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ASSESSMENT OF CORRELATION BETWEEN SIMULATIONS AND STANDARDIZED TESTS OF THERMOPLASTICS FROM DIFFERENT TRUE STRESS-STRAIN EQUATIONS

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Abstract. *The literature demonstrates von Mises model is not suitable for ductile thermoplastics. In addition, some Finite Element solvers still lack constitutive models that accurately simulate the thermoplastics behavior. However, it is known there are different formulations to estimate true stress. Thus, this study aims to evaluate the correlation between numerical simulations and standardized tests by comparing results from different true stress formulations. It also proposes a combination of these formulations, using the von Mises constitutive model available in ABAQUS® solver. The physical tests were carried out with Polypropylene specimens. The methodology was divided into three stages, the first relating to the data treatment, being the data acquired from standardized tensile tests and the combination of true stress formulations performed by parameters calibration. Then, finite element analyses were run for the following four tests: Tensile, Compression, Three-Point Bending, and Erichsen. Finally, an evaluation was done to determine which model fits better, considering the Normalized Root Mean Square Error as main metric. In conclusion, it is inferred that the combination of the true stress equations ISO 18872 and DuBois' showed better correlation than the others for this selected material, even though using the von Mises Classical Metal Plasticity constitutive model available.*

Keywords: *thermoplastic, true stress-strain, structural simulations, standardized test.*

1. INTRODUCTION

The use of ductile thermoplastic materials in various industrial sectors has become increasingly common. One of these sectors is the automotive industry, where approximately 10% of its components, both interior and exterior, are manufactured using these polymers (Greene, 2021). The utilization stems from the fact these materials have characteristics tend to improve the design, such as mass reduction, increased flexibility, and cost reduction, when compared to similar components made of metals.

To design components made of thermoplastics meeting market demands, it is necessary reliable results from virtual simulations, which means values close to those observed in physical tests. Once the correlation is proved, new configurations may be simulated, without raw material expenses. However, what is common in literature are simulations involving ductile thermoplastics through von Mises Classical Metal Plasticity constitutive model, which is well-established for metals and available in commercial Finite Element (FE) solvers, such as ABAQUS® and LS-DYNA®.

Although some references point out the ductile thermoplastics' behavior differs from the metals, particularly in the compression region of the yield surface (Dowling, 2017), some solvers do not provide constitutive models specifically for thermoplastics. An exception is the LS-DYNA® solver, it has the Semi-Analytical Model for Polymers or SAMP-1 (Kolling et al., 2006). Additionally, it is known the true stress-strain curve that is used as input in most constitutive models has a significant impact on the results.

It is usual to propose several formulations to improve the correlation between physical tests and simulations through the same constitutive model, especially when analyzing the plastic region, where hardening and necking phenomena may occur. For metallic components, a common approach is to combine two formulations, such as Gosh and Hockett-Sherby (Shin et al., 2022), or Swift and Hockett-Sherby (Chen et al., 2019). From engineering stress-strain data, certain parameters are calibrated, adjusting the simulated test results to the physical test values. About thermoplastics, the equations for true stress-strain are typically established using engineering stress-strain data and the Poisson's ratio, such as the ASTM E646 and ISO 18872 standards, as well as Du Bois (Lobo et al., 2013) equation.

Therefore, the main goal of this paper is to assess the different combinations of true stress equations, through the von Mises Classical Metal Plasticity constitutive model available in ABAQUS® solver, aiming to improve the correlation between physical and virtual tests. The physical tests were carried out with specimens made of Polypropylene (PP). To determine which formulation provides greater accuracy, the Normalized Root Mean Square Error (NRMSE) is used in conjunction with the following tests results: Tensile, Compression, Three-Point Bending, and Erichsen.

2. METHODOLOGY

The methodology applied to this study is divided into three fundamental parts: Data Treatment and Formulation Combination (MATLAB®), Structural Simulations (ABAQUS®), and Assessment of Correlation through the NRMSE (MATLAB®). Figure 1 exemplifies the methodology steps.

