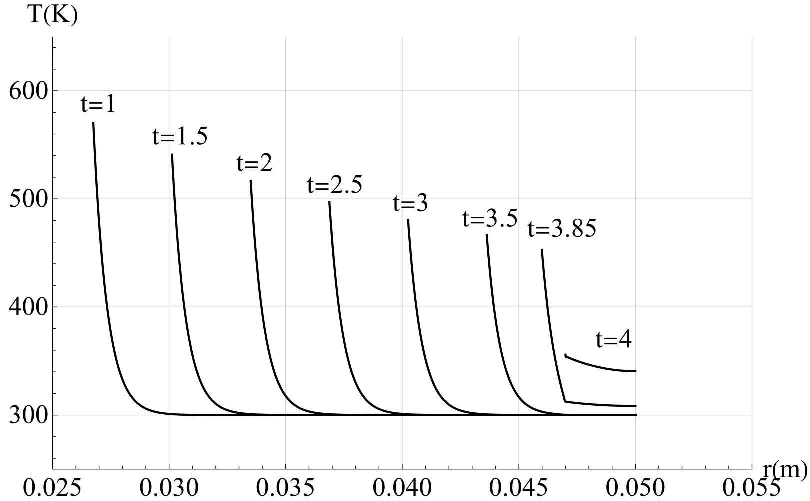


Figure 3. Temperature distribution considering 5% of propellant $H_{reac}$

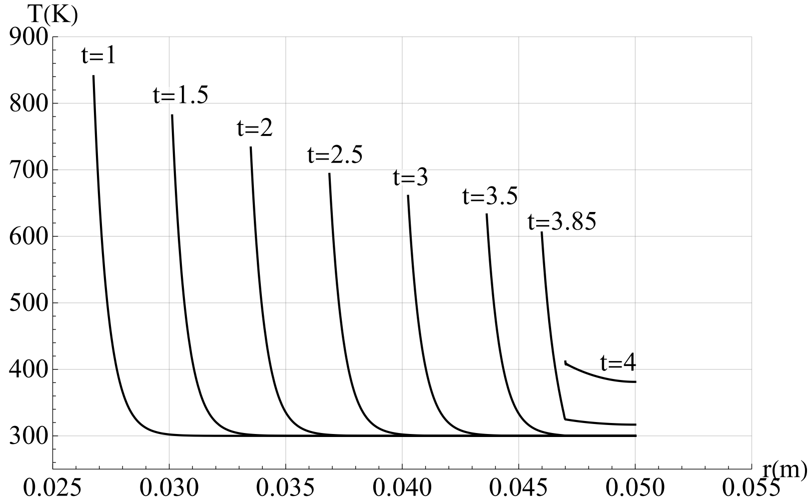


Figure 4. Temperature distribution considering 10% of propellant $H_{reac}$

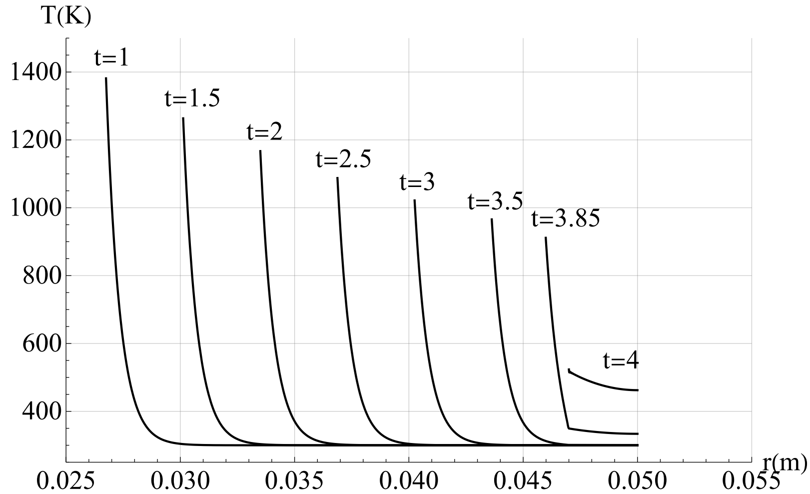


Figure 5. Temperature distribution considering 20% of propellant $H_{reac}$

Figure 6 corresponds to the logarithmic graph of the error presented in equation (30) at different points on the cylinder. It can be observed that the moving point was the one with the worst convergence. The inner region ($R_b$) showed an oscillatory convergence. As can be seen in the figure , the truncation of 100 has already resulted in a good convergence in the problem. The error was calculated using the following formula:

$$\varepsilon(r, n_{max}) = \frac{T_{n=100}(r,1) - T_{n=n_{max}}(r,1)}{T_{n=100}(r,1)} \tag{30}$$

