Research, Society and Development, v. 11, n. 12, e585111234937, 2022
(CC BY 4.0) | ISSN 2525-3409 | DOI: http://dx.doi.org/10.33448/rsd-v11i12.34937

Evaluation of polymers for upper limb orthosis through computer simulation

Avaliação de polímeros para órtese de membro superior através de simulação computacional

Evaluación de polímeros para órtesis de miembro superior mediante simulación por computadora

Received: 09/04/2022 | Revised: 09/16/2022 | Accepted: 09/18/2022 | Published: 09/25/2022

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Abstract
Material selection is one of the most relevant and challenging steps in engineering projects. In this study, we focused on selecting polymers with low density and stiffness for upper limb orthoses that help in the recovery of patients who have undergone cerebrovascular accident (CVA). CES EduPack 2011 software was used to compare the density and Young's modulus of different polymers. The merit index aided in the classification of these materials, which were applied to 3D orthosis models for computer simulations in FreeCAD 0.19.4 software. Using the simulation data, a decision matrix was developed using the Pahl & Beitz method to classify polymers according to the weighted property index. The decision matrix using the simulated and merit index data indicated polyethylene terephthalate (PET) and polylactic acid (PLA) as the best polymers for upper limb orthoses. The weighted property index values were 127.34 and 123.19, respectively. It is noteworthy that polyethylene terephthalate glycol (PETG - adaptation of PET) is an alternative to 3D printing filaments, and PLA is one of the main filaments.
Keywords: Materials selection; Merit index; Computer simulation; Orthopedic appliance; Orthosis.

Resumo
A seleção de materiais é uma das etapas mais relevantes e desafiadoras nos projetos de engenharia. Neste estudo, tem-se o foco da seleção de polímeros de baixa densidade e boa rigidez para órteses de membro superior que auxiliem na recuperação de pacientes que sofreram acidente vascular cerebral (AVC). O software CES EduPack 2011 foi utilizado para comparar a densidade e o módulo de Young de diferentes polímeros. O índice de mérito auxiliou na classificação destes materiais, os quais foram aplicados aos modelos de órteses 3D para simulações computacionais no software FreeCAD 0.19.4. A partir dos dados de simulação, foi desenvolvida uma matriz de decisão utilizando o método de Pahl & Beitz para classificar os polímeros de acordo com o índice de propriedade ponderada. A matriz de decisão utilizando os dados simulados e de índice de mérito apresentou o polietileno tereftalato (PET) e o ácido polilático (PLA) como os melhores polímeros para órteses de membros superiores. Os valores do índice de propriedade ponderada foram 127,34 e 123,19, respectivamente. Destaca-se que o polietileno tereftalato glicol (PETG - derivação de PET) é uma alternativa para filamentos de impressão 3D, além do PLA ser um dos principais filamentos.
Palavras-chave: Seleção de materiais; Índice de mérito; Simulação computacional; Dispositivo ortopédico; Órtese.

Resumen
La selección de materiales es uno de los pasos más relevantes y desafiantes en los proyectos de ingeniería. En este estudio, el enfoque está en la selección de polímeros de baja densidad y buena rigidez para ortesis de miembros superiores que ayuden en la recuperación de pacientes que han sufrido un accidente cerebrovascular. Se utilizó el software CES EduPack 2011 para comparar la densidad y el módulo de Young de diferentes polímeros. El índice de mérito ayudó en la clasificación de estos materiales, que se aplicaron a modelos de órtesis 3D para simulaciones por computadora en el software FreeCAD 0.19.4. A partir de los datos de simulación, se desarrolló una matriz de decisión utilizando el método de Pahl & Beitz para clasificar los polímeros según el índice de propiedad ponderado. La matriz

de decisión que utilizó los datos del índice de mérito y simulado mostró que el tereftalato de polietileno (PET) y el ácido poliláctico (PLA) eran los mejores polímeros para ortesis de miembros superiores. Los valores del índice de propiedad ponderado fueron 127,34 y 123,19, respectivamente. Cabe destacar que el polietilen tereftalato glicol (PETG - derivado del PET) es una alternativa para los filamentos de impresión 3D, además de que el PLA es uno de los principales filamentos.
Palabras clave: Selección de materiales; Índice de mérito; Simulación por computadora; Dispositivo ortopédico; Órtesis.

