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MULTIPHASE MODELING OF SOLID PROPELLANT DETONATION MOVING PROJECTILES

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Abstract. *This study investigates the combustion dynamics of nitrocellulose, a solid propellant, within combustion chambers, focusing on the pressure behavior during the propulsion of a projectile through a barrel using 12.7x99mm NATO ammunition. Employing the first law of thermodynamics, the research examines two hypotheses: partial and total grain combustion. The findings indicate that partial combustion results diverge from the literature in terms of energy loss, whereas total combustion, occurring at 0.32 meters from the barrel, aligns closely with experimental data. The maximum pressure observed was 330.9 MPa, within normative limits and corroborated by experimental results. Key parameters such as heat generation, internal energy variation, kinetic energy, and energy loss were consistent with established studies. The model highlights the critical influence of the amount of propellant converted to gas on the overall system performance and energy loss.*

Keywords: *Solid propellants, thermodynamics, energy loss, projectile, nitrocellulose.*

1. INTRODUCTION

The combustion of solid propellants is a complex and extensive phenomenon with significant implications in ballistics and the overall performance of systems utilizing this type of fuel. This study aims to expand the understanding of this process by focusing on modeling the combustion dynamics of this solid propellant and the associated thermal phenomena. Thus, a model of the solid propellant detonation moving a projectile within a tube/barrel was used to comprehend better the burning process of the propellant.

Studies involving solid propellant modeling are recent and scarce. Understanding their behavior implies optimizing systems involving multiphase phenomena. Examples of areas that can benefit from analyses related to these phenomena include propulsion engineering, defense systems, and space propulsion.

Maximum pressure is one of the primary factors in such analyses as it directly influences the selection of materials for components. Therefore, theoretical methods for determining pressure peaks are of extreme value.

Successful studies proposing models for the detonation of granular solid propellants were able to model the behavior of the flame front propagation using the finite element method (López-Munoz et al., 2019). This study used physical and numerical methods to describe the phase transitions. The modeling was done with continuity, momentum, and energy equations for both phases. To determine the model's reliability, the results were compared with experimental results. The results showed divergences from experimental tests, indicating that the problem's initial conditions generated sufficient disturbances to interfere with the result.

Another method used for prediction is a thermochemical approach by Değirmenci and Dirikolu (2012). This approach can model the behavior of various combustion products parameters from the propellant combustion. A disadvantage of the method is the need for a large number of inputs about the gases' behavior and it does not predict the percentage of solid propellant mass converted into gas.

In the studies of Moreal-González et al. (2017), the existence of unburned particles by the propellant combustion law was considered. Conservation equations were adopted, and the equation of state proposed by Noble-Abel, considering a co-volume, was used. Additionally, Moreal-González et al. (2017) also modeled the behavior of inter-granular stresses, forces, and heat transfer at interfaces. To solve this problem, a code in the UXGun software was used.

The modeling by Moreal-González et al. (2017) allows for the evaluation of the behavior of quantities such as speed and pressure over time and the analysis of solutions from different authors for the inter-granular stress law. To assess the system's reliability, the results were compared with experimental data and were found to be close.

The research by Zhen et al. (2019) analyzed the same behaviors of quantities measured by Moreal-González et al. (2017), but did not consider the existence of a projectile. Comparative verifications between the two phases of the propellant and different meshes were carried out. Characteristics of the DDT process of high-energy solid propellant were obtained, providing a better understanding of the effects of solid volume friction and the pressure exponent on the DDT of a solid propellant.

To obtain these results, conservation equations of mass, momentum (for both phases), the Noble-Abel equation of state for gas, and the Helmholtz equation of state for the solid phase were used. This indicates that, unlike other studies, the solid phase can be modeled with equations different from the gas phase, allowing verification of the most suitable for each case in question. With the modeling, it was possible to relate the grain shape to the maximum generated pressure. The combustion and compression processes were observed in both the deflagration and detonation stages. In both stages, the combustion zone's thickness is greater than the compressed bed's thickness, and the two thicknesses in the detonation stage are smaller than those in the deflagration stage (Zhen et al., 2019).

Otón-Martínez et al. (2021) used a FORTRAN code in the OpenFOAM software to predict the three-dimensional behavior of solid propellant combustion. Eulerian approximations were made to model the problem. The equations used were mass, momentum, and energy conservation (for the gas), reaction rate, and the Noble-Abel equation of state.

