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A COMPARATIVE EVALUATION OF SUITABLE CONSTITUTIVE MODELS FOR THERMOPLASTICS WITH THOSE BASED ON THE VON MISES CRITERION

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Abstract. *Thermoplastics have characteristics that differentiate them from metals, becoming challenging to simulate their structural behavior. Besides, literature demonstrates the elastoplastic model based on von Mises criterion is not suitable to represent the polymers behavior. Therefore, for structural simulations involving thermoplastics, a proper selection of the constitutive model is required to obtain reliable results. Thus, this work aims to evaluate constitutive models available in LS-DYNA[®] solver, through the correlation with physical tests. The methodology is divided into three stages. First stage concerns the data treatment and fitting, obtained from standardized tests of tensile and compression, carried out with polypropylene specimens. These data are inputs of the assessed constitutive models: Piecewise Linear Plasticity and Semi-Analytical Model for Polymers (SAMP-1). A SAMP-1 derivation was also studied by activating the damage curve. The second step consists in running finite element analyses for each constitutive model and verifying which one best correlates with the following physical tests: Tensile, Compression, Three-Point Bending and Erichsen. Finally, the Normalized Root Mean Square Error was used to determine the best constitutive model. In conclusion, the results indicated the SAMP-1 predictions are more assertive than those from Piecewise Linear Plasticity, the one based on von Mises criterion.*

Keywords: *thermoplastics; finite element method; constitutive model; numerical simulation; standardized test.*

1. INTRODUCTION

Since the 20th century, with the onset of the second industrial revolution and the subsequent technological advances, the use of plastic materials in various industrial sectors has become indispensable, including the automotive industry (Mathijssen, 2016). Some attributes justify the ever-increasing use of thermoplastics in structural components, such as low density, low cost, and the possibility of manufacturing complex geometries. Conversely, these materials are quite sensitive to thermal variations and strain rates, in addition to not being isochoric during plastic flow. These characteristics differentiate them from metallic materials, imposing challenges regarding the prediction of their structural behavior. This distinct behavior may be observed in the dissimilarity between the yield ranges under tension and compression loadings (Kurudimath et al., 2021).

The deep knowledge about how to simulate thermoplastics behavior through Finite Element Method (FEM) is one of the main challenges for structural engineering to meet the needs of the industry. A proper selection of the constitutive model allows optimized designs, reduced physical testing costs and consequently, increased companies' profitability. Nowadays, constitutive models based on the classical von Mises criterion are commonly used by the industry to represent polymers. It occurs because these models are minimally able to describe plastic behavior and are widely available in FEM solvers. However, they may not show good correlation with physical tests, since they were developed based on the metals' elastoplastic behavior.

Considering this context, the LS-DYNA[®] solver emerges as a robust FEM tool that provides a wide variety of material cards, including the Semi-Analytical Model for Polymers (SAMP-1). This constitutive model is suitable to represent the polymers' distinct behaviors when under tension and compression, as well as capturing the high strain rate sensitivity, volume dilatation after yielding, and stiffness loss due to damage accumulation (Kolling et al., 2005).

Therefore, this work compares SAMP-1 (MAT187) with a constitutive model based on the von Mises criterion, the Piecewise Linear Plasticity (MAT024), in order to evaluate the correspondence between physical tests and numerical

simulations. Tensile and compression standardized tests data are acquired from polypropylene specimens. They are treated for being used by the aforementioned constitutive models. Thus, FEM analyses are performed for the following tests: Tensile (T), Compression (C), Three-Point Bending (TPB), and Erichsen (ERI), where the effects of using the MAT187 along with damage curve are also investigated. Finally, the Normalized Root Mean Square Error (NRMSE) is used to determine the best constitutive model.

2. METHODOLOGY

Among the studied constitutive models, MAT024 was originally developed for metals and describes material behavior based on J2 plasticity, which uses a formulation based on the von Mises criterion (Kurudimath et al., 2021). In this model, the elastic region is modeled independently of strain rates up to an arbitrary or fixed yield point. From this point, the minimum strain rate of interest is decomposed into an elastoplastic model. This is possible because the plastic region can be defined by inputting true stress vs true plastic strain curves for different strain rates (Reithofer et al., 2018).

Conversely, MAT187 was developed exclusively for polymers characterization. Although it represents the elastic region and strain rate dependence similarly to MAT024, it can also capture viscoelastic and viscoplastic behavior, non-isochoric plastic strain, stiffness losses of the material due to damage, and different behavior in compression, tensile, and shear (Kolling et al., 2005). This constitutive model allows the representation of permanent volumetric strain, as the hardening of thermoplastics is anisotropic and plastic strain does not occur at constant volume, which means that it does not satisfy the incompressibility condition. Therefore, the tensile test needs to be processed with optical methods such as Digital Image Correlation (DIC) to obtain the point-wise plastic Poisson's ratio (Nutini and Vitali, 2008).

Damage processes, such as cracks or voids, may result in volumetric expansion of deformed polymeric specimens. Thus, this paper presents an extra scenario using damage curve available in MAT187, based on the application of the effective stress curve (Nutini and Vitali, 2008). Subsequently, the results arising from this parameter activation are compared with MAT024 and MAT187 results.