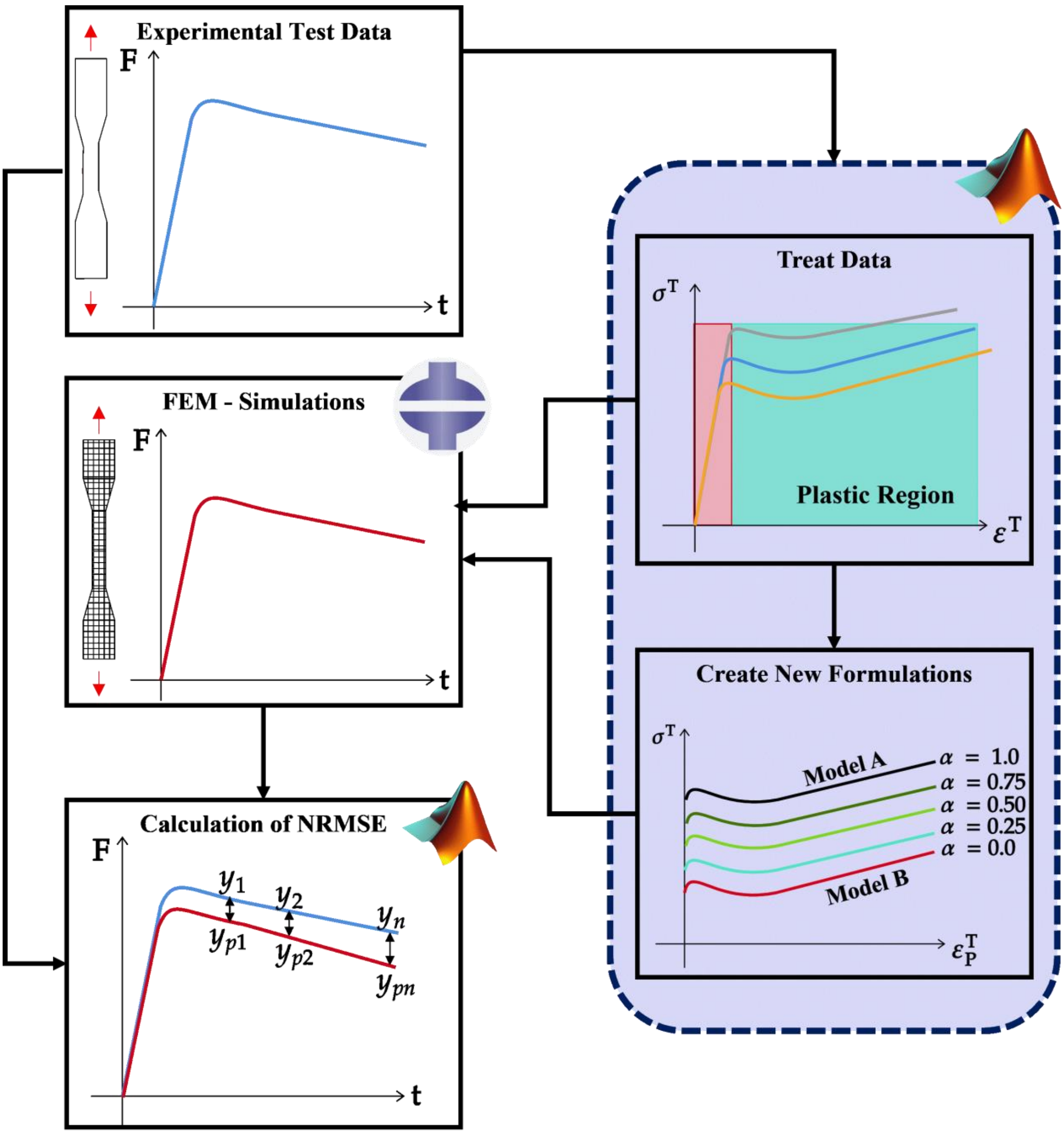

Figure 1. Methodology illustration: from experimental data acquisition to NRMSE calculation.

2.1 Data Treatment and Formulation Combination

For data treatment, the parameters requested by the von Mises Classical Metal Plasticity model were taken into consideration. The following mechanical properties were determined: elastic Poisson's ratio, Young's modulus, density, and the true stress-strain curve. For quasi-static dynamic analyses, it is possible to consider different strain rates and use multiple curves. The tensile tests of this study were performed at three different speeds: 1 mm/s, 10 mm/s and 200 mm/s, and the strain rates are, respectively: 0.0482 s^{-1}, 0.5123 s^{-1} and 10.1184 s^{-1}.

Initially, the data were treated considering the formulations: ISO 18872 (M1), Du Bois (M2), and ASTM E646 (M3). For the lowest strain rate test, longitudinal (ε_l) and axial (ε_a) strain values were collected, allowing point-to-point Poisson's ratio (ν) calculation, which can be mathematically expressed as Eq. (1):

$$\nu = -\frac{\varepsilon_l}{\varepsilon_a}, \tag{1}$$

in this case, the elastic Poisson's ratio is taken as the value obtained at the peak, separating the elastic region from the plastic region, and the Poisson's ratios curve (ν) is used for true stress calculation of M1 and M2, for all strain rates. Considering (ε_e) as the engineering strain, the true strain (ε_T) is obtained by Eq. (2):

$$\varepsilon_T = log(1 + \varepsilon_e). \tag{2}$$

From the tensile physical test results and the specimen's geometry, it is known the point-to-point force (F) and the initial area (A_0). Therefore, the engineering stress (σ_e) is defined by Eq. (3):

$$\sigma_e = \frac{F}{A_0}, \tag{3}$$

allowing the true stress calculation (σ_T). Model 1 (M1) is obtained by Eq. (4):

$$\sigma_{T1} = \frac{\sigma_e}{(1-\nu\varepsilon_e)^2}, \tag{4}$$

Model 2 (M2) by Eq. (5):

$$\sigma_{T2} = \sigma_e(1 + \varepsilon_e)^{2\nu}, \tag{5}$$

Model 3 (M3) by Eq. (6):

$$\sigma_{T3} = \sigma_e(1 + \varepsilon_e). \tag{6}$$

The elastic region for all formulations is similar, following ISO 527-1 standard, the Young's Modulus (*E*) is obtained within strain range from 0.05% to 0.25%. Once *E* is known, the true plastic strain (ε_{PX}) is determined by Eq. (7):

$$\varepsilon_{PX} = \varepsilon_T - \frac{\sigma_{TX}}{E}, \tag{7}$$

where the subscript X refers to formulation identification numbers.

