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COMBUSTION SIMULATION OF A PARAFFIN BASED SOLID FUEL WITH GASEOUS OXYGEN INSIDE A HYBRID ROCKET MOTOR

Paulo Gabriel Cunha Martins *LCPE, Aeronautics Institute of Technology*
Rene Gonçalves *Dept. of Chemistry, Aeronautics Institute of Technology*
Cristiane Aparecida Martins *LCPE, Aeronautics Institute of Technology*
Leonardo Henrique Gouvêa *Dept. of Propulsion, Aeronautics Institute of Technology*
paulomartins92@gmail.com
renefbg@ita.br
cmartins@ita.br
gouvea@ita.br
Praça Marechal Eduardo Gomes, 50 - Vila das Acacias, São José dos Campos - SP, 12228-900, Brazil

Abstract. During the past two decades, the state of art of hybrid rocket propulsion area has been in research of blends containing paraffin-based fuels because paraffin itself shows higher regression rate compared to traditional fuels commonly used, such as hydroxyl-terminated polybutadiene or polyethylene, but it does not have good mechanical properties, which increases the risk of grain cracking and rupturing. With the objective to benefit the database development of paraffin-based hybrid rocket propulsion, this work is devoted to present a numerical study of the combustion process of paraffin and gaseous oxygen during the propulsion of a 100 newtons hybrid rocket motor. The paraffin solid wax was chosen for the simulation since it exhibits more data about the regression rate with gaseous oxygen in literature. The simulations utilize a mesh with around 100000 quadrilaterals elements, with an average orthogonal quality of 96.5% and an average skewness of 11% . An axis-symmetric volume domain is considered. Paraffin is studied as hexadecane $(C_{16}H_{34})$ using a reduced reaction mechanism of diesel from "Creck-modeling". Paraffin is evaluated as a gas at 0, 5 and 10 seconds during a test of the hybrid rocket motor and the results of the simulations are compared. The results analyzed are temperature, pressure and velocity profiles inside the hybrid rocket motor. The nozzle and the plume of the exhaust product gases are as well evaluated. This work will contribute to a project of a hybrid rocket motor, where it will operate with paraffin solid wax and other paraffin-based blends on a laboratory test bench.

Keywords: Hybrid rocket motor, Combustion simulation, Paraffin and gaseous oxygen, k-ω SST turbulence model, Nozzle analysis

1 Introduction

This work aims to simulate the operation of a hybrid rocket motor designed to be built and operate in a horizontal test stand. The numerical simulation was necessary due to the complexity of geometry and difficulty to obtain the physicochemical properties of the propellant analytically in each portion of the motor, as well to validate the results obtained during the design. The flow behavior inside the combustion chamber and nozzle was obtained through numerical simulation using the software ANSYS Fluent and it was explained on the ”Computational procedures” section.

In the section ”Analytical procedures” the preliminary steps to design the hybrid rocket motor were explained. The thermodynamic analysis was done in order to choose a proportion of gaseous oxygen to paraffin for a given performance. This step was done using the program NASA CEA from Gordon and J. McBride [1], which returns all the thermodynamic properties of the mixture for a given oxidizer to fuel ratio. The next step was done by the analysis of the regression rate of Paraffin, which results in the oxidizer to fuel ratio as the main result. The final step corresponds to the temporal analysis, which uses the result from the latter analysis in the first one to get the thermodynamics properties, internal ballistics geometry and theoretical performance of the hybrid rocket motor at the end.

In the section of ”Computational procedures” the methodology of simulation is briefly explained, including the chose of turbulence model and combustion reaction model, the configurations of spatial discretization for the equations, the control volume with the boundary conditions and the mesh. In the final section the results for pressure, temperature, and velocity over time are presented. Contours on the control volume of simulation and the area-weighted average of the same properties along the convergent and divergent parts of the nozzle are presented. The results showed a fast pressure drop along time inside the combustion chamber, somewhat unrealistic, however, showed that the nozzle is approximately adapted over time resulting in high propulsive efficiency.

2 Analytical procedures:

During the project development of the hybrid rocket motor of 100 newtons, some preliminary analyses were performed in order to define the internal ballistics of the motor, such as thermodynamic analysis, regression rate analysis and temporal studies of propulsive performance.