The flowchart shown in Figure 1 depicts the methodology, starting from the experimental data treatment to obtain the minimum information required by the constitutive models, then FEM models are built and run for all tests, ending with the assessment through the NRMSE.

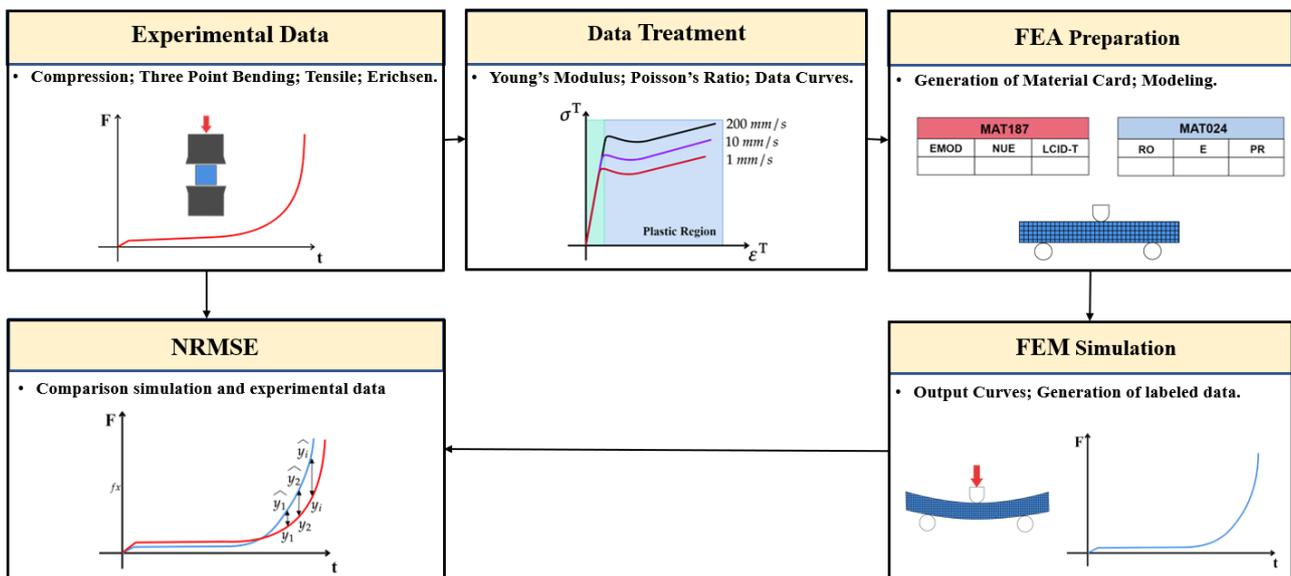


Figure 1. Flowchart of the methodology.

2.1 Constitutive Models and Data Treatment

As mentioned, each constitutive model requires specific information to be filled in, such as mechanical properties, curves, or calibration constants. Therefore, Figure 2 illustrates the MAT187 formulation, highlighting the boxes that were filled during this work. For the empty fields, the default values set by the software were used.

```

*MAT_SAMP-1
PP
$#      MID      RHO      NULK      GMOD      EMOD      NUE      RBCFAC      NUMINT
      1      1.00E-09
$#      LCID-T      LCID-C      LCID-S      LCID-B      NUPE      LCID-P      INCDAM
      1      6      8
$#      LCID-D      EPFAIL      DEPRPT      LCID-TRI      LCID_LC
      7
$#      MITER      MIPS      INCFAIL      ICONV      ASAF
$#      LCEMOD      BET      FILT      -Constant Parameters
                                     -Material Curves to be calibrated
    
```

Figure 2. Example of the material card MAT187.

Figure 3 illustrates the MAT024 formulation, highlighting the boxes that were filled during this work. For the empty fields, the default values set by the software were used.

```

*MAT_PIECEWISE_LINEAR_PLASTICITY_TITLE
PP
$#      MID      RO      E      PR      SIGY      ETAN      FAIL      TDEL
      1      1.00E-09      1269.0      0.377
$#      C      P      LCSS      LCSR      VP
      1
                                     -Constant Parameters
                                     -Material Curves to be calibrated
    
```

Figure 3. Example of the material card MAT024.

Standardized test results were used for the polypropylene characterization. They were obtained from reports provided by Ford Motor Company. These reports contained information such as specimen dimensions, tests response data, and fundamental mechanical parameters. To use this information in the LS-DYNA[®] solver, it is necessary to apply data treatment to avoid the presence of unwanted data, such as noise or excessive data points (Lobo et al., 2013), as well as conversion to true stress-strain curves. Table 1 shows the available data for each test and the number of specimens.

Table 1. Available physical tests data.