Five samples for each test were used. The average curve was calculated for each strain rate extrapolating the plastic strain up to 300% to make sure there were an equal number of equidistant points in all cases. True stress vs true plastic strain diagrams are presented in the Figure 2, for all test speeds and M1, M2, and M3 formulations.

Once the true stress vs true plastic strain curves are generated, combinations between the curves are established with a parameter to be calibrated. Therefore, models 4 (M4), 5 (M5), and 6 (M6) are formulated according to Eq. (8), Eq. (9), and Eq. (10), respectively:

$$\sigma_{T4} = \alpha\sigma_{T1} + (1 - \alpha)\sigma_{T2}, \tag{8}$$

$$\sigma_{T5} = \alpha\sigma_{T1} + (1 - \alpha)\sigma_{T3}, \tag{9}$$

$$\sigma_{T6} = \alpha\sigma_{T2} + (1 - \alpha)\sigma_{T3}, \tag{10}$$

it should be noted the true plastic strain range is the same for all formulations, from 0% until 300%, as extrapolated.

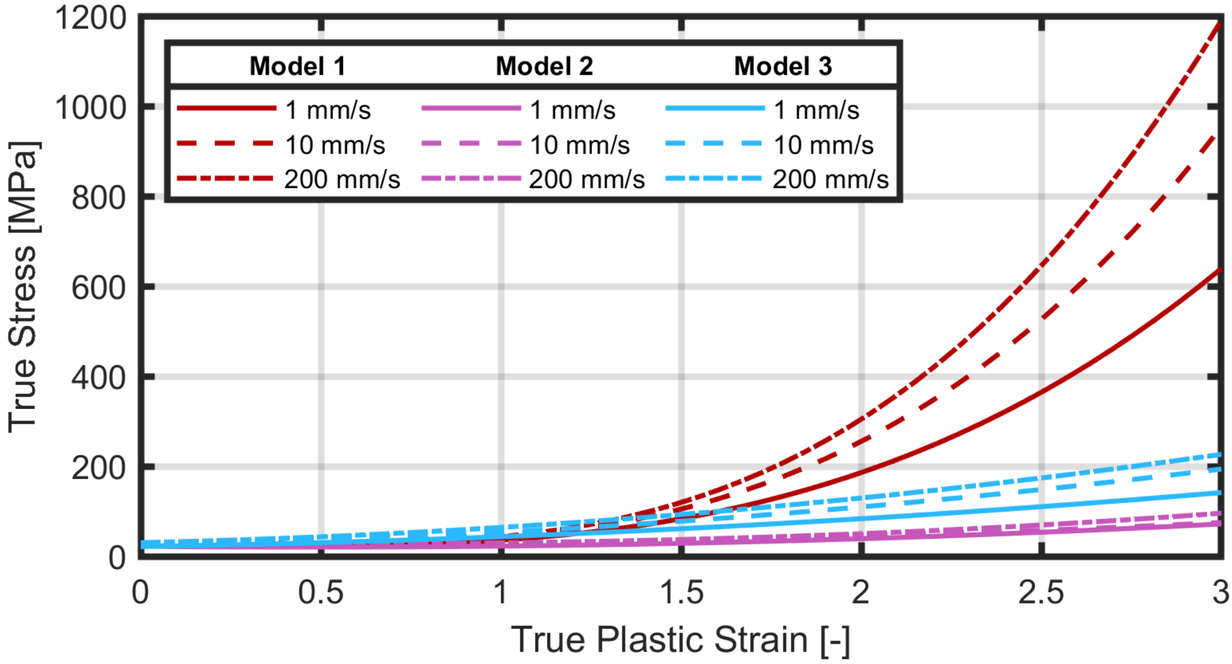

Figure 2. Formulation curves for each test speed: 1 mm/s, 10 mm/s, and 200 mm/s.

Values for α are within the interval from 0.0 up to 1.0, i.e., α ∈ [0.0, 1.0]. When α reaches the max or min value, the formulation will correspond to one of the original literature relationships. Figure 3 shows the three combinations for the speed of 1 mm/s, with α ranging from 0.0 up to 1.0, with an increment size of 0.05.