The thermodynamic analysis was performed using the program NASA CEA from Gordon and J. McBride [1], in which the characteristic velocity by the oxidant fuel ratio is determined and is present at the figure 1, where the blue circles represent frozen flow, red stars represent equilibrium flow and the black dots the operational performance theoretically considered to the project.

Regression rate analysis regards the mean rate that paraffin is burnt with gaseous oxygen. A suitable equation that quantifies the burning rate is the following, Humble et al. [2].

$$\dot{r} = aG_{ox}^{n} \tag{1}$$

$$G_{ox} = \frac{\dot{m}}{\pi r^2} \tag{2}$$

where $\dot{r}$ = space-time averaged regression rate (m/s), a = regression-rate coefficient, n = regression-rate exponent and G_{ox} = oxidizer mass flux rate through port area ($kg/m^2 s$).

The coefficients a and n are determined directly experimentally and depend on the propellants, grain configuration, and the type of injector used. Attention must be given to the G_{ox} range evaluated experimentally since the coefficients a and n are only true within the limits. For Paraffin and Gaseous oxygen in the range of 15 to 105 of G_{ox} the space-time averaged regression rates law chosen for this simulation corresponds to the paraffin-based fuel (SP-1) tested at Stanford university by Karabeyoglu et al. [3], and is given by the following equation:

$$\dot{r} = 0.091 G_{ox}^{0.69} \tag{3}$$

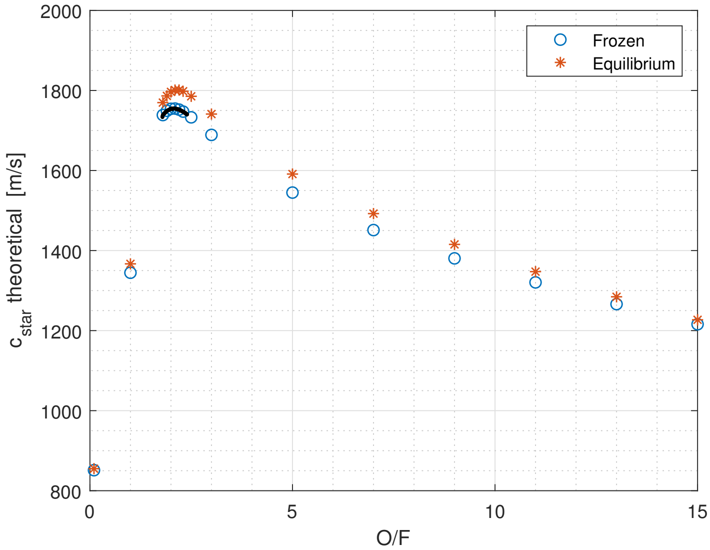

Figure 1. Characteristic velocity varying with O/F ratio at frozen and equilibrium conditions, for a Paraffin/GOX combustion.

The temporal studies of propulsive performance consist of the use of the regression rate equation and the results obtained in the NASA CEA program. The regression rate analysis provides the burning rate of paraffin for a given quantity of oxygen, which results in the oxidizer to fuel ratio over time. Interpolating the data obtained from the NASA CEA program, such as the exit pressure, exit velocity, the heat capacity ratio and the characteristic velocity of the mixture and using some rocket propulsion equations, such as the thrust, specific impulse, thrust coefficient and nozzle throat area, the internal ballistics of the hybrid rocket motor is defined. An example of the application of this methodology was done by Genevieve et al. [4]. One of the results obtained through this methodology is present in the following figure 2.

Because of $n > 0.5$ results in a decreasing regression rate of paraffin, which leads to an increasing O/F ratio overall. O/F ratio decreases downstream the grain because it is consumed through the combustion. This effect is not considered in the calculations since it was considered that the paraffin is equally burned over time following the equations rdot. However, this effect is accounted for in the numerical simulation.

3 Computational procedures:

The numerical simulation was performed with a commercial software fluent from ANSYS. The RANS equations for single-phase multicomponent turbulent reacting flows are solved with a control volume-based technique and a pressure-based algorithm.