Experiment	Samples	Force	Displacement	Time	Transverse Strain	Axial Strain
Tensile at speed of 1mm/s	5	X	X	X	X	X
Tensile at speed of 10mm/s	5	X	X	X	X	X
Tensile at speed of 200mm/s	5	X	X	X	X	X
Compression	4	X	X	X	-	-
Three-Point Bending	4	X	X	X	-	-
Erichsen	4	X	X	X	-	-

To convert the results of the physical tests to the parameters shown in Figures 2 and 3, the data treatment is performed using equations derived from technical standards and literature references. The data treatment focuses on the MAT187 parameters, once its inputs can be also used by MAT024. The details of the equations are presented below. The point-to-point Poisson's ratio (ν) is calculated from the tensile test values at a speed of 1 mm/s, as shown in Eq. (1), being the negative ratio between the transverse strain (ϵ_x) and the axial strain (ϵ_y):

$$\nu = -\epsilon_x/\epsilon_y. \quad (1)$$

Additionally, the true strain (ϵ_T) can be calculated using the Eq. (2):

$$\epsilon_T = \ln(1 + \epsilon_y). \quad (2)$$

Since the specimen geometry is known, the engineering stress (σ_e) can be calculated by Eq. (3), where F represents the applied force and A_0 is the initial cross-sectional area:

$$\sigma_e = F/A_0. \quad (3)$$

The Young's modulus is usually set according to ISO 527, so the true plastic strain (ε_p) can be defined by Eq. (4):

$$\varepsilon_p = \varepsilon_T - \sigma_e/E. \quad (4)$$

This work used the Du Bois equation to obtain the true stress that fills the tensile field, a commonly used approach for SAMP-1 constitutive model, as described in Lobo et al. (2013). The n is an index that considers the point-to-point Poisson's ratio. Additionally, the compression true stress is determined using the ASTM E646 standard. Then, for both tensile (σ_{Tn}) and compression (σ_{Tc}) the values are determined by Eq. (5) and Eq. (6), respectively:

$$\sigma_{Tn} = \sigma_{en} \cdot (1 + \varepsilon_{yn})^{2\nu_n}, \quad (5)$$

$$\sigma_{Tc} = \sigma_e \cdot (1 + \varepsilon_y). \quad (6)$$

Particularly for SAMP-1, the damage curve (d) may be activated, being defined by the parameter of the Eq. (7):

$$d = 1 - e^{-m}, \quad (7)$$

where in case the strains ε_x and ε_z are equal, the volumetric strain (m) can be given by Eq. (8):

$$m = 2 \cdot \varepsilon_x + \varepsilon_y. \quad (8)$$

Nutini and Vitali (2008) indicate the damage occurrence requires the effective stress (σ_{eff}), given by Eq. (9):

$$\sigma_{eff} = \frac{\sigma_{Tn}}{1-d}, \quad (9)$$

The ordinary parameters were density ($\rho = 1.0E-6$ t/mm³), Young's modulus ($E = 1269$ MPa), and elastic Poisson's ratio ($\nu = 0.377$). 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.

Finally, the true stress-strain curves were calculated. The true plastic strain values were extrapolated up to 300% to ensure there were an equal number of equidistant points in all cases. It is important to highlight two models were developed for MAT187, one that uses damage curve and effective stress (from Eq. 5 until Eq. 9), and another that does not use damage curve and effective stress (only Eq. 5 and Eq. 6). This paper referred them as Effective Du Bois (EDB) and Real Du Bois (RDB), respectively. Figures 4 and 5 show the curves obtained for MAT187 by this data treatment, for each tensile test speed (LCID-T), compression (LCID-C), plastic Poisson's (LCID-P), and damage (LCID-D). The RDB tensile curves were used in MAT024.

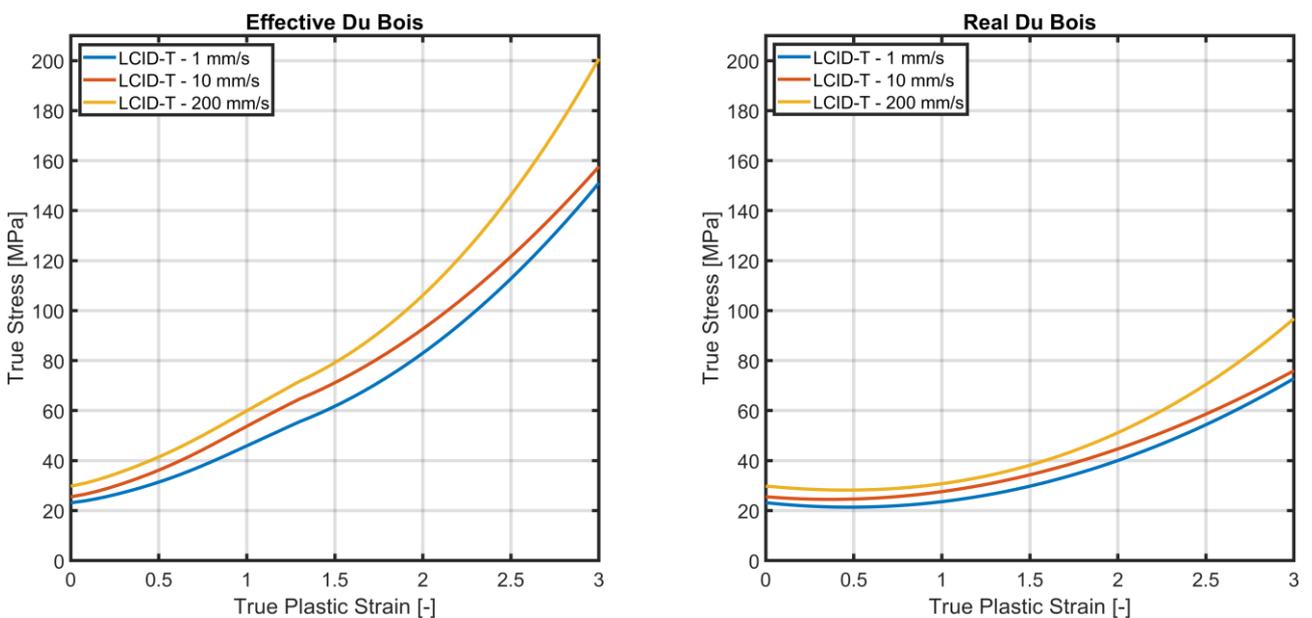


Figure 4. LCID-T (MAT187) curves for Effective Du Bois and Real Du Bois, named as LCSS in MAT024.