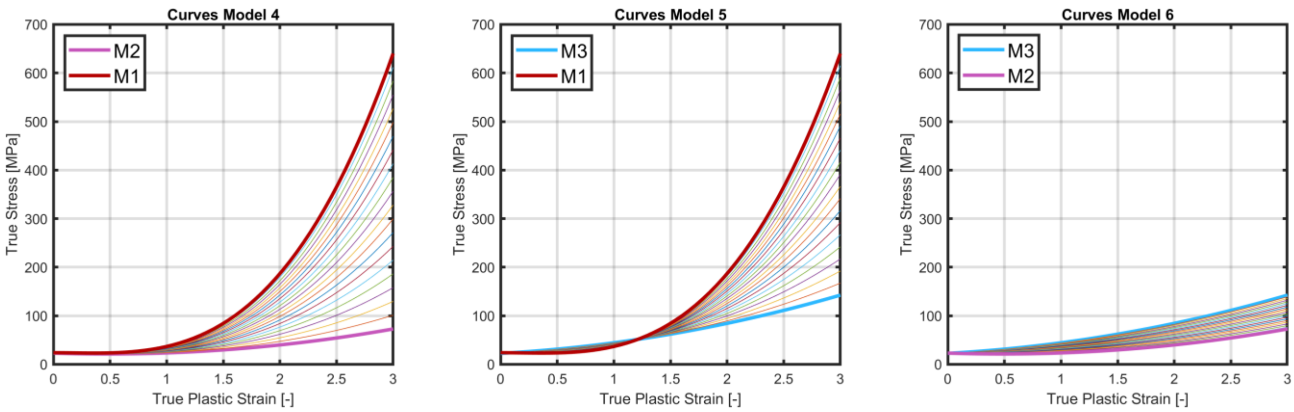

Figure 3. Curves generated by the equation combinations (for the test speed of 1 mm/s only).

Not necessarily within this range, the same value of α will produce the best result for all models. For this reason, an assessment was conducted with several α numbers, aiming the identification of a global minimum.

2.2 Structural Simulations

FE models were created for each standardized test. Thus, four test configurations were considered: Tensile (T) at 1 mm/s, Compression (C) at 0.05 mm/s, Three-Point Bending (TPB) at 0.25 mm/s and Erichsen (ERI) at 0.23 mm/s. A simplified representation of each scenario is shown in the Figure 4. The Young's modulus, elastic Poisson's ratio and density, obtained from the tests, are presented in Table 1.

Implicit quasi-static analysis was used to represent and run the structural simulations. The specimens were modeled using elements type C3D8I, that are of continuum three-dimensional with 8 nodes and complete integration type. For all cases, a mesh convergence study was carried out, at which time the meshes were gradually refined until they reached stable results, and at this point, force and time data for this paper were collected. Table 2 present information about the models and elements used for each specimen to perform the simulations.

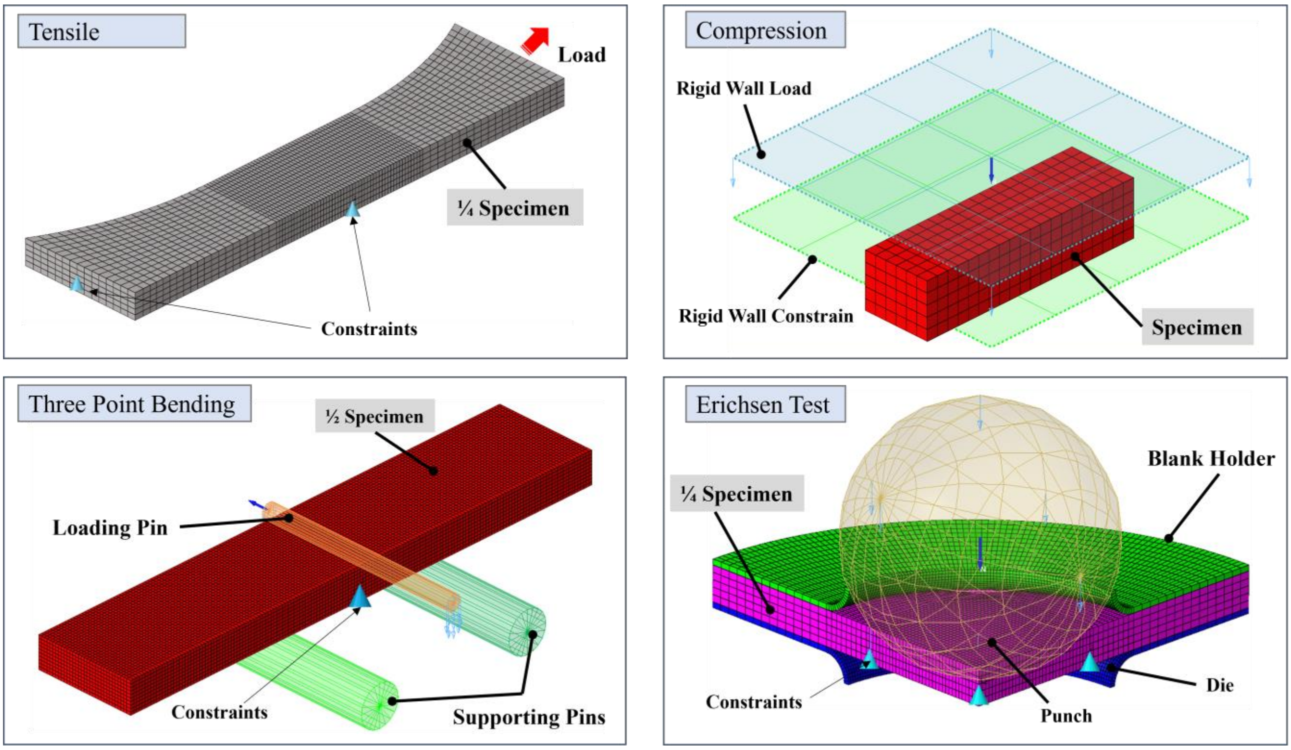

Figure 4. FE models, constraints, and loadings. Some were simulated by symmetry, so the force values were multiplied by the scalar of symmetry (i.e., 1/2 symmetry implies $F_{test} = 2 * F_{simulation}$).

