3D simulation of orthodontic tooth movement

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Abstract

Objective: To develop and validate a three-dimensional (3D) numerical model of a maxillary central incisor to simulate tooth movement using the Finite Element Method (FEM). **Methods:** This model encompasses the tooth, alveolar bone and periodontal ligament. It allows the simulation of different tooth movements and the establishment of centers of rotation and resistance. It limits the movement into the periodontal space, recording the direction, quantifying tooth displacement and initial stress in the periodontal ligament. **Results:** By assessing tooth displacements and the areas that receive initial stress it is possible to determine the different types of tooth movement. Orthodontic forces make it possible to quantify stress magnitude in each tooth area, in the periodontal ligament and in the alveolar bone. Based on the axial stress along the periodontal ligament and the stress in the capillary blood vessel (capillary blood stress) it is theoretically possible to predict the areas where bone remodeling is likely to occur. **Conclusions:** The model was validated by determining the modulus of elasticity of the periodontal ligament in a manner consistent with experimental data in the literature. The methods used in building the model enabled the creation of a complete model for a dental arch, which allows a number of simulations involving orthodontic mechanics.

Keywords: Finite elements. Periodontal ligament. Tooth movement. Orthodontic forces. Axial stress.

INTRODUCTION

The finite element method (FEM) enables the investigation of biomechanical issues involved in orthodontic treatment[14] and stimulates the currently increasing scientific interest in tooth movement. The development of a numerical model makes it possible to quantify and evaluate the effects of orthodontic loads applied in order to achieve initial tooth movement. One of the main features of the finite element method lies in its potential to analyze complex structures. This is possible when the numerical model behaves in a manner equivalent to the structure one wishes to analyze. In the case of tooth movement, the numerical model should respond in a manner equivalent to the clinical behavior of a moving tooth

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in terms of stress, strain and displacement. Additionally, FEM can be used to determine, through reverse calculations, the mechanical properties of tissues such as the periodontal ligament.[10]

The periodontal ligament is a dense fibrous connective tissue composed primarily of collagen fibers arranged in bundles, vascular and cellular elements, and tissue fluids.[5,6,19] The periodontium comprises the root cementum, periodontal ligament and alveolar bone. The periodontal ligament mediates the process of bone resorption and neoformation in response to orthodontic forces, although the mediator of the tooth movement per se is not force itself, but rather the magnitude of the stress generated in the periodontium.[3] The stress-strain experienced in the periodontium due to orthodontic forces contribute to alveolar bone remodeling through the recruitment of osteoblastic and osteoclastic cells, ultimately bringing about tooth movement.[5,9,12,18] Melsen et al[16] argue that it is the changes caused by stress-strain of the periodontium, and not any compression or tension forces, that release a cascade of biological reactions leading to tooth movement. They demonstrated that the stress exerted by the stretching of periodontal ligament fibers induces bone remodeling and that the stress generated by the application of force tends to create areas of tension and compression around the tooth, whose boundaries cannot be easily demarcated.

Because orthodontic treatment involves the delivery of forces to produce movements we can base our analysis on biomechanics. The analysis should begin by determining the properties of the materials involved and, with the aid of FEM, we can quantify the phenomena involved in tooth movement. Several tissues and materials used in orthodontics have had their properties identified, such as bones, teeth and stainless steel. However, the properties of the periodontal ligament are not fully known.

Several authors have described periodontal ligament properties using different methods. Experimental tests have been performed in vivo and in vitro using animals and humans.[5,12,18] Linear, homogeneous and isotropic features have been ascribed to the periodontal ligament and used to describe its behavior.[3,4,8-11,20,21,22] Some authors have determined the coefficient of elasticity of the periodontal ligament using FEM in specific and unique situations.[5,10,18,21] Others[2,16] have attributed nonlinear mechanical properties to the periodontal ligament, based on micro-CT scans of anatomical specimens, although these features are dependent on individual morphological and anatomical variations. As emphasized by Geramy,[7] the literature contains a wide range of values for the modulus of elasticity of the periodontal ligament. Therefore, with the aid of FEM and by determining the modulus of elasticity of the periodontal ligament it will be possible to investigate or evaluate the relationship between tooth movement and orthodontic forces. This method enables the quantification not only of the force system being applied, but also the stress-strain experienced by the tissues that comprise the periodontium.