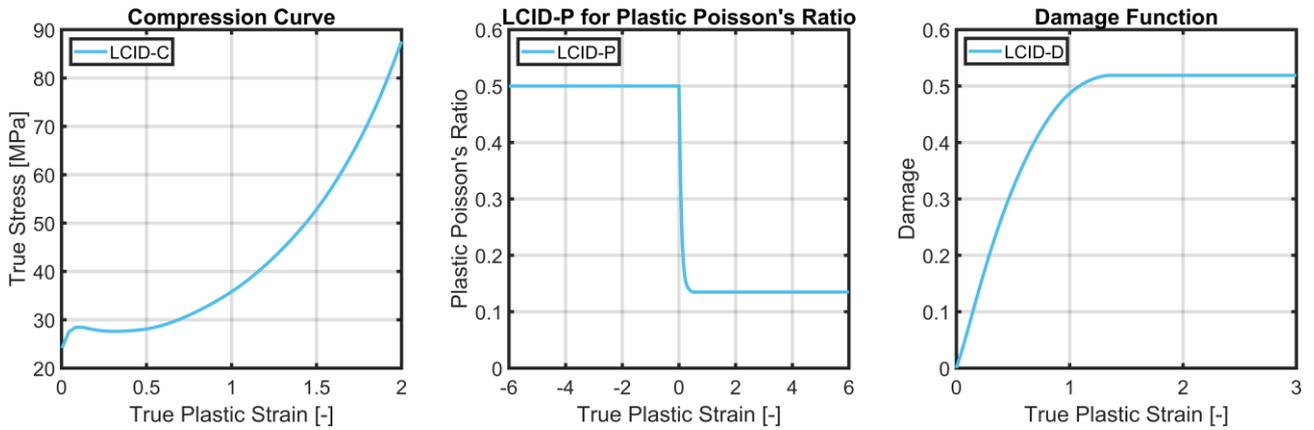


Figure 5. LCID-C, LCID-P, and LCID-D, available only in MAT187.

2.2 Finite Element Analysis Setup

Considering the high number of elements, the analyses were run considering symmetry techniques, so the force values were multiplied by the scalar of symmetry (i.e., 1/4 symmetry implied $F_{test}=4 \cdot F_{simulation}$). This approach provided consistent values and reduced computational costs. Therefore, 1/4 of the geometries were considered for Tensile and Erichsen tests, 1/2 for the Three-Point Bending, and the whole geometry was considered for Compression, as shown in Figure 6.