Table 1: Polypropylene (PP) mechanical properties.

Young's Modulus (MPa)	Poisson's Ratio	Density (kg/mm^3)
1269.0	0.377	1.0 E-06

Table 2: Representation of specimen, volume by element, total volume of specimen, number of nodes and total number of elements corresponding to each of standardized tests for FE model.

Test	**Symmetry**	**Volume by Element, mm^3 Smaller/Bigger**	**Total Volume, mm^3**	**Nº Nodes**	**Total Nº Elements**
T	1/4	0.0207/0.0896	251.967	8736	6750
C	-	0.1200/0.1200	72	882	600
TPB	1/2	0.0296/0.0444	1550	58806	51520
ERI	1/4	0.0842/0.2829	2118.722	18636	15040

2.3 Correlation through the Normalized Root Mean Square Error (NRMSE)

To assess whether the models provided a good correlation with the physical tests, the Normalized Root Mean Square Error (NRMSE) calculation was adopted. This technique was used because it is known each mechanical scenario has distinct values of force. To avoid outliers, a normalization was performed using the maximum value of each test. Mathematically, the NRMSE for a particular test is given by Eq. (11):

$$NRMSE_{Test} = \frac{\sqrt{\frac{1}{n}\Sigma\left(y-y_p\right)^2}}{y_{max}}. \tag{11}$$

In this case, the values correspond to the force obtained in the physical test (y) and in the simulation (y_p), where n is the total points compared, and (y_{max}) is the physical test maximum force. To consider a general mathematical model, the NRMSE average results for each scenario is calculated, as shown in the Eq. (12). The closer the Total NRMSE result is to zero, the better the mathematical model to represent the represent the true mechanical behavior of the test via the simulation.

$$NRMSE_{total} = \frac{1}{4}(NRMSE_T + NRMSE_C + NRMSE_{TPB} + NRMSE_{ERI}), \tag{12}$$

3. RESULTS

Initially, tests were simulated considering only the true stress formulations given by equations Eq. (4), Eq. (5) and Eq. (6) or M1, M2 and M3. The mechanical tests results are presented in Figure 5. It is noted the M2 is the one that best correlated, although it deviates for the Tensile test. The total NRMSE values of the formulations were calculated using Eq. (12). These results are presented in Table 3.