1. Introduction

Patients who have had a cerebrovascular accident (CVA) might experience sequelae that lead to difficulty moving a certain body part. An example of a sequela is spasticity, which causes muscle stiffness and consequently prevents or impairs movement of the affected region (Radomski & Latham, 2013). In this study, we sought materials aimed at developing 3D printing-based upper limb orthosis to assist patients in recovering from CVA-related muscle stiffness in the forearm, hand, and wrist. Orthoses are components that aid in physiotherapy for patients with certain physical disabilities or prevent the aggravation of such disabilities (Baronio, et al., 2016; Silva, et al., 2017; Shih, et al., 2017). These orthopedic devices can be integrated into different segments of the human body, such as limbs, organs, and tissues, allowing support, immobilization, correction of deformities, alignment, tissue protection, and stability. Specialized professionals manufacture these devices according to the patient's needs to avoid movements that may hinder recovery (Carvalho, 2013; Radomsksi & Latham, 2013; Silva, et al., 2017; Souza, et al., 2022).

The materials that can be used to manufacture orthoses are diverse. Materials such as leather, metal alloys, thermoplastics, foams, viscoelastic polymers, and carbon fibers are commonly used, depending on the desired application, properties, characteristics of each element (Carvalho, 2013), and patient needs (Garros, et al., 2010). Moreover, the additive manufacturing can be applicated due high degree of orthoses customization (Hale, et al., 2020; Łukaszewski, et al., 2020; Poier, et al., 2021). An example is the use of PLA for 3D printing of modular wrist, hand, finger and low-cost orthoses, made by Poier et al. (2021).

In this study, we focused on polymers and performed material selection using the CES EduPack 2011 software, merit index, and decision matrix. In addition, the finite element method (FEM) was applied for the 3D model computer simulation of the upper limb orthosis. Simulations were performed with material properties from various polymers using FreeCAD 0.19.4 software and analyzed according to the stress required for orthosis use. The FEM has been increasingly applied in biomechanical research (Driscoll, 2019; Ali, et al., 2021; Tiwari, et al., 2022), such as studying the biomechanical behavior of biological structures. Preventive medicine is another field that has been using various FEM resources for applications such as medical visualization, data monitoring to build a model of a part of the anatomy and physiology of an individual, and manufacturing of prostheses (Fish & Belytschko, 2009).

2. Methodology

2.1 Materials selection

For material selection through the merit index and decision matrix, steps are conducted to find the best combination of desired profiles in the project with profiles of existing materials, that is, to establish the link between material and function (Ashby, 2011). To identify the material selection requirements, boundary conditions were established based on the orthotic function, possible restrictions, objectives, and free variables (Table 1). In this case, the function of the orthosis is to withstand the flexion effort caused by the patient's upper limb. The restriction is the value applied in the computer simulation, which will be explained in the next section. The objective is mass reduction for comfort and adaptation to the patient's limb. Consequently, the free variable is density.

Table 1. Identification of requirements.

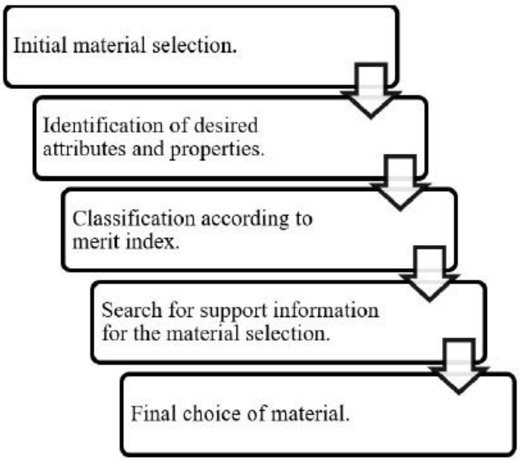
Function	The orthosis must withstand the longitudinal bending caused by the patient's upper limb.
Restriction	The value applied to longitudinal bending.
Objective	Mass reduction.
Free variable	Density.