The stationary Navier-Stokes equations were supported by the $k - \omega$ SST turbulent model. The $k - \omega$ SST turbulent model was created by Menter [5] and was chosen because it is a low Reynolds model and has two functions: near the wall it calculates the properties of the fluid more precisely using the standard k-ω model from Wilcox [6], and in the core of the fluid it uses the k-ϵ model from Jones, W P; Launder [7], which results in the best performance of both models. This model is well presented in ANSYS manual Ansys [8],Ansys [9],Ansys [10] and in the article Martino et al. [11].

To model the species reactions inside the hybrid rocket motor the reduced diesel combustion model available on Stagni et al. [12] was chosen. This reaction mechanism has 201 species with 4240 reactions, among them $C_{16}H_{34}$ and O_2 considered both in gaseous phase as Paraffin and injector inlets. The species were modeled considering non-premixed combustion with steady diffusion flamelet since the simulation is in steady-state and chemical equilibrium could lead to unrealistic results, the energy treatment was non-adiabatic and the compressibility effects were as well considered.

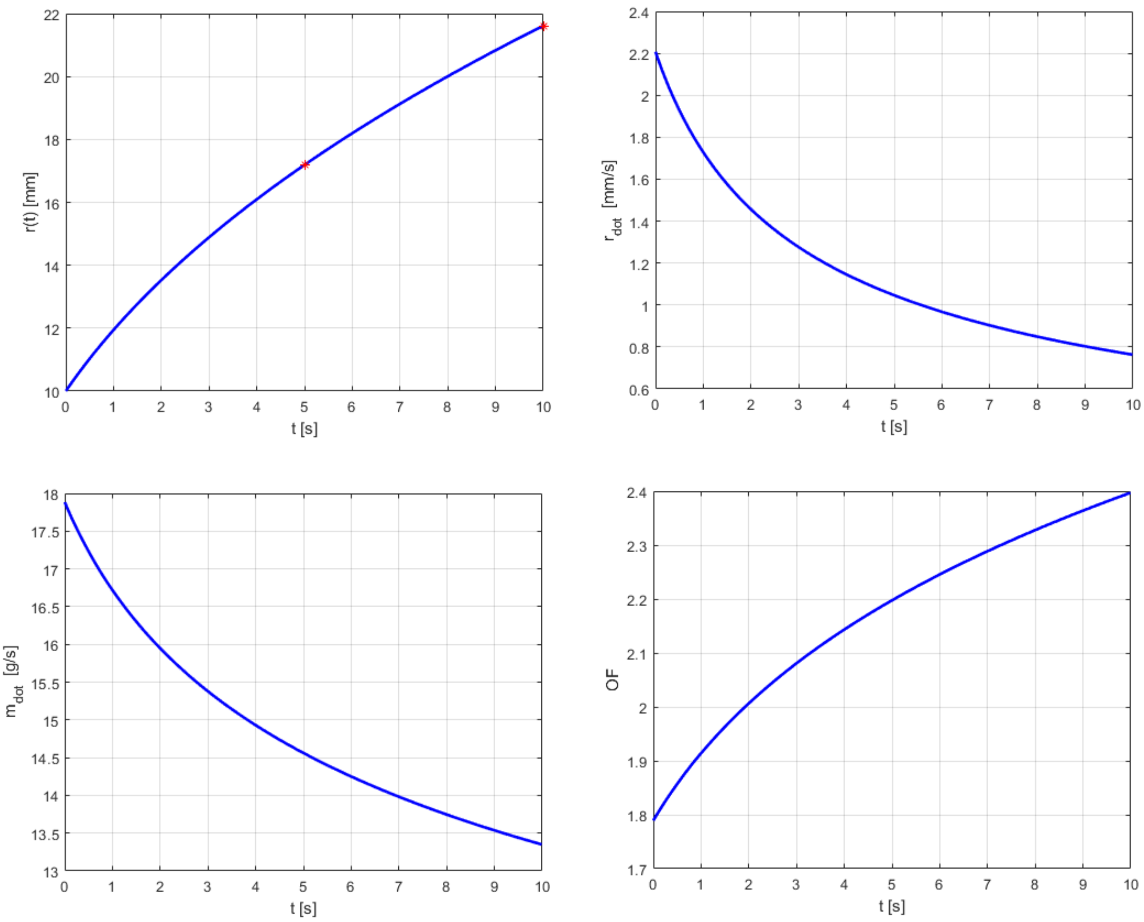

Figure 2. [A] radius, [B] regression rate, [C] fuel mass ow rate, and [D] O/F ratio varying along the burning time.