The purpose of this study is to validate a three-dimensional numerical model using Finite Elements to assist in studies involving orthodontic mechanics. To this end we created a three-dimensional model of a maxillary central incisor tooth taking into account the periodontal ligament "fibers".

MATERIAL AND METHODS

Properties

The mechanical properties of organic tissues and orthodontic materials were drawn from the orthodontic literature.[4,5,7,9,10,12] The properties are the input data required for the numerical model, which is based on the finite element method. The structures that make up this model are composed of organic tissues and metallic materials with different mechanical properties in terms of characteristics and values, as following.

Teeth

In order to simplify the tooth structure as a single body to suit the desired analysis, the values used to characterize tooth properties were: 20,000 N/mm^2 for the modulus of elasticity[8,9,11,18] and 0.30 for the Poisson's ratio.[10,12,21,22]

Bone

The dental alveolus is composed of a thin layer of cortical bone which communicates directly with the periodontal fibers.

Several authors describe it as a homogeneous and isotropic material with a linear and elastic behavior. The mechanical properties found in the literature[4,11,12,22] assign to the alveolar cortical bone a mean value of 13,800 N/mm^2 (modulus of elasticity) and 0.30 (Poisson's ratio).

Brackets

Orthodontic brackets are made of stainless steel and have defined properties such as 180,000 N/mm^2 for the modulus of elasticity and 0.30 for the Poisson's ratio.[8]

Periodontal ligament

Since the literature comprises a wide array of values assigned to the modulus of elasticity of the periodontal ligament[7] the modulus of elasticity had to be determined using reverse calculations. The results were compared with values obtained experimentally by Jones et al,[10] who quantified the initial tooth displacement in vivo by subjecting it to an orthodontic force.

The mean value for tooth displacement obtained experimentally served as a basis for comparison with the displacements obtained in computer simulations in this study. Based on this comparison the modulus of elasticity of the periodontal ligament was determined.

Finite elements

The FEM-based numerical model that represents this system was developed with the computer program Ansys, version 8.1.[24,25] Each component comprised in the model was discretized into finite elements.[4,14]

The tooth and alveolar cortical bone

The tooth[27] and alveolar cortical bone were discretized into Shell63 elements with a thickness of 0.25 mm. Figure 1 shows the model of the tooth and the alveolus using finite elements.

Periodontal ligament

The fibers of the periodontal ligament were discretized into Beam4 elements. The geometric properties attributed to the fibers of the periodontal ligament were established, noting that a large portion of the ligament (75%) is composed of collagen fibers arranged in bundles that extend from the root cementum to the alveolar cortical bone.[5] Thus, to represent a bundle of fibers, we assigned a value of 1 mm diameter to each fiber drawn in the model, which amounts to about 75% of intra-alveolar space filled with periodontal fibers. Figure 2 shows the connection between the tooth and alveolus through the periodontal fibers (A), with emphasis on the apical (B) and cervical (C) areas.

TABLE 1 - Materials properties.

Properties	Tooth	Alveolus	Bracket	Periodontal Ligament
Modulus of Elasticity (MPa)	20,000	13,800	180,000	0.059
Poisson's ratio	0.30	0.30	0.30	0.49

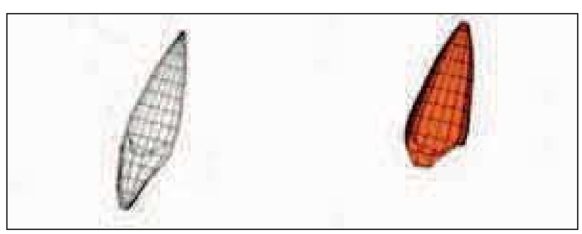

FIGURE 1 - Tooth and alveolus models in finite elements.