Studies focusing solely on the gas phase can contribute to improving the gas phase modeling of this study. Zhou et al. (2020) contributed to studies involving projectile movement in ducts. In this study, the modeling was generated using the transient one-dimensional Navier-Stokes equation. Additionally, conservation equations of mass, momentum, energy, the Peng-Robinson equation of state for gas, a thermal diffusivity equation, and a reaction rate equation were used. The fuel tested was a hydrogen-oxygen reaction. By solving the equations using MATLAB code, it was possible to trace the behavior of the flame front position over time and the flame front's temperature and pressure along the fluid's length in the tube. The projectile's speed in the tube was also obtained by solving the equations (Zhou et al., 2020).

Propellant combustion laws were presented by Cronemberger et al. (2014). Based on the propellant combustion law combined with a thermodynamic approach, it was possible to determine the pressure behavior along the barrel with solid propellant burning while moving a projectile. These parameters are of high importance due to the high magnitude of energy released, which, if poorly dimensioned, can cause accidents. For this study, a condition of total propellant combustion before the projectile exits the barrel was adopted, this factor directly influences the obtained results.

Following Cronemberger et al.'s (2014) studies, Akçay (2017) expanded the understanding of propellant combustion functions, resulting in similar outcomes but with lower propellant load. Unlike Cronemberger et al.'s (2014), partial propellant combustion was adopted, resulting in unburned powder.

Thus, it is evident that studies addressing such phenomena are recent and complex due to involving more than one phase. There is no consensus on the most suitable way to model the solid phase, making it necessary to enrich research in the area to expand the understanding of these phenomena for obtaining more optimized and reliable systems.

A highly influential factor in the results is the amount of propellant converted from solid to gas. There is a lack of advanced studies on this behavior across different calibers, which is essential for more accurate modeling and a broader understanding of this phenomenon. Understanding the combustion quantity can directly influence the percentage of lost energy, and this factor can be crucial for the development of more efficient systems, benefiting further studies.

Analysis involving solid propellant detonation in ducts is of extreme utility. Considering this need, this study proposes a formulation to determine the pressure behavior generated by the solid propellant combustion through the percentage of burned propellant, and an analysis of the burned quantity and the percentage of lost energy.

2. METHODOLOGY

To obtain a model capable of predicting maximum pressure values in the solid propellant combustion process in barrels moving projectiles, a one-dimensional model considering the energy equation of the first law of thermodynamics was used.

Predictability of pressure peaks is directly related to the combustion behavior of this propellant. For this calculation, two hypotheses of propellant combustion behavior were analyzed: the first considers that the solid propellant burns entirely upon reaching a distance equivalent to 34% of the barrel length. The other hypothesis considers that when the projectile leaves the barrel, the propellant has not yet fully burned (Cronemberger et al., 2014; Akçay, 2017;).

The analyzed propellant was nitrocellulose (single-base powder) arranged in cylindrical grains. The model used considered the 12.7x99mm NATO ammunition. A one-dimensional modeling was performed in which various parameters were analyzed as a function of time and the distance traveled by the projectile in the barrel. The results obtained from the modeling were compared with experimental data.

2.1 Assumptions Adopted

For the proposed model, the following assumptions were adopted:

- Constant cross-section of the barrel;
- Incompressible solid phase;
- High Reynolds numbers;
- Temperature-independent specific heats;

Additionally, the following boundary conditions were used:

- Initial condition: t=0; x=0; $P = P_a$;
- Final condition: t=t_1; x=L; $P = P_e$;

Where t is time, x is the distance traveled by the projectile, P is pressure, P_a is atmospheric pressure, t_1 is the time the projectile exits the barrel, L is the total length of the barrel, and P_e is the pressure at the moment the projectile leaves the barrel.

2.2 Proposed Method

The proposed method equates the energy provided by the propellant combustion to the system (Q), which can be correlated with other factors by the first law of thermodynamics. The energy provided by the system is converted into kinetic energy imparted to the projectile (W), variation of the internal energy of the gas (ΔU), and lost energy (E_{lost}).

$$Q = \Delta U + W + E_{lost} \tag{1}$$

The properties presented above can all be related to the impulse imparted to the projectile (F), the specific heat ratio (γ), and the ignition energy required to start the propellant combustion (E_i). This relationship can be expressed by the following equation:

$$Q = \frac{m_g F}{\gamma - 1} + E_i \tag{2}$$

The energy provided by the system considers the impetus imparted to the projectile, which is a factor difficult to measure (Schweitzer and Ziegler, 1964). A possible simplification is to adopt it as a constant value.