Regarding the solution methods, the simulation was solved with a pressure-velocity coupled scheme, with a Rhie-Chow flux type. The spatial discretization was considered second order for pressure, density, momentum, turbulent kinetic energy, specific dissipation rate, energy, mean mixture fraction and mixture fraction variance.

The two-dimensional control volume of the simulation is shown in figure 3. In order to simplify the numerical calculations, the simulation was treated as 2D axisymmetric and therefore, the effect of injection can't be realistic calculated and with that, the results obtained in the pre-chamber are a suitable approximation.

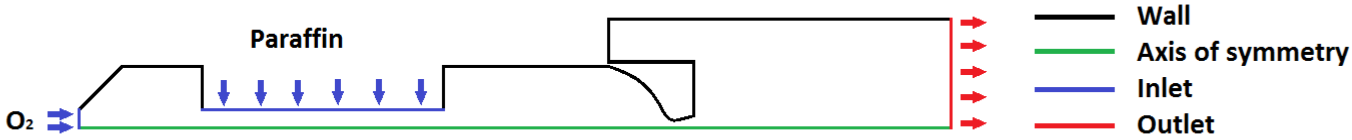

Figure 3. Boundary faces of the combustion chamber and nozzle.

In color blue are the injectors with a constant mass flow rate of gaseous O_2 and paraffin treat as gaseous $C_{16}H_{34}$. In black color is the solid wall with non-slipping shear condition and adiabatic, in green is the axis of symmetry for rotation of the surfaces described and in red color is the pressure outlet with ambient pressure and the environment downstream the nozzle is considered as pure O_2 instead of air because is not possible to deal with more than two species in the simulation.

The parameters of the combustion chamber port radius and mass fluxes of paraffin over time considered for the simulations were taken from the analytical studies, figure 2, at 0, 5 and 10 seconds during the firing test. This simulation was designed to visualize the quantities of the properties, such as pressure, temperature, and velocity when this hybrid motor is working in the test stand, disregarding the effects of gravity.

One of the mesh for this simulation is shown in Figure 4 and consists of around 100000 elements, its distribution has a higher density near the walls in order to satisfy the $k - \omega$ turbulence model that require $y^+ \simeq 1$ and enough nodal points (> 10) within the buffer region and sub-layers in order to optimally detail the boundary layer. The present mesh presents y^+ between 0.5 and 15 inside the combustion chamber, which is not a problem at all. Thanks to the work of [13], in the current software (ANSYS Fluent, CFX) the $k - \omega$ SST turbulence model uses a hybrid function that uses or not the wall functions depending on the value of y^+. In locations where $y^+ > 1$, the wall functions are automatically activated, thus allowing the use of this turbulence model with a less refined mesh without losing the quality of the results, as can be observed in the paper of [14].

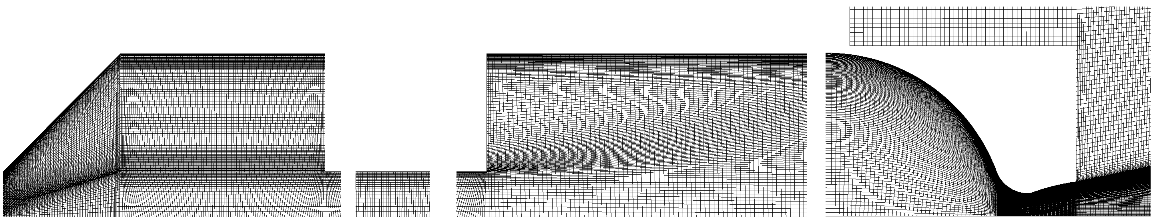

Figure 4. Distribution of the elements in the mesh over all the control volume and near the wall.

The model FLUID81 implemented in ANSYS Fluent was used to generate this mesh. This model is considered to be appropriate for the axisymmetric simulations of fluids inside pipes, where the variation of pressure and temperature influence on the structure of the turbulences and the interaction between wall and fluid, [15].