Source: Authors.

Ashby charts, which are diagrams or maps of resulting material properties, synthesize a large volume of information and present correlations between material properties. Furthermore, Ashby charts aid in selecting materials, which contributes to the analysis and development of orthoses. Using the CES EduPack 2011 software, Ashby charts can be generated by correlating the properties and limits of material selection. In this study, Young's modulus (GPa) vs. density (kg/m³) plot facilitated the choice of materials that are light and have good stiffness.

Subsequently, the materials were classified according to the merit index (Ashby, 2011), a fraction defining a property or group of properties that quantify the project performance. In this index, the numerator and denominator represent the characteristics or properties to be maximized and minimized, respectively; Young's modulus was the numerator and density was the denominator. Rigid polymers with low density were expected for this study. This classification aided in sorting the materials according to their properties. Thus, materials that were best suited for the project were selected. Furthermore, the necessary supporting information for the selection was sought, as shown in Figure 1.

Figure 1. Steps for material selection.



Source: Adapted from Ashby (2011).

The application of the decision matrix contributed to the selection of the materials. This matrix aided in comparing candidate materials, requirements, material properties, and weighting factors and thereby generated a material classification (Ferrante, et al., 2000). The systematic approach with quantitative properties suggested by Pahl e Beitz (Pahl, et al., 2007) was then applied. Based on the identification and description of previously designed products, the primary requirements and evaluation criteria were established according to the objectives and functions of the orthosis (Table 2). Values for weighting factors are established according to their importance to the desired material profile.

Table 2. Primary requirements and evaluation criteria.

Criteria			
Primary requirements	**Weighting factor**	**Rating criteria**	**Weighting factor**
Density	0.40	Low density	0.40
Price	0.30	Approximate price	0.30
Performance	0.30	Maximum displacement	0.15
		Maximum principal stress	0.15

Source: Authors.

The density and approximate price per kilogram of material were obtained using the CES EduPack 2011, whereas the maximum displacement and maximum principal stress criteria were obtained from the first 3D orthosis simulation results. With the defined primary requirements and evaluation criteria, the decision matrix was developed by gathering the candidate materials, evaluation criteria, proportionality factors, scale factor, and weighted property index, which resulted in the classification of materials (Findik & Turan, 2012).

The scale factor (β) is a property balancing factor with the aim of making all properties within the same numerical range. Generally, the maximum dimensionless value adopted for the scale factor is 100. Equation 1 demonstrates how the calculation for the scale factor is performed:

$$\beta = \frac{v*100}{p} \tag{1}$$

where: β = scale factor; v = numerical value of the property; p = highest value among property values.

In cases where the lower value is better for the evaluation, such as lower cost and lower density, the following equation (Equation 2) must be applied

$$\beta = \frac{p*100}{v} \tag{2}$$

where: β = scale factor; b = lowest value among property values; v = numerical value of the property.

The weighted property index (γ) allows classifying materials according to scale factors and proportionality factors for each material, as shown in Equation 3:

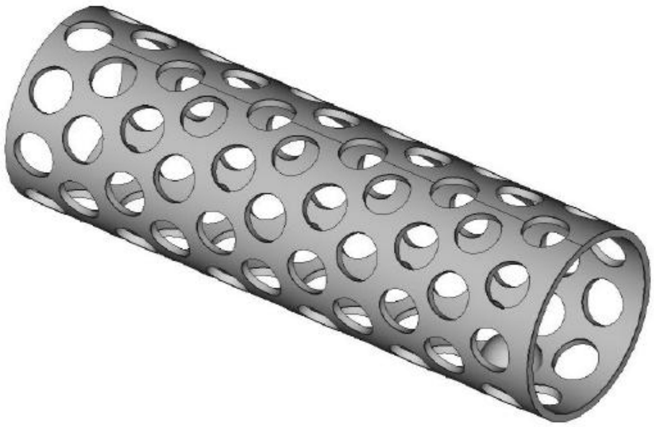
$$\gamma = \sum_{i=1}^{n} \beta_i w_i \tag{3}$$

where: γ = weighted property index; n = number of material properties; β = scale factor; w = proportionality factor.