The kinetic energy imparted to the projectile and the variation in the gas's internal energy are given by the following equations, respectively:

$$W = 0{,}5\, M\, V^2 \tag{3}$$

$$\Delta U = \frac{P}{\gamma - 1}\left(Vol_g - m_g\, c\right) \tag{4}$$

The variation in the gas's internal energy is a crucial parameter as it allows the measurement of pressure. This equation relates, besides pressure and specific heat ratio, the gas volume (Vol_g), gas mass (m_g), and co-volume (c). The equation for kinetic energy relates the mass (M) and velocity (V) of the projectile.

The specific heat ratio values can be replaced by measured values to compensate for lost energy, ranging from 1.19 to 1.24, as presented by Akçay (2017). For this study, theoretical values for the specific heat ratio will be adopted, and losses will be considered separately. The reason for considering losses in an equation and separately is to allow quantification, making the results closer to experimental data. This factor is fundamental for the following analysis as, with such distinct combustion percentages, the lost energy can vary significantly. Thus, the lost energy is given by the following equation:

$$E_{lost} = X\, \frac{m_g F}{\gamma - 1} \tag{5}$$

The percentage of lost energy (X) can vary greatly for each literature, ammunition, or analyzed conditions. As one of this study's objectives is to investigate the amount of propellant burned in the process, the lost energy value was different for each combustion hypothesis adopted.

From the presented equations, it is possible to obtain a function for pressure:

$$P = \frac{(\gamma - 1)(Q - W - E_{lost})}{Vol_g - m_g c} \tag{6}$$

The volume occupied by the gas (Vol_g) can be determined by the following dimensional relation between the combustion chamber volume (Vol_{cc}), specific mass (ρ), tube diameter (D), distance traveled by the projectile (S), and solid and gaseous propellant masses:

$$Vol_g = Vol_{cc} - \frac{m_p}{\rho} + \pi \frac{D^2}{4} S + \frac{m_g}{\rho} \tag{7}$$

The gas mass (m_g) is determined by multiplying the propellant mass (m_p) by the burned percentage (z).

$$m_g = m_p\, z \tag{8}$$

Determining the burned propellant percentage is distinct for each combustion hypothesis. The first hypothesis of total propellant combustion is given by a linear regression of the nitrocellulose grain size until the projectile travels 34% of the barrel length, after which the grain combustion is total. The 34% value is close to those used by Cronemberger et al. (2014).

The second hypothesis, assuming partial propellant combustion, defines the percentage of nitrocellulose converted to gas by the combustion function established by Akçay (2017) by the Combustion Equation present on the following equation:

$$\frac{dz}{dt} = B_a \varphi(z) \left(\frac{P}{P_a}\right)^n \tag{9}$$

This combustion equation considers a combustion grain shape function ($\varphi(z)$) which is equivalent to 1 for cylindrical propellant grains, as in the proposed case. The equation relates a pressure ratio between the pressure at a specific point in the tube/barrel (P) and atmospheric pressure (P_a) raised to a burn rate exponent and multiplied by a burn rate coefficient (B_a) to obtain the burned propellant percentage behavior (z) converted to gas over time.

The values of each parameter used in the modeling are presented in Tab. 1.

Table 1. Values of Parameters Used in the Modeling

Parameter	**Value**
Projectile Diameter (D)	12.7 mm
Projectile Mass (M)	42 g
Propellant Mass (m_p)	14.5 g
Propellant Density (ρ)	1577.8 kg/m^3
Grain Diameter	0.28 mm
Burn Rate Coefficient (B_a)	0.000000787 $\left(\frac{m}{s}\right) Pa^{-a}$
Contained Pressure in Propellant (n)	0.69
Propellant Impetus (F)	1250 kJ/kg
Specific Heat Ratio of Gas (γ)	1.24
Combustion Chamber Volume (Vol_{cc})	18303.955 mm^3
Propellant Shape Function ($\varphi(z)$)	1
Covolume (c)	0.001 m^3/kg
Ignition Energy (E_i)	69 J

By adopting each established hypothesis for the solid propellant converted to gas behavior, it is possible to establish the pressure behavior at each point in the barrel using the one-dimensional modeling. To analyze the data, experimental tests were conducted to verify the proposed model's reliability.