4 Results:

The criterion of results convergence considered was the residuals values of each simulation as presented in figure 5. It was considered that, when the residuals of energy were below the limits of 10^{-4} and the corresponding values of continuity, x-velocity, y-velocity, k, omega, fmean and fvar were stabilized, the solution had converged and the results were determined.

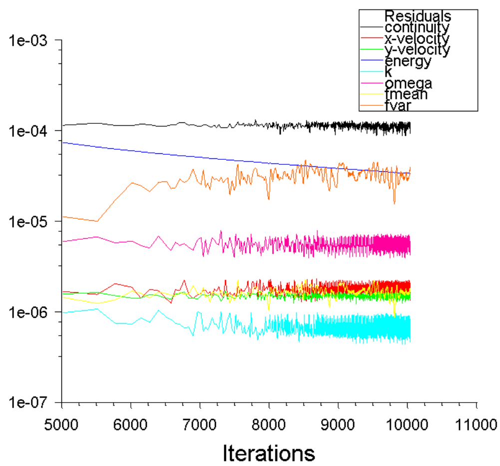

Figure 5. Simulation residuals.

The results obtained in this simulation were the values of pressure, temperature, and velocity inside the hybrid rocket motor and nozzle. The contour of absolute pressure is present in figure 6. The values inside the hybrid rocket motor distinguish a little, representing a diminishing of pressure over time. The exact value for static pressure inside the combustion chamber will be presented later in figure 9.

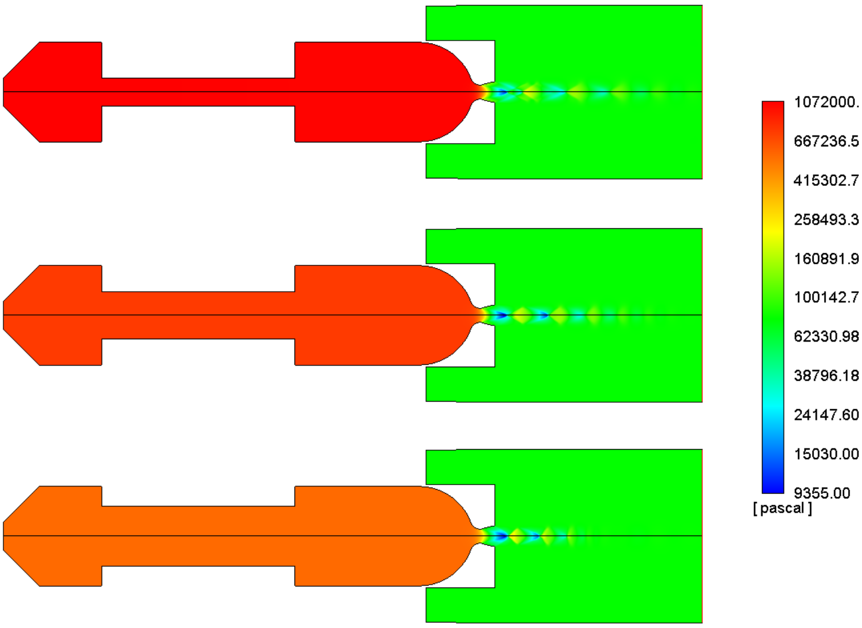

Figure 6. Pressure distribution on the control volume.

In figure 7 are presented the values of the temperature inside the hybrid rocket motor. The results in the pre-chamber for any property cant be believed since the injector wasn't well described by the axisymmetric simulation, but it is a good initial step. The values of temperature in general increase in the pre-chamber and decrease through the combustion chamber port, post-combustion chamber, and nozzle.