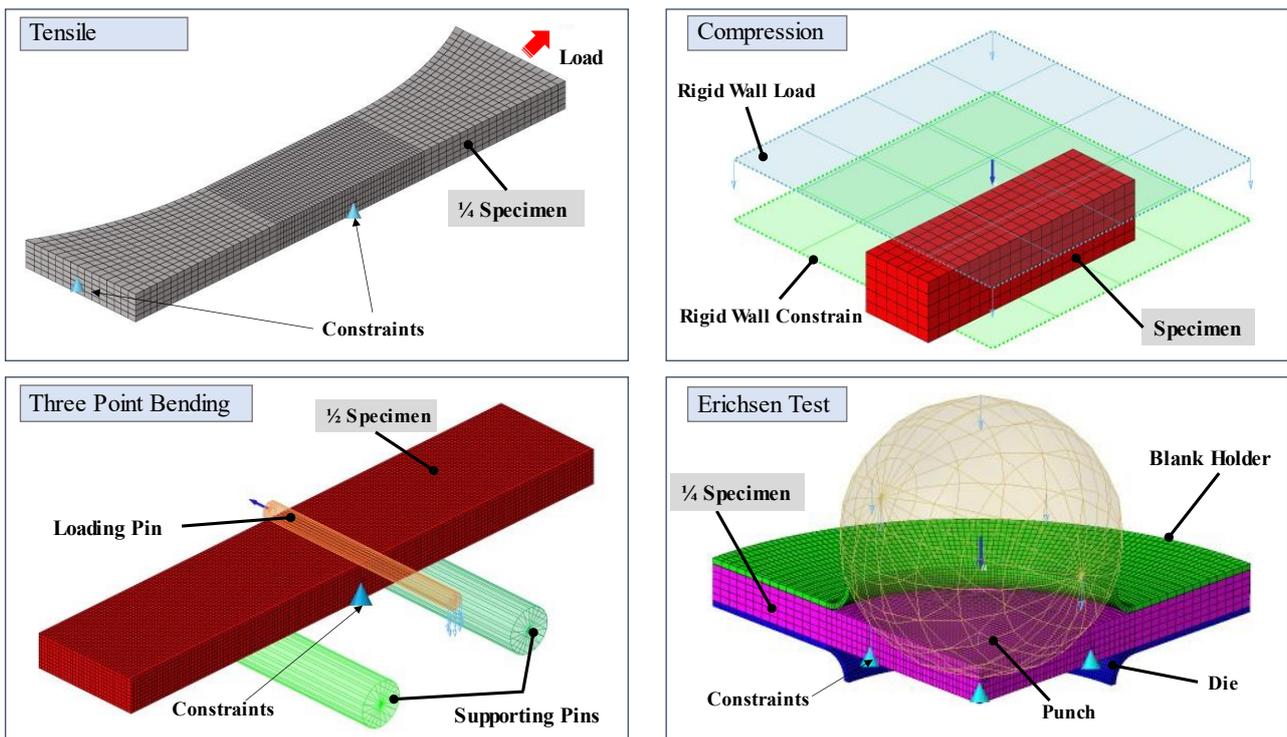


Figure 6. FEM models, constraints, and loadings.

The loading condition was based on the displacement-time data available for each specimen and physical test, as presented in Table 1. Rigid walls were used for Compression, Three-Point Bending, and Erichsen simulations, while displacements were applied for the tensile test through defined node sets for motion. In addition, hexahedral elements were chosen for most elements. It is worth mentioning the additional parameters, such as `*CONTROL_HOURLGLASS`, where its absence would result in elements with zero energy deformation modes that could distort and impair the solution. Also noteworthy is the use of mass scaling by the keyword `*CONTROL_TIMESTEP`. It was used to control the timestep size, and its use required an evaluation of the mass increase applied to the FEM models.

2.3 Normalized Root Mean Square Error

To assess the results obtained, the Root Mean Square Error (RMSE) metric was used, which is commonly used to evaluate the accuracy of a predictive model in relation to observed values. In summary, it is a measure of the dispersion of error between the model's predictions and the corresponding actual values. A lower RMSE value indicates better performance. The calculation is given by the square root of the mean of the squared errors, as shown in Eq. (10):

$$RMSE = \sqrt{\frac{\sum_{i=1}^n (\hat{y}_i - y_i)^2}{n}}, \quad (10)$$

where \hat{y}_i represents the predicted value by the model and y_i represents the actual observed value. However, for comparison between different models that have different variables and scales, it is necessary to use the normalized form, known as the Normalized Root Mean Square Error (NRMSE). The normalization is done by dividing the RMSE by the maximum (y_{max}) value of the target variable. Mathematically, the NRMSE of a particular test is given by Eq. (11):

$$NRMSE = \frac{RMSE}{y_{max}}. \quad (11)$$

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. This allowed a general observation of which model better represents the behavior of the studied polypropylene:

$$NRMSE_{Total} = \frac{1}{4} (NRMSE_{Tensile} + NRMSE_{Compression} + NRMSE_{TPB} + NRMSE_{Ericksen}). \quad (12)$$

3. RESULTS

Figure 7 presents some results. It is worth noting that only one sample of each test was chosen for this graphical representation. By analyzing the curves, and considering only the elastic region, it is possible to notice the proximity and similarity in the behavior of the virtual simulations in relation to the physical tests. This can be justified by using a constant value of Young's modulus for both models. However, when analyzing the plastic region, significant differences can be observed between MAT187 and MAT024, especially for the tensile and compression curves.