2.2 Finite Element Method (FEM)

The FEM simulation was performed in FreeCAD 0.19.4 software with two 3D models of the upper limb orthosis developed by our group. The models were developed with cylindrical shapes and dimensions similar to those used for rehabilitation and physiotherapy treatment, adapting to the forearm, hand, and cuff (Figure 2). The models were 240 mm long and had an internal radius of 35 mm. A thickness of 3 mm and 5 mm were chosen for the first and second models, respectively.

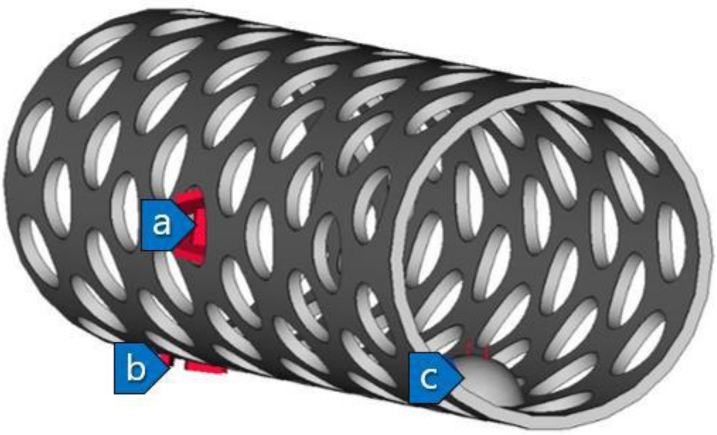
Figure 2. 3D model of an orthopedic appliance for forearm, hand, and wrist.



Source: Authors.

The analysis was performed according to the downward movement of the patient's hand to obtain maximum stress and displacement values. For the boundary conditions, the model was considered to be fixed at two points, the lateral region by Velcro (a) and the inferior region (b) where the forearm was located, which was also the region furthest from the force application region (c) (Figure 3). As this was a simulation of the patient's hand movement, a force of 100 N was applied to the lower inner region of the orthosis (c). This intensity was selected to obtain results close to the maximum stress of the part in the simulation (Dantas, 2019).

Figure 3. Fixation and force application regions of 3D model orthopedic appliance: (a) and (b) fixed region; (c) force application region.



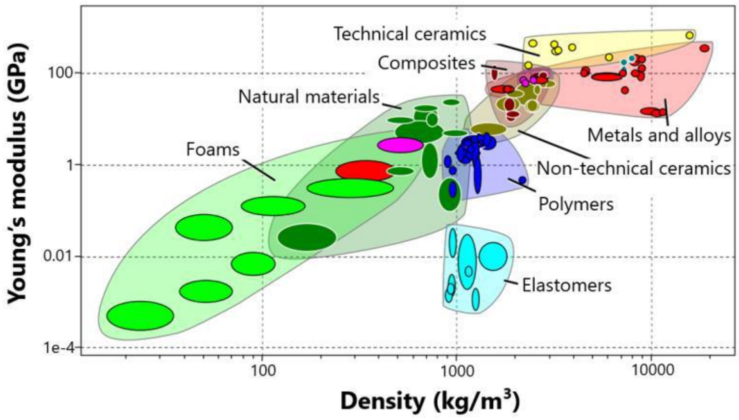
Source: Authors.

3. Results

3.1 Initial materials selection

In the initial selection of materials, the CES EduPack 2011 software was used to plot the Ashby chart comparing Young's modulus to density. Figure 4 represents the obtained data and the families of the materials indicated by different shades.