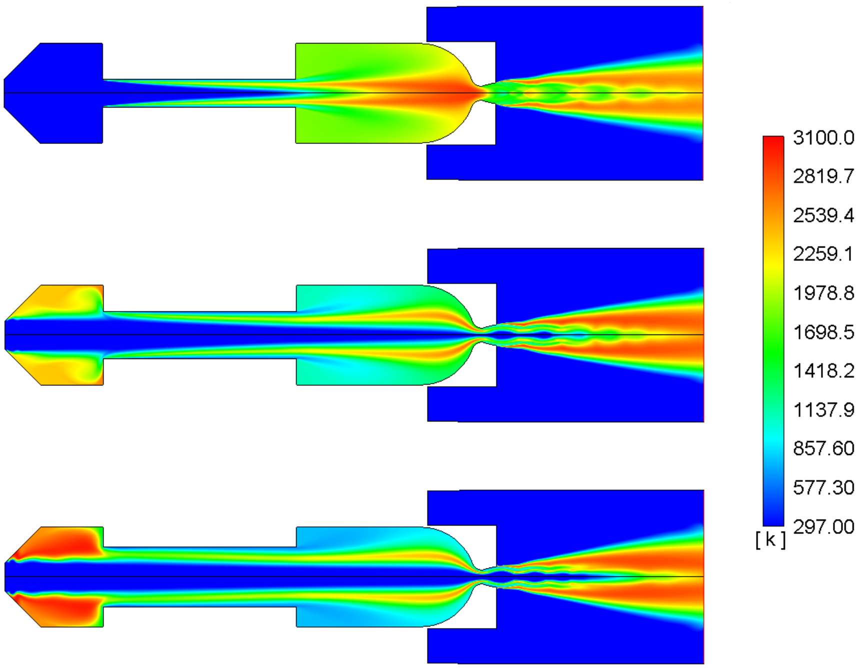

Figure 7. Temperature distribution on the control volume.

The distribution of velocity inside the hybrid rocket motor is presented in figure 8. Inside the pre-chamber, combustion port, post-combustion chamber and the convergent part of the nozzle the values of velocity are low, in the throat the mixture is accelerated to reach Mach 1 and on the divergent part the flow reach supersonic velocities.

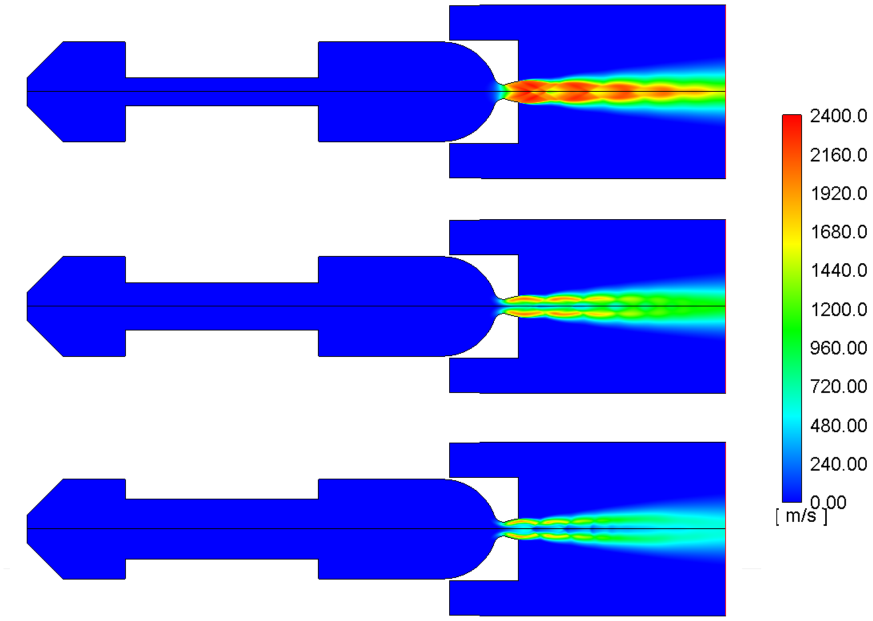

Figure 8. Velocity distribution on the control volume.

The area-weighted averaged of the properties pressure temperature and Mach number along the convergent and divergent part of the nozzle were calculated. Those values obtained for each simulation were compared with each other and are presented in figure 9.

The values observed in the last results can be better evaluated through figure 9. Over time all the values decrease at some point towards the nozzle exit. The diminishing of the pressure and temperature on the combustion chamber is due to the growth of the combustion port, increasing the volume of the flux during the propulsion process. For the divergent part of the nozzle, it is noted that pressure and temperature decrease and the velocity increase over time, according to the theory of compressible flow, [16]. However the decrease of pressure inside the combustion chamber during the experimental tests may happen, those values won't decrease so quickly like the values presented in figure 9.