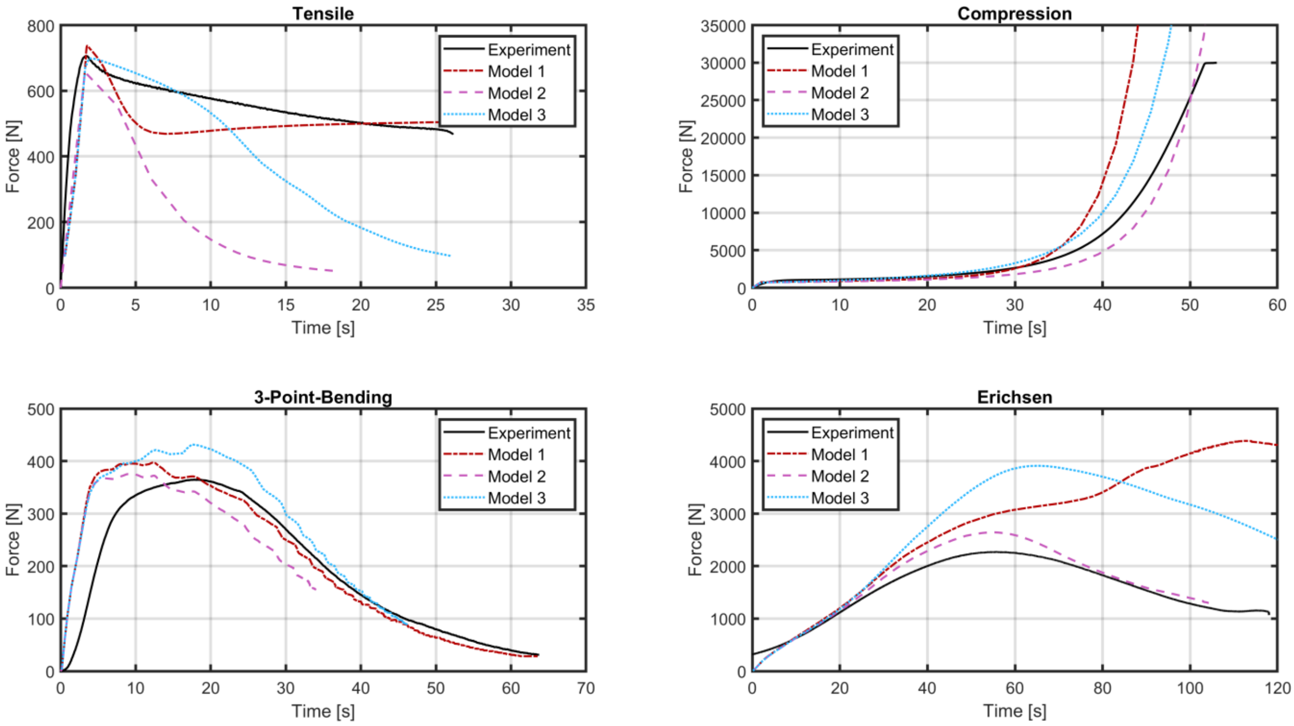

Figure 5. Model 1, Model 2 and Model 3 results along with physical tests.

Table 3. Total NRMSE values for the literature equations: Eq. (4), Eq. (5), and Eq. (6).

Formulation	**Model 1**	**Model 2**	**Model 3**
$NRMSE_{Total}$ [-]	0.2612	0.1865	0.2853

Subsequently, several configurations were simulated combining the M1, M2 and M3 formulations with different α values. For each physical test and model, the NRMSE values were calculated according to Eq. (11), so the Total NRMSEs of the formulations were determined using Eq. (12). Relationships between error and the α parameter are shown in Figure 6. As expected, the α values that minimize each model's error are different. Table 4 shows these minimum values along with the Total NRMSE value. Figure 7 presents the obtained NRMSE values for all equations and tests.

Table 4. Initial α values that minimize the Total NRMSE of each formulation.

Description	**Model 4**	**Model 5**	**Model 6**
α	0.20	0.35	0.95
$\boldsymbol{NRSME_{Total}}$	0.1700	0.2427	0.1849

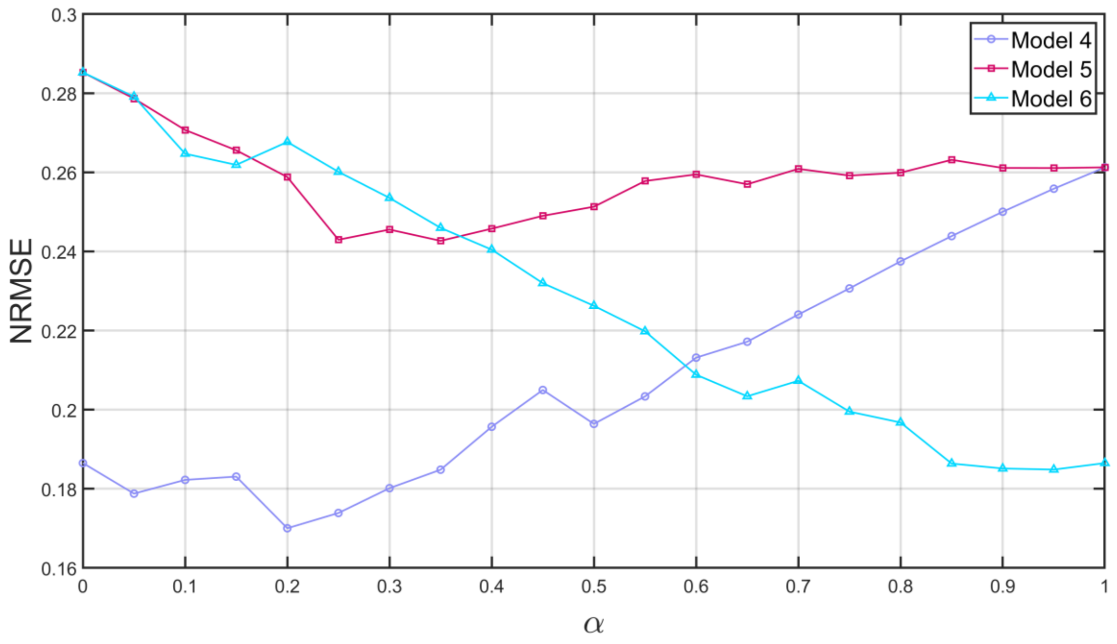

Figure 6. NRMSE variation in function of α parameter for M4, M5, and M6.