Bracket

The bracket was discretized into Shell63 elements with a thickness of 1.40 mm, which corresponds to the distance between the bracket base and the bracket slot.

Finite element model

The numerical model consists of 1,026 finite elements distributed among tooth, alveolus, periodontal fibers and bracket. Figure 3 shows the complete model and its respective reference axes. The tooth dimensions were obtained from the dental anatomy literature.[27]

Boundary conditions

Boundary conditions were applied in an attempt to replicate the conditions of the experiment conducted by Jones et al,[10] who used a device that produced a constant 0.39 N force in the midpoint of the labial surfaces of one central incisor in ten experimental patients. The initial displacements were measured at a site in the incisal edge of the tooth crown with the aid of a laser beam measuring apparatus.

To reproduce the experimental conditions, the alveolar area of the model had its movements restricted in all directions, thereby limiting tooth movement within the periodontal space (Fig 4). Furthermore, a 0.39 N force was applied to the midpoint of the bracket in the model, as properly described by its directional components x, y, z.

RESULTS AND DISCUSSION

Model validation

To validate the three-dimensional numerical model, tooth displacement results were compared

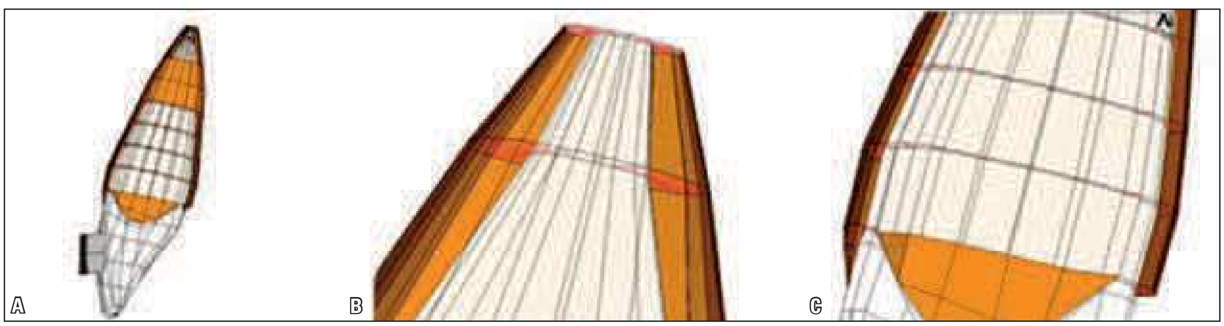

FIGURE 2 - Finite element model with the periodontal fibers connecting the tooth and alveolus.

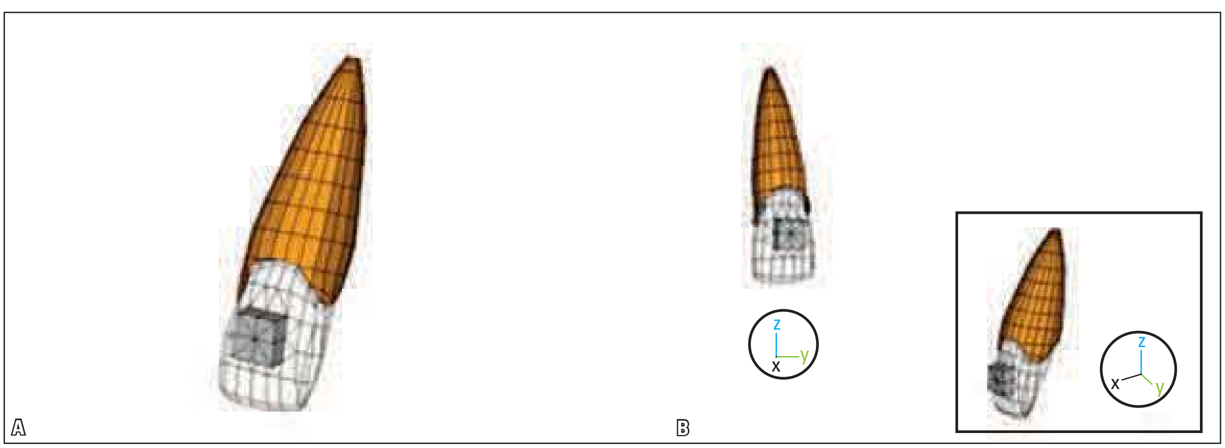

FIGURE 3 - Complete finite element model.