5 Conclusions and discussion:

The present work has presented a combustion modeling of paraffin with gaseous oxygen inside a hybrid rocket motor. Paraffin was treated as gaseous hexadecane $C_{16}H_{34}$ to avoid multiphase flows but still uses a higher alkane to better represent the paraffin combustion. With this simulation, it was possible to evaluate the flow properties inside the hybrid rocket motor and nozzle, such as pressure, temperature, and velocity.

The pressure drop inside the combustion chamber over time is due to the volume expansion of the port. However this may happen during experimentation, the rate of pressure drop in the simulation was evaluated as unrealistic. Moreover, the nozzle was evaluated as approximately adapted, slightly over-expanded due to the pressure drop. The simulation results help to improve the quality of the design project of a hybrid rocket motor of 100 newtons. In future, this simulation should be checked and validated with the experimental results.

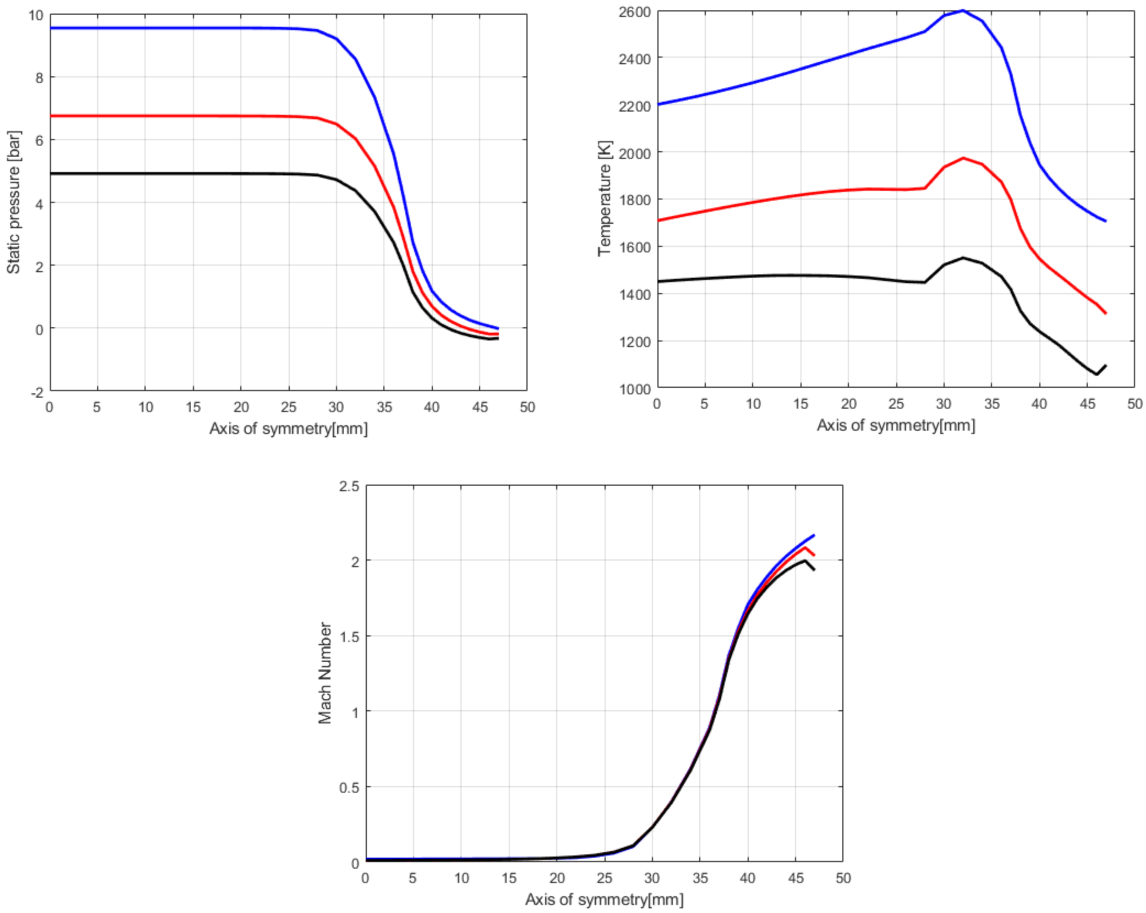

Figure 9. Area-weighted average of the properties pressure, temperature and Mach number along the nozzle.

Acknowledgements

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