Experimental tests were conducted according to specific standards for this type of ammunition, MOPI AEP-94. The tests were conducted in test barrels equipped with high-resolution pressure transducers. The ammunition tested was 12.7x99mm NATO caliber with single-base powder (nitrocellulose). The projectile velocity outside the barrel was measured according to the standard, measured at 24 meters from the barrel's muzzle.

3. RESULTS

Adopting the total and partial combustion hypotheses made it possible to establish the behavior of the solid propellant mass fraction profile converted to gas. Besides these two hypotheses, similar to partial combustion calculations, a modeling was performed in which the powder reaches percentages close to 100% at the barrel exit. This modification was made to better understand the energy lost in the process. The nitrocellulose combustion percentage behavior for each adopted hypothesis is shown in Fig. 1.

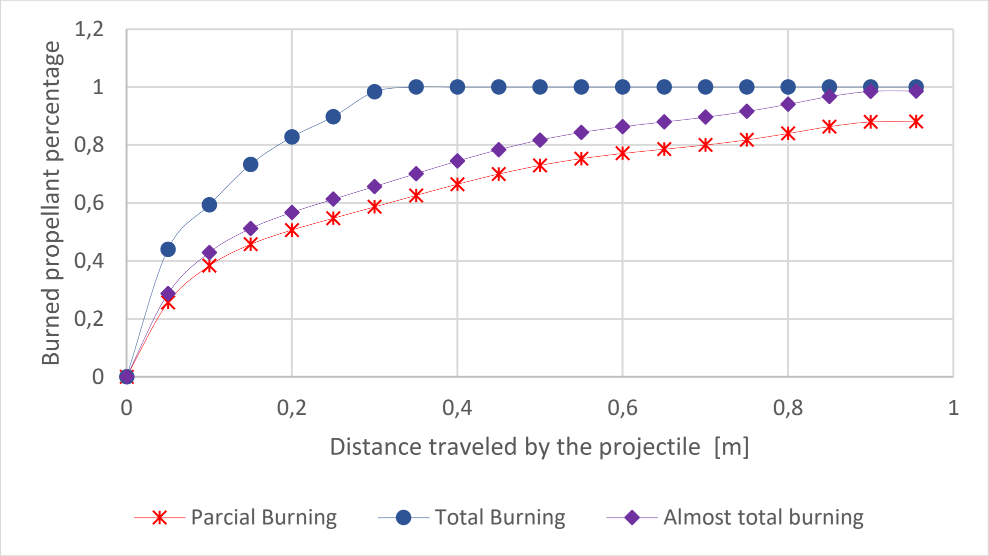

Figure 1. the Burn Percentage of Propellant for Each Hypothesis Analyzed by the Distance Traveled by the Projectile.

In the total combustion hypothesis, when the projectile has advanced approximately 0.32 meters, the propellant is fully burned. Diverging from the total combustion behavior, which quickly converts all the fuel's energy into kinetic energy, the behavior of the partial combustion hypothesis shows a lower and gradual solid fraction conversion into gas. This phenomenon is visible in the presented graphs and justifies variations in lost energy.

The analyzed properties behavior present in the first law's equation diverged for each hypothesis. The behavior of each parameter analyzed for the total propellant combustion hypothesis is presented in Fig. 2.