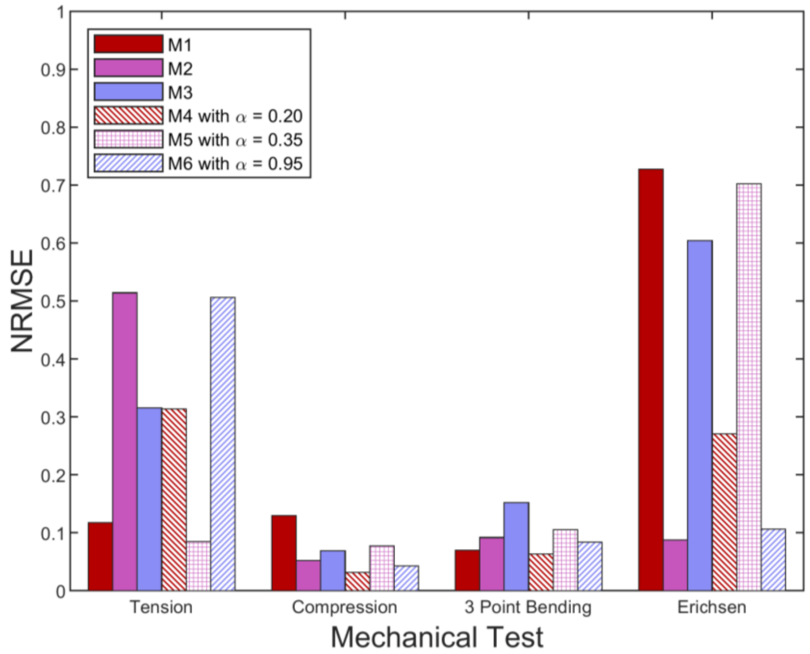

Figure 7. NRMSE values with the α parameters that minimized the Total NRMSE of each configuration.

As M4 formulation showed the lowest Total NRMSE when α is equal to 0.2, a new investigation was conducted further exploring α values ranging from 0.15 to 0.25, with increments of 0.01, therefore adding eight new studied points. The results are presented in Figure 8. It was noticed the error reduced slightly, leading the M4 with α = 0.22 to achieve an NRMSE of 0.1690, which is the lowest error among all configurations and formulations.

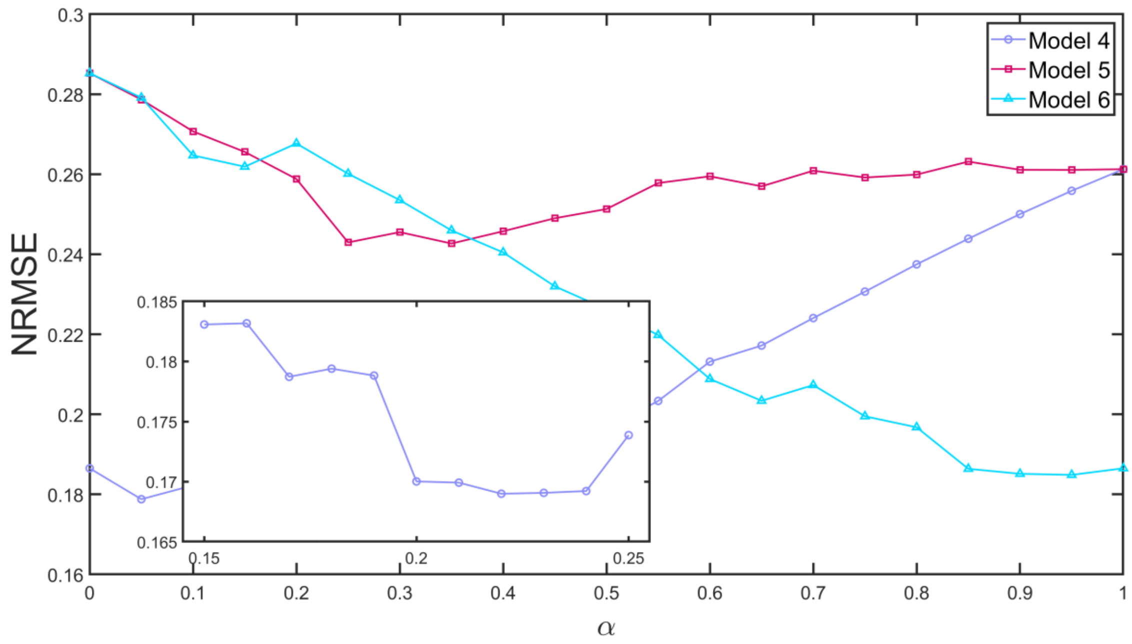

Figure 8. New M4 results around the minimum region (α ranging from 0.15 to 0.25).

Figure 9 present the results for experimental tests as well as the results for simulations with M4 (α = 0.22), M5 (α = 0.35) and M6 (α = 0.95) formulations. Upon analyzing each physical test, it becomes evident the configuration that achieved the lowest overall NRMSE is not necessarily the one that reached minimum values in each test, but rather the one that best fits them in a general sense. This is comprehensible when examining the Tensile and Erichsen curves in Figure 9, where the M5 equation with α = 0.35 would be the best proposal for the Tensile test, and the M6 formulation with α = 0.95 is the best for the Erichsen test.