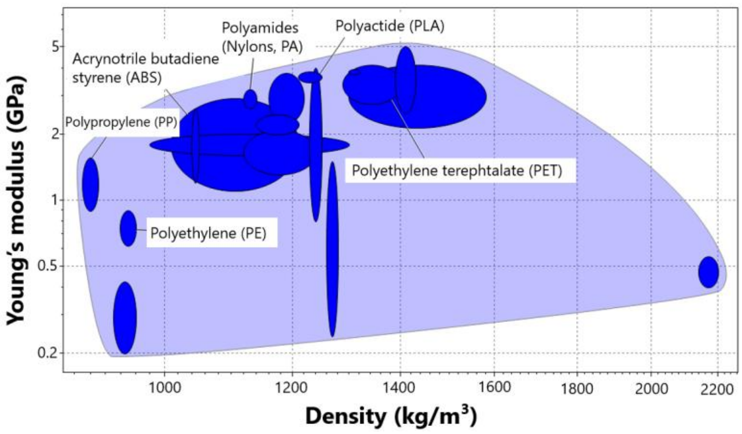
Figure 4. Ashby chart depicting the Young's modulus plotted against density for the materials families.



Source: CES EduPack 2011.

In agreement with the values, the polymers met the desired requirements, with density values ranging from 890–2200 kg/m³ and Young's modulus between 0.2–5 GPa. A new Ashby map comparing Young's modulus vs. density was plotted for the group of polymeric materials. The elements were graphically arranged in blue, as shown in Figure 5.

Figure 5. Ashby chart depicting the Young's modulus plotted against density for polymers under consideration.



Source: CES EduPack 2011.

From the Ashby chart data, the materials could be classified according to their merit index (MI). Table 3 presents the ten highest-ranked polymers based on the optimal relationship between the elastic modulus and density. The first five materials, polylactic acid (PLA), polyetheretherketone (PEEK), polyoxymethylene (POM), polyamide (PA), and polyethylene terephthalate (PET), were selected for further simulations.

Table 3. Classification by merit index.

Polymers	MI
Polylactic acid (PLA)	2.959
Polyetheretherketone (PEEK)	2.939
Polyoxymethylene (POM)	2.660
Polyamide (Nylon, PA)	2.575
Polyethylene terephthalate (PET)	2.565
Polymethylmethacrylate (PMMA)	2.538
Polyvinyl chloride (PVC)	2.181
Polyhydroxyalkanoates (PHA)	1.935
Polycarbonate (PC)	1.889
Polystyrene (PS)	1.818

Source: Authors.

3.2 Simulation of longitudinal bending of 3D models

The computational simulation by FEM was performed by applying the material properties of the five main polymers classified by the merit index. Table 4 presents the simulation results performed with PLA properties for the 3- and 5-mm thick models.

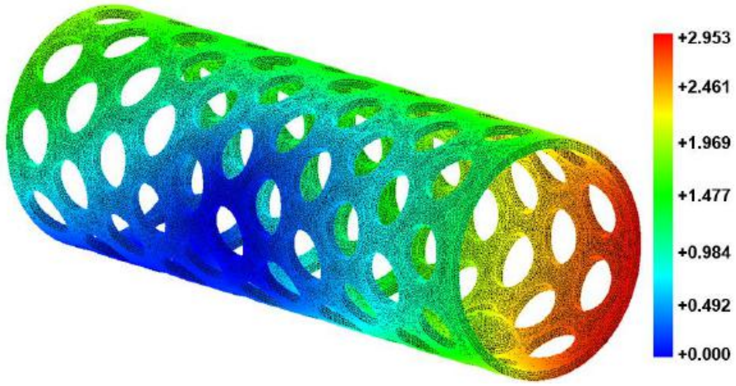
Table 4. Simulations performed for the 3D model with PLA properties.

Model	Thickness (mm)	Von Mises (MPa)	Max. principal stress (MPa)	Maximum displacement (mm)
Model 1	3	29.00	42.00	2.95
Model 2	5	13.52	18.01	1.08

Source: Authors.

Figure 6 highlights the location where the maximum displacement occurs in the piece (model 1), with a value of 2.95 mm (red color).