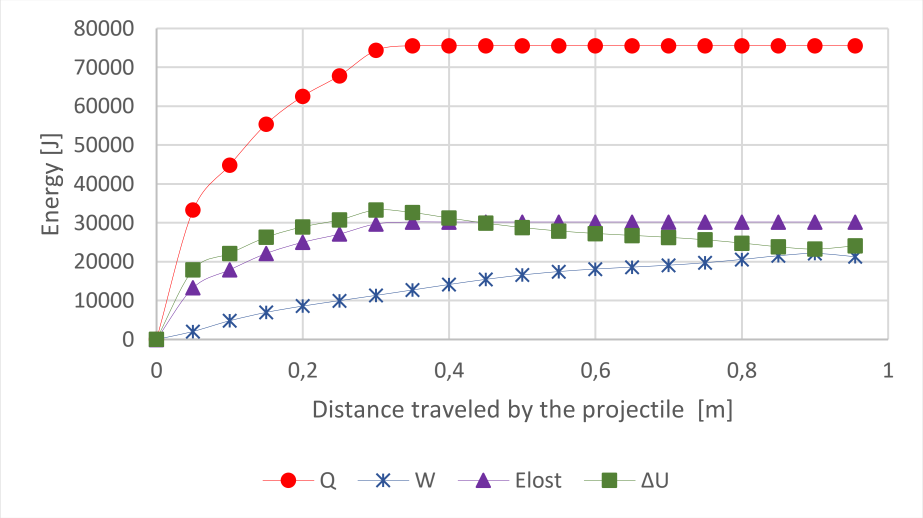

Figure 2. The Properties Used for Modeling by the Distance Traveled by the Projectile Inside the Barrel for the Hypothesis of Total Propellant Burn Occurring at 34% of the Total Barrel Length.

It is evident that the energy provided to the system and the lost energy behavior has a noticeable stagnation for the total fuel combustion condition. The kinetic energy gradually increases as the projectile advances in the barrel, while the variation in the gas's internal energy decreases after the total combustion of the propellant is achieved.

The behavior of each parameter analyzed for the parcial propellant combustion hypothesis is presented in Fig. 3.

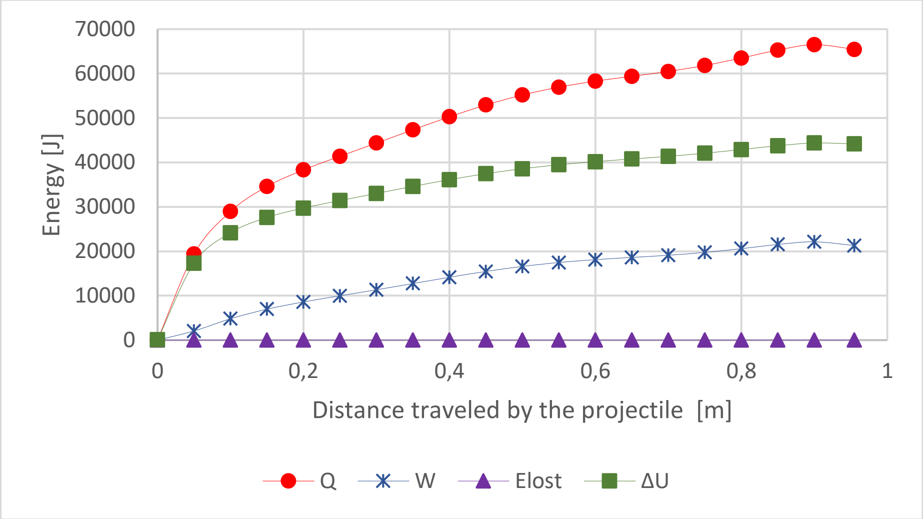

Figure 3. The Properties Used for Modeling by the Distance Traveled by the Projectile Inside the Barrel for the Hypothesis of Partial Propellant Burn

In partial combustion case, part of the fuel's contained energy was not used, the total loss values were significantly lower. For the partial combustion hypothesis, even when assuming the system has no losses, the maximum pressure values were still lower than those obtained experimentally. Therefore, it was necessary to test the condition where the propellant combustion approaches totality when the projectile leaves the barrel. Thus, higher loss values were obtained but still significantly lower compared to the total propellant combustion hypothesis. The results for this hypothesis are presented in Fig. 4.