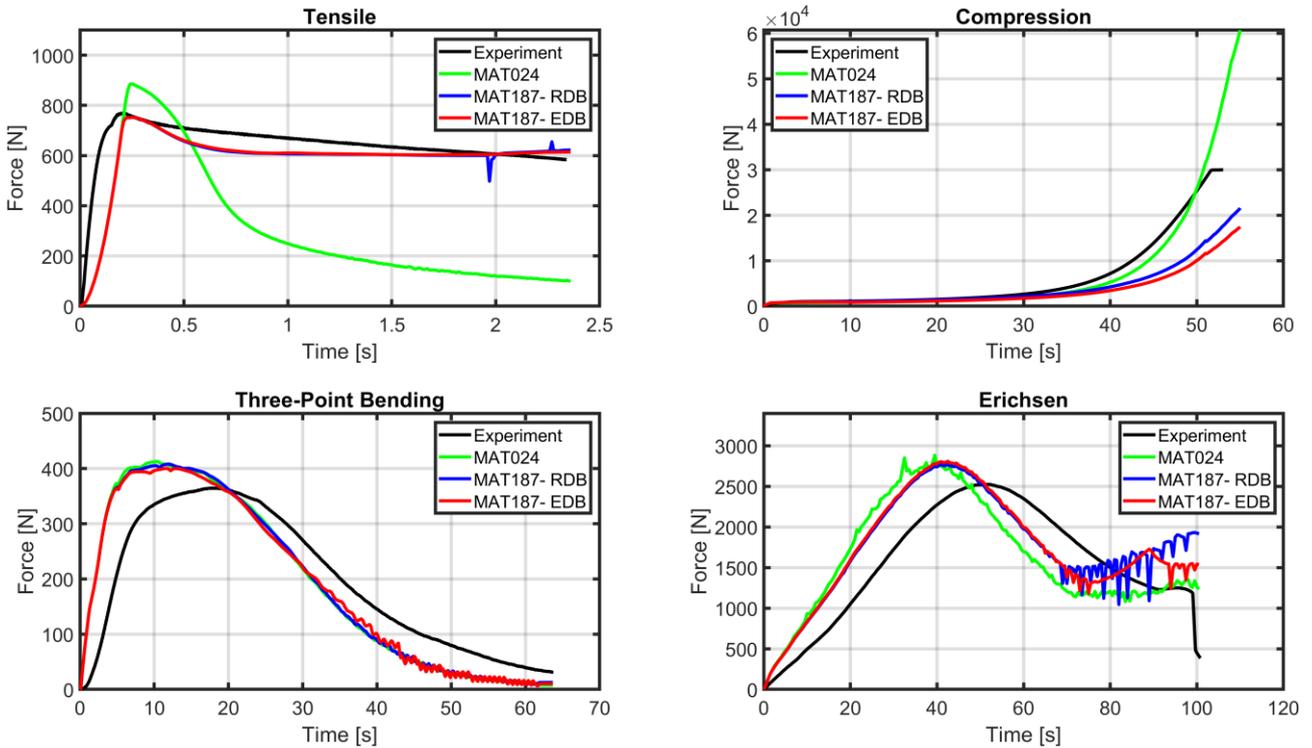


Figure 7. Physical and simulated results for Tensile, Compression, Three-Point Bending, and Ericksen.

For tensile, the difference between the models can be justified by the fact the MAT024 formulation does not consider specimens volume changes. Moreover, discontinuities are observed in the MAT187 - RDB curve, which can be explained by the absence of damage curve. In compression, MAT024 performed better than MAT187, however after the peak force of the physical test, a divergent behavior is observed for MAT024 towards the end of plastic region.

Furthermore, a good correlation can be observed for Three-Point Bending and Erichsen, although the Erichsen's results showed noise throughout the MAT024 and at the end for MAT187. This is due to the mass addition associated with the preset timestep. In order to quantify the observed differences and enhance the results comparison of the remaining samples, it is necessary to evaluate the values obtained by applying NRMSE. This involves obtaining the error values from Eq. (11) for each of the specimens, shown in Figure 8.

