Linear, bilinear, and hyperelastic comparison for the periodontal ligament modeling

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Abstract. One of the most relevant parameters to assess orthodontic and prosthodontic treatments is the biomechanical behavior of periodontal ligament. Due to the challenges associated with the experimental studies to test new devices and techniques and evaluate the periodontal ligament reactions, numerical studies are an alternative and complement for in vitro and in vivo studies. Very often, the contribution of the periodontal ligament is neglected or described using simplified models. In this study, the feasibility of simplified analysis of the periodontal ligament is evaluated using linear, bi-linear, and hyperelastic models on a central mandibular incisor, applying an orthodontic force of 1.4142 N in ANSYS 19. Although the hyperelastic model shows a realistic behavior of the periodontal ligament, this model demands more significant computational time than the other models. But in cases when the aim of the study is not to analyze the periodontal ligament, the linear model characterizes the periodontium’s behavior adequately.

1. Introduction
The periodontal ligament (PDL) is a connective tissue of great importance in analyzing the mechanical behavior of the periodontium [1]. It is a tissue located between the tooth and the cortical bone responsible for the distribution of masticatory forces. Although there is not complete clarity about the mechanical properties of the PDL, it is a crucial component that cannot be excluded from the numerical analysis of the periodontium [2].

Biomechanics provides a better understanding of the human body through rigorous mathematical and physical analysis. By this approach in previous studies are shown variations between the different constitutive models that best represent the real behavior of the PDL, among which the most used models are: linear [1, 3–5], bilinear [6–8], and hyperelastic [2,9]. Therefore, to predict the outcomes of orthodontic, prosthodontic, and some periodontal treatments, it is essential to characterize this particular element correctly.

Therefore, comparing these constitutive models was made to identify the one that can accurately describe the PDL’s behavior and decide when it is possible to use simplified models to save computational time. The different models were evaluated using the finite element analysis (FEA) method. The first part of this article describes the conditions under which these models were evaluated, then it discusses the results obtained in the FEA simulations, and finally, it presents conclusions and recommendations for future research.
2. Method and materials
A three-dimensional model of a mandibular incisor, a PDL, surrounded by its cortical and alveolar bone was used, as shown in Figure 1. The PDL has a thickness between 100 µm and 500 µm [3, 10]; for this study, a uniform thickness of 500 µm was chosen. According to the literature, the thickness of the cortical bone varies between 0.5 mm and 2 mm [11, 12]. In this study, a thickness of 1 mm was chosen. The bone structures were extended double in size, to avoid interference of border conditions in the behavior of the periodontal system.

![Figure 1. Tridimensional model of the periodontium under a force of 1.4142 N.](image)

FEA provides a detailed analysis of biomechanical behaviour conditions on structural bodies [13, 14]. The numerical analysis was made using ANSYS (version 19) with different constitutive models of the PDL. An orthodontic force of 1.4142 N at 45° was simulated on the tooth’s crown, as shown in Figure 1. The contact between the different components was assigned as bonded, which avoid the relative displacement among surfaces, and fixed conditions were assigned to the sides of both cortical and alveolar bone. In total, a mesh of 53485 elements, mostly hexahedral, and 186138 nodes describe the model’s geometry. A converge analysis with an error of 5% was carried out. It was considered an orthotropic linear behavior for the cortical and trabecular bone, and for the tooth, it was considered an isotropic linear behavior, as shown in Table 1 [15–17].

| Table 1. Mechanical properties for the components of the periodontium. |
|-------------------|-----------------|-----------------|-----------------|
|                   | Cortical bone   | Alveolar bone   | Tooth           |
| Young modulus (MPa) | $E_X$ 19400  | 1148  | $E$ 18000        |
|                   | $E_Y$ 12600  | 210   |                 |
|                   | $E_Z$ 12600  | 1148  |                 |
| Poisson’s ratio   | $\nu_{xy}$ 0.253 | 0.01 | $\nu$ 0.45     |
|                   | $\nu_{xy}$ 0.253 | 0.32 |                 |
|                   | $\nu_{xy}$ 0.300 | 0.05 |                 |
| Shear modulus (MPa) | $G_{xy}$ 5700  | 51.0  | $G$ - - -       |
|                   | $G_{xy}$ 5700  | 325.5 |                 |
|                   | $G_{xy}$ 4850  | 51.0  |                 |
Previous studies assume a linear model for the PDL with a Young modulus between 0.01 MPa and 100 MPa [3]. For the linear analysis, three models were analyzed, each one with anisotropic behavior and Young modulus of 50 MPa, 10 MPa, and 3 MPa, respectively. The average Poisson ratio of the PDL is between 0.4 and 0.49 due to its incompressibility [1]. For all the linear models, a Poisson ratio of 0.45 was chosen.

The literature on bilinear models agrees on the mechanical properties of the PDL. The Young modulus of the initial expansion ($E_1$) is between 0.04 MPa and 0.05 MPa, and the Young modulus of the second phase ($E_2$) is between 0.16 MPa and 0.20 MPa [6, 7, 11]. For this analysis, an $E_1$ of 0.05 MPa and an $E_2$ of 0.28 MPa were chosen, along with a Poisson ratio of 0.45 at a temperature of 37 °C. The PDL is generally characterized as a nonlinear material, which is considered hyperelastic behavior [18]. A first-order Ogden model was used since it is widely used in the literature [9]. The constants used in the simulation are presented in Table 2.

| Table 2. Hyperelastic constants of PDL. |
|---------------------------------------|
| Constant | Value  |
|----------|--------|
| $C_1$    | 375.450|
| $C_2$    | 24.203 |
| $C_3$    | 0.000  |

3. Results and discussions

Figure 2 shows the results of the linear simulations and Figure 3 shows the results of the bilinear and hyperelastic simulations obtained for two elements of the periodontium, the cortical and PDL. The Figure 2 and Figure 3 present the $\mu$-strains of the cortical bone, the von Mises stress, the maximum principal stress, and the minimum principal stress of the PDL. The results obtained using the hyperelastic model represented the best real behavior of the PDL compared with the literature [2, 9, 12–14, 18]; therefore, the hyperelastic model is used as reference to compare the behavior of the linear and bilinear models.