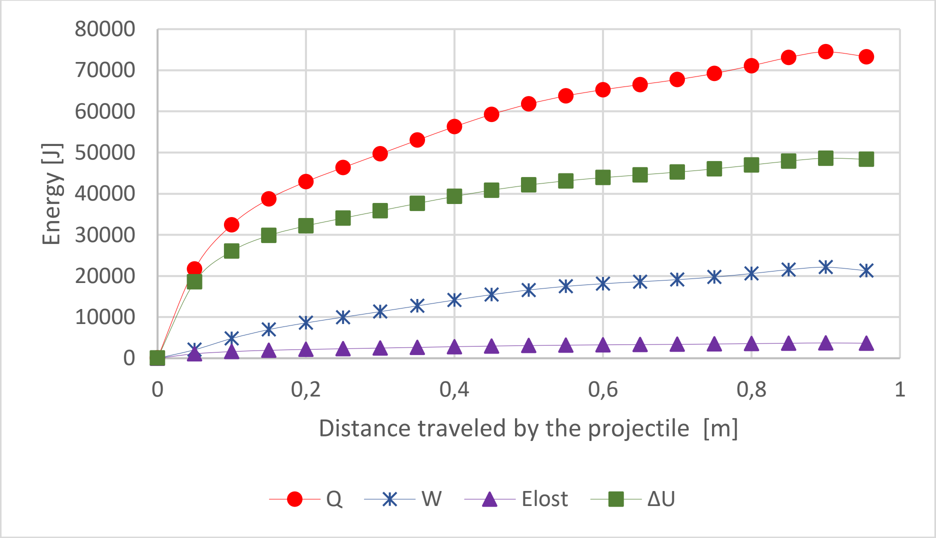

Figure 4. The Properties Used for Modeling by the Distance Traveled by the Projectile Inside the Barrel for the Hypothesis of Partial Propellant Burn Reaching Close to 100% When the Projectile Exits the Barrel.

Comparing the three simulated hypotheses, the kinetic energy imparted to the projectile increased gradually in all cases. Another divergent factor between the hypotheses is the percentage of energy lost.

For the total combustion hypothesis, 40% of the energy was lost. The result of 40% is significantly higher than the losses in 7.62x51mm NATO ammunition, which are 26% (Farrar and Leeming, 1983). This increase can be justified by the fact that 12.7x99mm NATO ammunition is significantly larger and more robust, losing much more energy through barrel friction and dispersing more energy through heat, light, and sound. The partial combustion hypothesis had low values compared to the literature, being 5% (Akçay, 2017).

Having the parameters' behavior involved in the proposed model equation, it was possible to model the pressure behavior along the barrel. The results were compared with experimental values and are shown in Fig. 5.

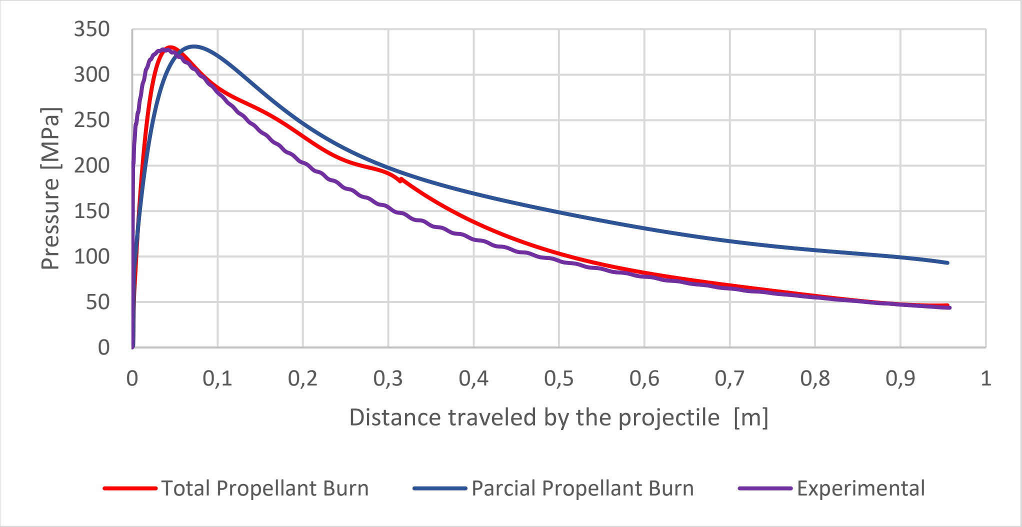

Figure 5. Comparison of Partial Burn, Total Burn, and Experimental Data Models, Analyzed in Terms of Pressure Generated by the Distance Traveled by the Projectile.

The pressure behavior of the models resembled that of the experimental tests, with the maximum pressure values in the model adopting partial combustion being close to the modeling adopting total combustion, and both values being higher than the experimental results. The results obtained are consistent with the literature and within the safety standards for this type of experiment (NATO, 2020).