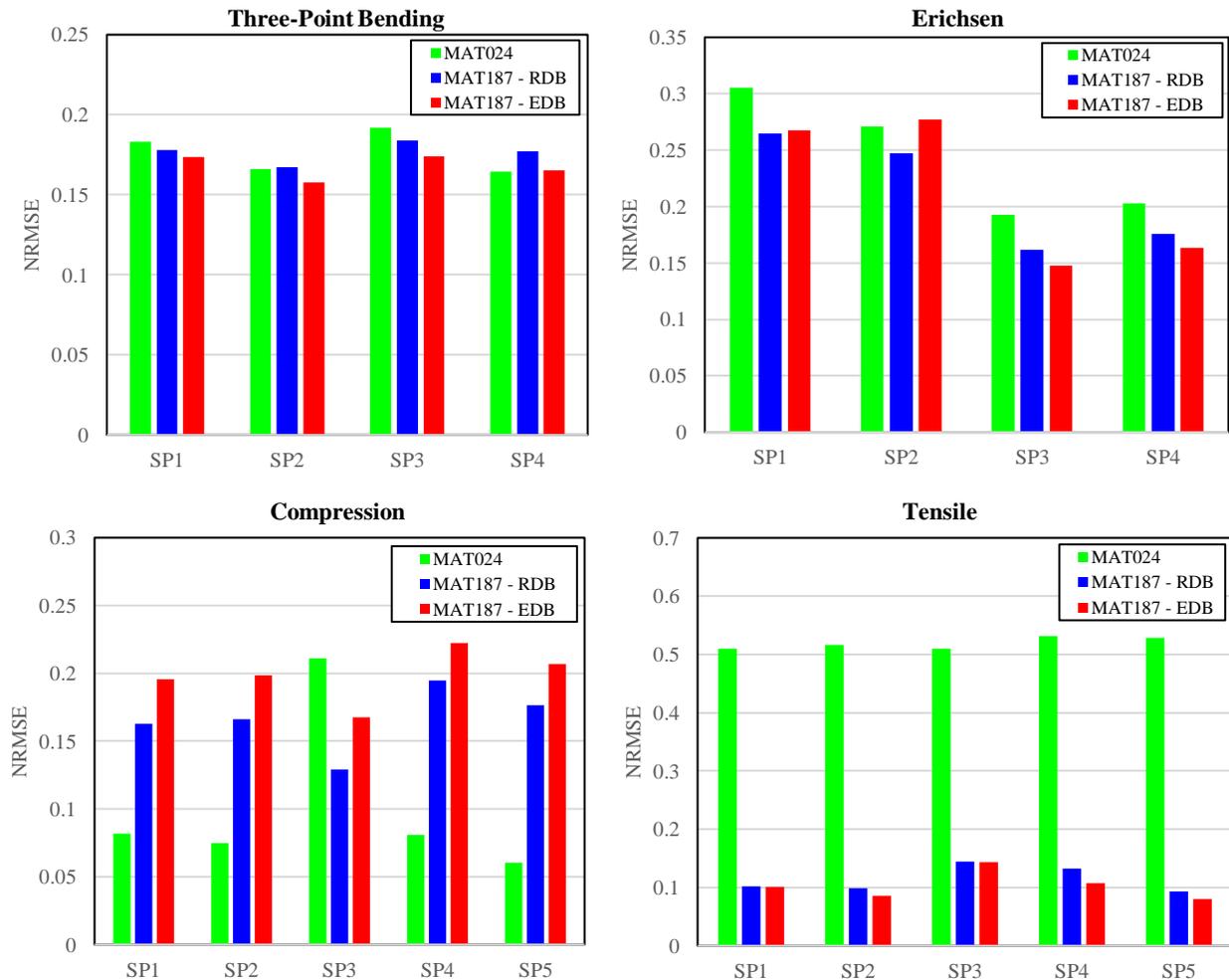


Figure 8. NRMSE of all specimens. (SP = Specimen)

The NRMSE discrepancies of different samples in the same test may be due to the chemical properties of the polypropylene, as its composition may affect the nature of the results (Nutini and Vitali, 2008). Nevertheless, a certain pattern can be observed, where the MAT187 RDB and EDB results show lower errors compared to MAT024, except for the compression test. For an overall analysis, the samples average was calculated for each test. Thus, a graph is obtained as shown in Figure 9a, and then Eq. (12) is applied to obtain the $NRMSE_{Total}$, represented in Figure 9b.

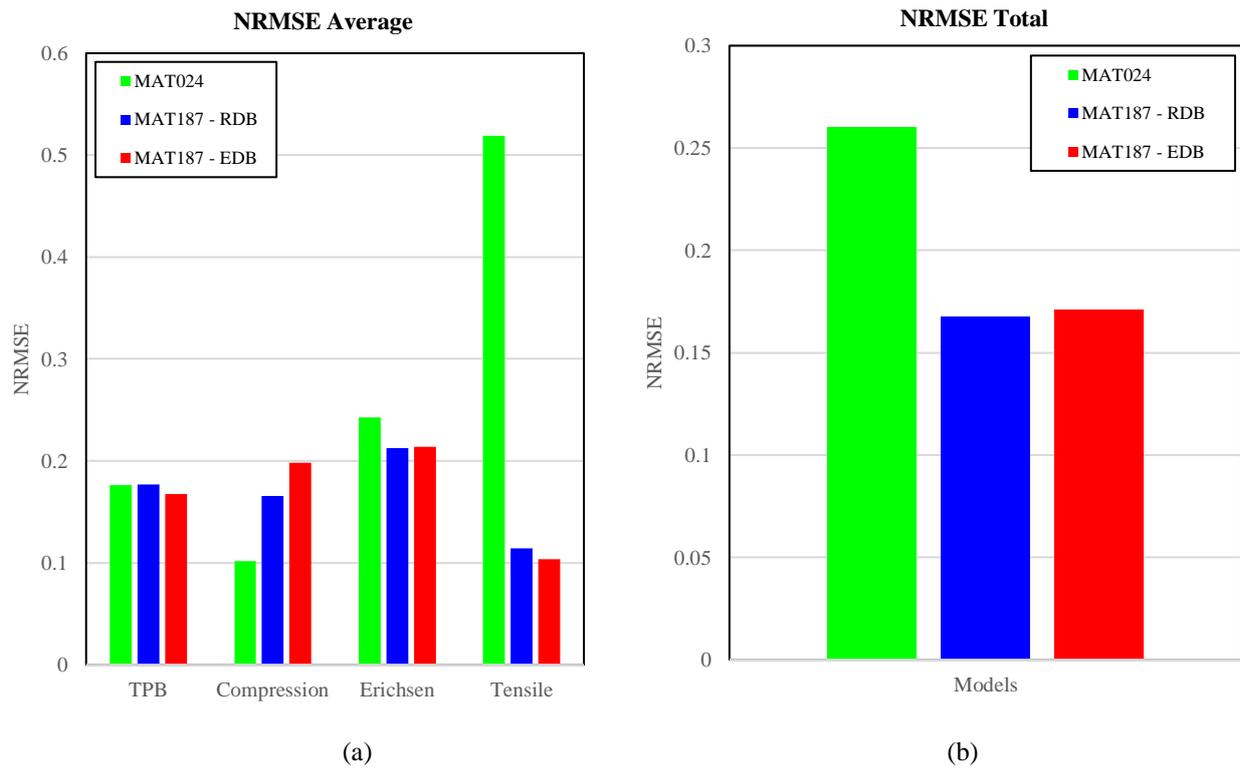


Figure 9. (a) NRMSE average of each test and (b) NRMSE total for all tests and specimens.

The evaluation of Figures 9a and 9b confirmed that MAT187 exhibits better correlation with the physical tests, as its $NRMSE_{Total}$ is lower than MAT024. However, about the Du Bois formulations comparison, it is not clear which one has better correlation with physical tests. An additional criterion was needed for this conclusion, the visual comparison of the post-processing animations, which can be seen in Figure 10. It can also be noticed that the absence of the damage curve leads to the emergence of results singularities, not observed in the NRMSE assessment. Furthermore, it is showed the inadequacy of MAT024 in representing volume variations, resulting in specimen distinct behavior, which can be seen by maximum stress values, higher in MAT024 (173.882 MPa) than MAT187 RDB (49.019 MPa) and EDB (38.105 MPa).