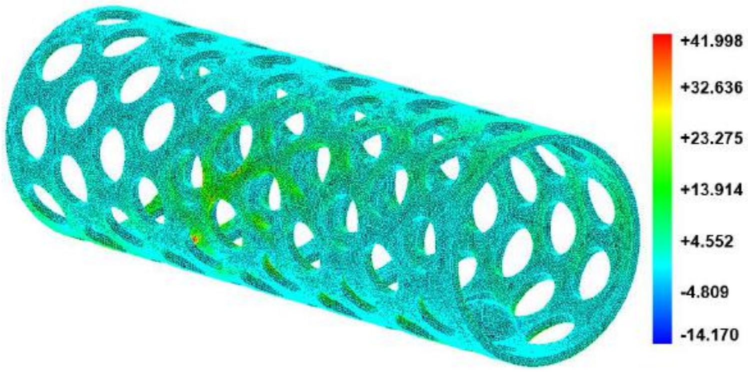
Figure 6. Result of the displacement analysis from the first 3D orthotic model with PLA properties.



Source: FreeCAD 0.19.4.

Figure 7 highlights the main stress points in model 1 (3 mm) of the orthosis, wherein the 100 N force was applied.

Figure 7. Maximum stress analysis results from the first 3D orthotic model with PLA properties.



Source: FreeCAD 0.19.4.

Table 5 represents the results obtained in the simulation of 3D models for the PLA, PEEK, POM, PA and PET. It is possible to observe that values obtained for Von Mises stress, maximum principal stress and maximum displacement for each model were similar.

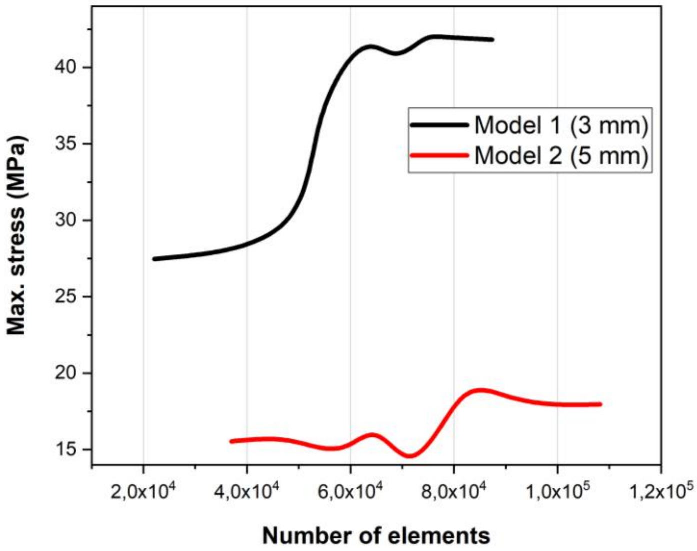
Table 5. Simulations performed for the 3D model with polymers properties.

Polymer	Model	Thickness (mm)	Von Mises (MPa)	Max. principal stress (MPa)	Maximum displacement (mm)
PLA	1	3	29.00	42.00	2.95
PEEK	1	3	29.03	43.73	2.79
POM	1	3	29.02	42.82	2.69
PA	1	3	28.99	41.25	3.71
PET	1	3	29.00	42.00	3.41
PLA	2	5	13.52	18.01	1.08
PEEK	2	5	13.37	19.35	1.02
POM	2	5	13.38	18.86	0.98
PA	2	5	13.40	18.03	1.35
PET	2	5	13.39	18.43	1.24

Source: Authors.

The mesh convergence study showed convergence between 74,000–87,000 elements and 97,000–108,226 elements for the first and second models, respectively (Figure 8).

Figure 8. Mesh convergence study for orthosis models.



Source: Authors.

3.3 Decision matrix

The decision matrix developed using the Pahl and Beitz method (Pahl, et al., 2007) indicated PET as the primary material in the classification by the weighted property index (γ), with a value of 127.34 (Table 6). PLA and PA showed similar indices of 123.19 and 122.78, respectively.

Table 6. Decision matrix.