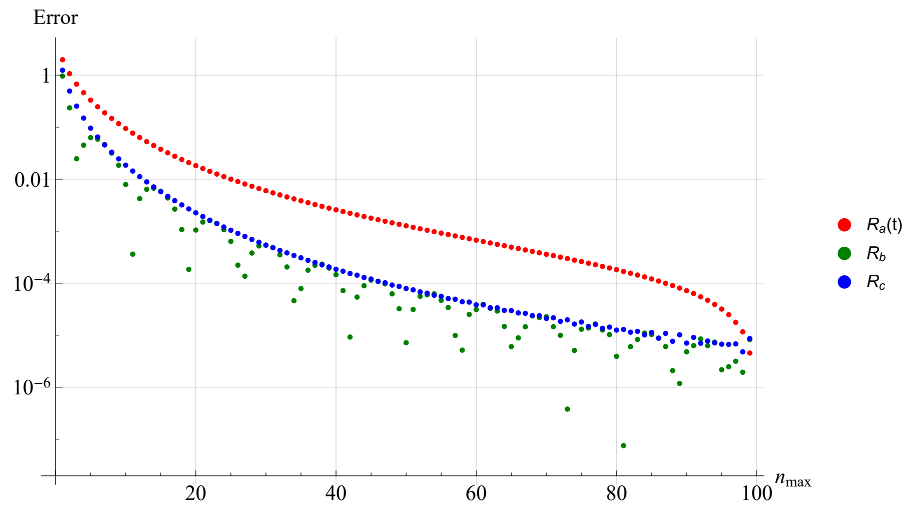

Figure 6. GITT Error at different positions for 5% of propellant $H_{reac}$

## 5. Conclusion

The main objective of this work was to obtain the temperature distribution of a rocket engine without the need of experimental data. For this, the heat released from combustion was calculated through the equation of heat and enthalpies of the reaction elements.

The Generalized Integral Transform (GITT) technique was used to obtain the temperature distribution in a moving boundary. To facilitate the solution of the eigenvalue problem, the solution was obtained in Cartesian coordinates instead of Cylindrical. With that, the transformed pair was chosen and the problem equation was developed, generating an infinite coupled system of ordinary differential equations (23) that were solved numerically by Wolfram Mathematica.

The results of the temperature distribution were as expected. It was observed that the moving point $R_a(t)$ decreases its temperature with time. As the thermal conductivity of the propellant is extremely low, the high-temperature internal point is consumed before its thermal energy reaches the outer layers. The insulating characteristic of the propellant thermally protected the engine until the end of its consumption. This is something that does not happen in practice, as the fuel is also consumed in the axial direction, preventing it from offering perfect protection.

For future work, one can evolve this study with more precise considerations. One of them is to seek alternatives to obtain the heat released during combustion. The second would be to develop a mathematical model that also considers the temperature distribution in the axial direction. It would also be interesting to consider the external convection during the rocket's flight.

## 6. REFERENCES

Chalhub, D.J.N.M., 2011. "Desenvolvimento de soluções para problemas de advecção-difusão combinando transformada integral e métodos discretos". *Dissertação (Mestrado) - Universidade Federal Fluminense, Niteroi-RJ*.

Chase, M., 1998. *NIST-JANAF Thermochemical Tables, 4th Edition*. American Institute of Physics, -1.

Mehta, R.C., 1981. "Estimation of heat-transfer coefficient in a rocket nozzle". *AIAA Journal, American Institute of Aeronautics and Astronautics*, Vol. 19, No. 8, pp. 1085–1086.

Nunes, A.P.C., 2017. "Estudo da distribuição de temperatura em motores foguete a propulsão híbrida". *Monografia, Universidade de Brasília*.

Silva, L.C., 2017. "Solução do problema de graetz conjugado em um duto ortotrópico por transformada integral". *Dissertação (Mestrado) - Universidade do Estado do Rio de Janeiro, Rio de Janeiro -RJ*.

Sutton and Biblarz, G.P., 2010. "Rocket propulsion elements". *John Wiley & Sons*.

Turns, S.R., 2011. *An Introduction to Combustion: Concepts and Applications*.

Vicentin, I.C.F.S., Marchi, C.H., Foltran, A.C., Moro, D., Silva, N.D.P., Campos, M.C., Araki, L.K. and Diógenes, A.N., 2019. "Theoretical and experimental heat transfer in solid propellant solid engine". *Journal of Aerospace Technology Management*, Vol. 11.

Wolfram, S., 2003. *The Mathematica Book*, Vol. 5.

Özisik, M.N. and Murray, R.L., 1974. "On the solution of linear diffusion problems with variable boundary condition parameters". *Journal of Heat Transfer*, Vol. 96, No. 1, pp. 48–51.

## 7. RESPONSIBILITY NOTICE

The authors José F. A. Avelino and Daniel J. N. M. Chalhub are solely responsible for the printed material included in this paper.