Figure 2 present for a linear model the $\mu$-strains of the cortical bone with $E = 3$ MPa, maximum = 42.049 MPa (Figure 2(a)), $E = 10$ MPa, maximum = 41.139 MPa (Figure 2(b)), $E = 50$ MPa, maximum = 37.209 MPa (Figure 2(c)); the equivalent stress von Mises of the PDL with $E = 3$ MPa, maximum = 0.1077 MPa (Figure 2(d)), $E = 10$ MPa, maximum = 0.1151 MPa (Figure 2(e)), $E = 50$ MPa, maximum = 0.1490 MPa (Figure 2(f)); the maximum principal stress ($\sigma_1$) of the PDL with $E = 3$ MPa, maximum = 0.1130 MPa (Figure 2(g)), $E = 10$ MPa, maximum = 0.1163 MPa (Figure 2(h)), $E = 50$ MPa, maximum = 0.1304 MPa (Figure 2(i)); the minimum principal stress ($\sigma_3$) of the PDL with $E = 3$ MPa, minimum = 0.1526 MPa (Figure 2(j)), $E = 10$ MPa, minimum = 0.1428 MPa (Figure 2(k)), $E = 50$ MPa, minimum = 0.1657 MPa (Figure 2(l)). Likewise, The

Figure 3 present the $\mu$-strains of the cortical bone for the bilinear model, maximum = 45.916 MPa (Figure 2(a)), hyperelastic model, maximum = 49.827 MPa (Figure 2(b)); the equivalent stress von Mises of the PDL for the bilinear model, maximum = 0.0722 MPa (Figure 2(c)), hyperelastic model, maximum = 0.10124 MPa (Figure 2(d)); the maximum principal stress of the PDL for the bilinear model ($\sigma_1$), maximum = 0.0898 MPa (Figure 2(e)), hyperelastic model ($\sigma_1$), maximum = 0.0778 MPa (Figure 2(f)); the minimum principal stress of the PDL for the bilinear model ($\sigma_3$), minimum = 0.1130 MPa (Figure 2(g)), hyperelastic Model ($\sigma_3$), minimum = 0.1163 MPa (Figure 2(h)).
Figure 2. FEA simulations results for linear models and maximum values under a force of 1.4142 N.
Figure 3. FEA simulations results for bilinear and hyperelastic models and maximum values under a force of 1.4142 N.
The maximum $\mu$-strain in the cortical bone for each model was presented in the alveolar buccal bone plate. Moreover, the maximum von Mises stress of PDL is presented in the vestibular zone in contact with the tooth. The maximum principal stress, also known as traction stress, was presented in the palatine zone of the PDL in contact with the cortical bone for the linear FEA simulations. For the bilinear and hyperelastic models, this stress was located on the vestibular zone of the PDL, near the apex. For the bilinear and linear model with a Young modulus of 3 MPa and 10 MPa, respectively, the minimum principal stress, also known as the compressive stress in the PDL was located on the apex. For the linear model with a Young Modulus of 50 MPa, this same stress was presented in the vestibular zone in contact with the tooth. The hyperelastic model presented the minimum principal stress in the vestibular zone in contact with the cortical bone.

3.1. Model comparison
The linear model with a Young modulus of 3 MPa, presented the lowest error among the other linear models compared with the hyperelastic model. However, the bilinear model compared with the hyperelastic model presented a lower error than the linear model. A comparison of the PDL and periodontium stress error in the linear and bilinear models compared with the results obtained in the hyperelastic model is presented in Table 3.

Table 3. Mechanical properties for the components of the periodontium.

|                      | Linear model $E = 3$ MPa | Bilinear |
|----------------------|-------------------------|----------|
|                      | PDL                     | Periodontium | PDL | Periodontium |
| Equivalent von Mises stress error (%) | 33.19                  | 2.59      | 55.24 | 1.49      |
| Maximum principal stress error (%)     | 45.19                  | 5.27      | 15.39 | 4.03      |
| Minimum principal stress error (%)      | 2.59                   | 6.82      | 5.51  | 5.45      |

3.2. Computational time comparison
The computational time required for the hyperelastic model is five times higher than the bilinear model and 105 times higher than the linear model.

3.3. Limitations and considerations
Previous studies have shown that the PDL can also be characterized with a viscoelastic or hyperviscoelastic model [19]. However, the assumptions made in the present study are valid since it has been demonstrated that the movement of the teeth is not associated with the nonlinearities of the PDL material behavior [19].

4. Conclusions
The main objective of this study was to identify a simplified model of the periodontium that saves computational time and approaches a real behavior of the PDL. According to the results, the behavior of PDL can be defined according to the necessities of each study. For example, if the study is focused on the PDL, then the best option is to assume the PDL with a hyperelastic constitutive model. However, if the objective in the numerical study is a different element of the periodontium or the periodontium itself, the linear model with a Young modulus of 3 MPa and the bilinear model can be used since the results approach the real behavior of the PDL under orthodontic forces. However, the linear model is 100 times more efficient in saving computational time.
Further analysis with hyperviscoelastic or viscoelastic behavior, anatomical geometries from segmentations, and validations with in vitro studies are required to have a broader understanding of the PDL and the periodontium. It is vital to continue researching with real geometries and conditions to correctly predict the outcomes of orthodontic, prosthodontic, and some periodontal treatments.

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