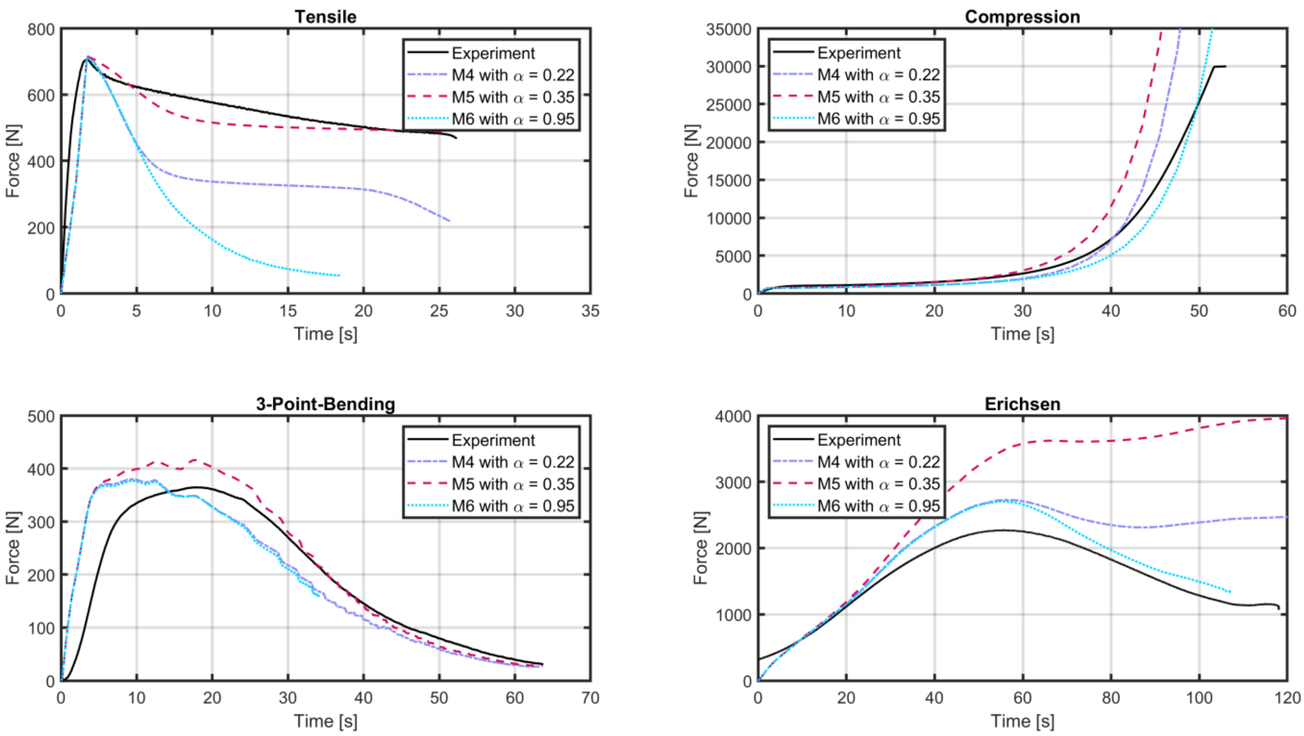

Figure 9. Model 4 (α = 0.22), Model 5 (α = 0.35) and Model 6 (α = 0.95) results along with physical tests.

Although the M4 configuration (α = 0.22) does not show the best results for each individual test, as summarized in Table 5, it is the one that best fits the tests in a global sense, thereby increasing the correlation between simulation and physical tests.

Table 5. NRMSE values per test, corresponding to the α parameters that minimize the Total NRMSE.

	Tensile	**Compression**	**TPB**	**Erichsen**
M4 ($\alpha = 0.22$)	0.2881	0.0364	0.0630	0.2885
M5 ($\alpha = 0.35$)	0.0852	0.0779	0.1054	0.7022
M6 ($\alpha = 0.95$)	0.5057	0.0432	0.0840	0.1065

4. CONCLUSION

An assessment of correlation between physical and simulated tests for Polypropylene (PP) was performed, combining true stress equations from the literature through the von Mises Classical Metal Plasticity constitutive model available in ABAQUS® solver. The evaluations were based on Normalized Root Mean Square Error (NRMSE) comparisons that consider the average of the following mechanical tests: Tensile, Compression, Three-Point Bending and Erichsen. The study aimed to investigate the sensitivity of the output data (Force vs Time) to the input data (True Stress vs True Plastic Strain). The input data were set from formulations based on ASTM E646, ISO 18872 standards, and the DuBois equation, besides several combinations of these original formulations through a calibration parameter (α).

The results considering only the literature equations indicated that the Du Bois formulation (Model 2) provides the best correlation, showing in Table 3 a Total NRMSE of 0.1865. However, when each test is analyzed individually, it is observed that this configuration has an error greater than 50% for the Tensile test. Therefore, combinations between the formulations were proposed to minimize the total error, as well as the singular errors of each mechanical test.

Upon new results, it was found that Model 4, the one that combines the ISO 18872 with the Du Bois equation by a parameter value of 0.22, achieved a Total NRMSE value of 0.169 and for each test did not exceed 0.3. It was observed that even though it is not the optimal formulation for the four tests simultaneously, as Model 5 with an α of 0.35 is the best for Tensile ($NRMSE_T$ = 0.0852) and Model 6 with an alpha of 0.95 is the best for Erichsen ($NRMSE_{ERI}$ = 0.1065), Model 4 delivers the better balance between all the tests.

Furthermore, even though the classical von Mises constitutive formulation is not recommended for simulating thermoplastics, the use of approximations for input data based on different true stress formulations results in values closer to reality, thus increasing the correlation between actual and simulated physical tests. For future work, it is suggested to study other formulations different from von Mises Classical Metal Plasticity, were other material properties and stress states dependence may present more corelated results between FE simulation to true thermoplastic behavior.

5. ACKNOWLEDGEMENTS

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