Candidate materials	Factor	0.4		0.3		0.15		0.15		Weighted property index (γ)
	Criteria	**Density**		**Approx. price**		**Maximum displacement**		**Max. principal stress**		
		β	kg/m³	β	R$/kg	β	mm	β	MPa	
PLA		100	1230.00	68	4.40	91.19	2.95	98.21	42.00	**123.19**
PEEK		94	1310.00	2	179.50	96.42	2.79	94.33	43.73	**99.83**
POM		87	1410.00	42	7.15	100.00	2.69	96.33	42.82	**110.57**
PA		100	1230.00	73	4.12	72.51	3.71	100.00	41.25	**122.78**
PET		91	1350.00	100	2.99	78.89	3.41	98.21	42.00	**127.34**

Source: Authors.

4. Discussion

Among the analyzed materials by the Ashby chart, polymers had an optimal Young's modulus vs. density ratio. In addition, these materials meet the desired requirements, such as low density and rigidity associated with malleability. Therefore, polymers were the class of materials chosen to perform the simulations.

The maximum stress values reached by the two models in the simulation were within the maximum stress limit of PLA (48–60 MPa) according to the range of values provided by the CES EduPack 2011 software. When performing a longitudinal bending simulation of two different orthotic models of the current work, a maximum stress of 36.37 MPa and 28.94 MPa were obtained for the first (3 mm) and second models (5 mm), respectively, using the properties of PLA (Dantas, 2019). Similar to PLA, the maximum stress values achieved by the two models in the simulation are within the other polymers maximum stress limit (Table 7).

Table 7. Comparison between maximum principal stress obtained through FreeCAD 0.19.4 software for model 1 (3 mm) and range of maximum stress limit given by CES EduPack 2011 software.

Polymer	Max. principal stress (MPa) - FreeCAD	Maximum stress limit (MPa) - CES EduPack
PLA	42.00	48-60
PEEK	43.73	70-103
POM	42.82	60-90
PA	41.25	90-165
PET	42.00	48-72

Source: Authors.

The maximum stress and displacement values directly depend on the applied force and part geometry, such as section thickness, length, and area. The results indicated a significant variation in the maximum stress and maximum displacement owing to the variation in the thickness. However, the two models have the same length and internal radius.

With the results of the decision matrix, PET and PLA were indicated as the best materials for 3D printing of upper limb orthosis. Although the most common composition of PET is not ideal for 3D printing, polyethylene terephthalate glycol

(PETG) is a suitable alternative for filaments (Besko, et al., 2017). Thus, a study by Santana et al. (2018) was conducted to compare the mechanical, thermal, and chemical properties of samples injected with PETG and PLA. This study demonstrated that PETG displayed better deformation at maximum stress. In contrast, PLA has superiority for maximum stress tolerance (52.32 MPa) and its rigidity (2.69 GPa) when compared to the injected PETG samples (49.78 MPa for maximum stress and 1.50 GPa for the elastic modulus) (Santana, et al., 2018). Polytrimethylene terephthalate (PETT) is another derivative of PET that is more rigid than PETG and has the potential for use in filaments (Besko, et al., 2017).

PLA is one of the main filaments used in 3D printing (Mikula, et al., 2021), as it is non-toxic, biocompatible, has biological absorption, good mechanical properties, and is biodegradable (Lanzotti, et al., 2019). Thus, it has a lower environmental impact than other filaments (Besko, et al., 2017; Santana, et al., 2018). Furthermore, PLA has applications in research areas such as biomedicine. These applications are exemplified by the manufacture of orthopedic parts, microspheres for controlled drug delivery, and tissue regeneration support (Thiré, et al., 2019; Górski, et al., 2020).

5. Conclusion

The study of materials for developing upper limb orthoses that help in the recovery of patients post-CVA was performed in two stages: material selection using merit index and decision matrix, and computer simulation using the finite element method. The results from the simulations were applied to the decision matrix to assist in selecting materials by adopting the Pahl and Beitz systematic approach. Finally, a weighted property index, representing a numerical value according to the criteria and weighting factors used, was obtained. Among the materials used in this study, PET/PETG and PLA are the best choices for designing upper-limb orthoses through 3D printing.

This evaluation contributes to the development of upper limb orthoses, with the aim of facilitating the production of orthopedic products through additive manufacturing. For future work, it is recommended to manufacture PLA, PET and PETG orthoses by 3D printing for biocompatibility comparison and realize clinical test with patients.

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