The maximum pressures obtained in the study for the partial, total, and experimental results were 330.9 MPa, 330.0 MPa, and 327.7 MPa, respectively. Being at most 3.2 MPa higher compared to experimental results, still within the CIP and SAAMI standards' limits. This discrepancy is reasonable and consistent.

The behavior obtained for heat generated, internal energy variation, kinetic energy, and lost energy are all similar to those modeled by other studies on different ammunition (Cronemberger et al., 2014).

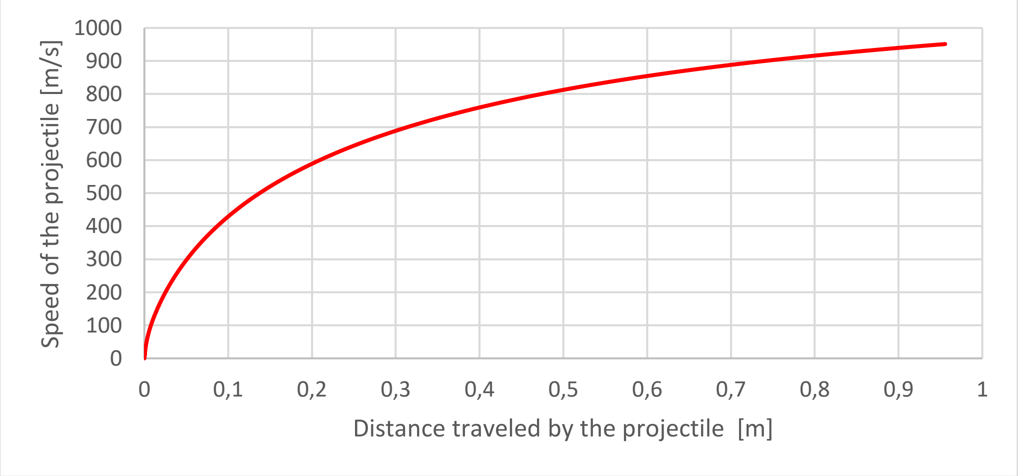

Figure 6. Behavior of the speed of the projectile in each distance traveled.

Analyzing the velocity profile by the distance traveled, as shown in Fig. 6, it becomes noticeable that at a distance of 0.1 meters, the projectile already reaches supersonic speeds, meaning that factors such as the compressibility of the fluid ahead of the projectile may be responsible for some of the losses. This factor was not considered in the present study, but it becomes a suggestion for future research.

4. CONCLUSION

This research presented an analysis of solid propellant combustion in a combustion chamber, focusing specifically on the pressure behavior within the barrel moving a projectile. Through an approach based on thermodynamic principles and analyzing two different hypotheses of combustion dynamics, it was possible to determine crucial system behaviors. This formulation allowed for determining the burned propellant percentage, essential for understanding the combustion process and its implications on system dynamics.

Applying the first law of thermodynamics proved crucial for quantifying the heat generated by combustion products, as well as determining the projectile's kinetic energy, lost energy, and the system's internal energy variation. From these data, it was possible to present a mathematical expression to determine pressure at each barrel point.

The results obtained based on two distinct hypotheses (partial grain combustion and total combustion) were of high importance. It was observed that partial combustion results showed inconsistencies concerning existing literature, as the lost energy values were lower than expected. On the other hand, total combustion results occurring at 0.32 meters from the barrel's beginning showed high coherence with experimental results. This alignment reinforces the proposed model's validity and the precision of the adopted hypotheses, being able to estimate 40% losses for this case.

The maximum pressures obtained in the study for the partial, total, and experimental results were 330.9 MPa, 330.0 MPa, and 327.7 MPa, respectively. Being at most 3.2 MPa higher compared to experimental results, still within the CIP and SAAMI standards' limits. This discrepancy is reasonable and consistent.

The behavior obtained for heat generated, internal energy variation, kinetic energy, and lost energy are all similar to those modeled by other studies on different ammunition.

The methods and results presented here offer a solid basis for future investigations, with the potential to further optimize the performance and safety of such systems. It is recommended for future studies to experimentally determine the amount of burned propellant. One way to achieve this is through tests that capture propellant particles at the barrel exit and burn them subsequently. This method is useful for determining the amount of unburned powder. Such an experiment can enhance this resolution's robustness.

5. ACKNOWLEDGEMENTS

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