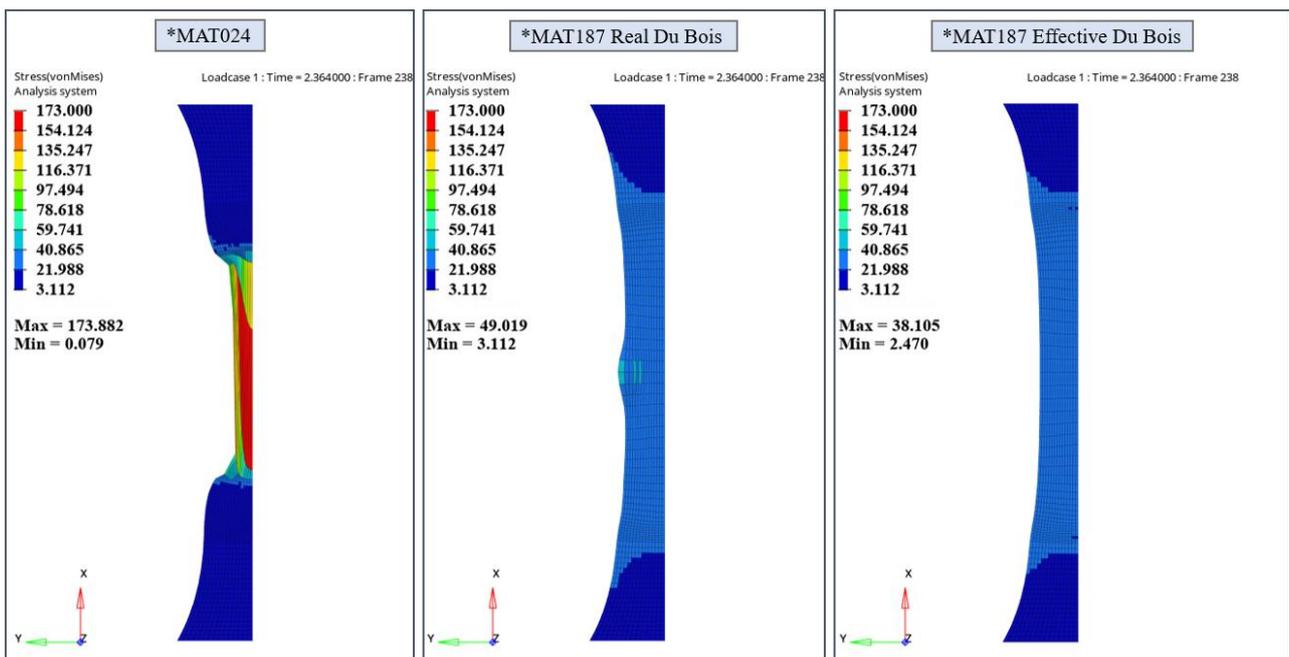


Figure 10. Stress comparison (same frame) for MAT024, MAT187 - Real Du Bois and MAT187 – Effective Du Bois.

4. CONCLUSION

Based on the curves obtained from physical tests, data treatment was performed to generate the inputs of the constitutive models. The polypropylene material was selected due to data availability provided by the Ford Motor Company. Tensile, Compression, Three-Point Bending, and Erichsen tests were performed, using stress-strain tensile curves at different speeds. The constitutive models were: MAT024 RDB, MAT187 RDB and MAT187 EDB. Additionally, the Young's modulus, elastic Poisson's ratio, and density constants were defined. The compression, plastic Poisson's ratio and damage curves were applied only to MAT187.

The MAT187 had a higher correlation with the physical tests than MAT024. A total of 18 samples were analyzed through the 4 physical tests and the results were compared by NRMSE. MAT024 performed better in compression, with an average NRMSE of 0.1017, while MAT187 had errors of 0.1658 (RDB) and 0.1981 (EDB). However, the largest difference was observed in the tensile test, where the average NRMSE was 0.5189 (MAT024), 0.1143 (MAT187 RDB), and 0.1036 (MAT187 EDB). This results difference can be attributed to the SAMP-1 ability of representing the sample volume variation, where the tensile sample's behavior difference at the simulation end could be noticed.

In addition, the use of the Effective Du Bois curve proved to be more appropriate when considering the visual post-processing results, since the absence of the damage parameter led to the emergence of singularities that were not observed in the NRMSE analysis. Therefore, further studies are needed to investigate the application of Real Du Bois in MAT187 without the use of the damage parameter.

In summary, conducting thermoplastics simulations with a constitutive model suitable for polymers resulted in a greater correlation with physical tests and underscored the importance of using these models instead of those based on von Mises criteria. Additionally, it is worth highlighting the importance of using a formulation that is compatible with the chosen constitutive model, such as the selection of the Real Du Bois and Effective Du Bois curves. In order to spread the application of SAMP-1, it is necessary to conduct future work with other polymeric materials, such as Acrylonitrile Butadiene Styrene (ABS) and Polyamide (PA).

5. ACKNOWLEDGEMENTS

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