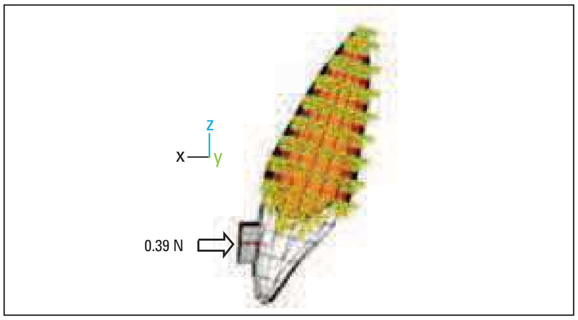

FIGURE 4 - Boundary conditions applied to the model: force of 0.39 N in the bracket and restrictions to alveolar movements.

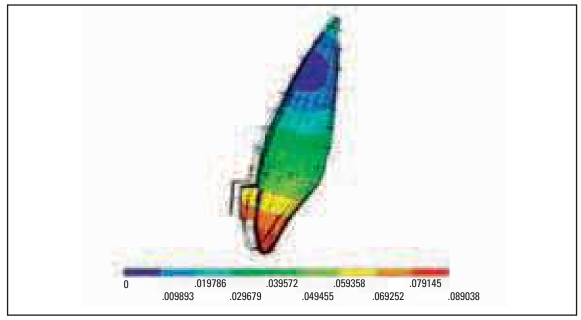

FIGURE 5 - Tooth displacement (mm) resulting from a 0.39 N load.

with those obtained by Jones et al,[10] in which the mean displacement found for the central incisors of the ten experimental subjects was 0.0877 mm with a standard deviation of 0.0507.

To determine central incisor displacement different values were assigned to the modulus of elasticity of the periodontal ligament fibers. With the value of 0.059 MPa, the incisal edge of the crown exhibited a tooth displacement of 0.089 mm (Fig 5). This value shows a difference of 1.46% compared with the value experimentally determined by Jones et al[10] (0.087 mm). Despite this difference, it is possible to validate the results obtained with the finite element model by considering the morphological and geometric differences and according to the standard deviation value found experimentally.

Based on this result it is valid to assign the value of 0.059 MPa to the modulus of elasticity of the periodontal ligament fibers. The validation of this model allows further study through variations in load parameters (forces and moments).

Table 1 summarizes the values assigned to the properties of the materials used in the numerical model.

Study of axial stress

In addition to the results found for tooth displacements, the axial stress of the periodontal fibers was also obtained.

The classical concept of "optimal force" advocates that in order to produce orthodontic movement in such a manner as to allow the periodontal ligament and alveolar bone tissue to restore normality, the root surface should undergo stress that is slightly higher than the stress exerted by the blood in the capillary vessel[6] (capillary blood stress) of 15 to 20 mm Hg or equivalent to 20 to 26 gf/cm^2 (0.0026 N/mm^2 or 0.0026 MPa). Vessel compression hinders blood flow in areas of tension and compression of the periodontal fibers.[19] Kawarizadeh et al[12] used histological analysis to conclude that the periodontal areas where greater stress arises from the application of orthodontic forces also promote a greater recruitment of bone tissue remodeling cells. Whenever an orthodontic force is applied to a tooth, the root moves closer to the alveolus wall, thereby stretching the periodontal ligaments on the side where the force was applied while compressing the opposite side. Thus, the vascular system that works naturally under local capillary blood stress is compressed and blood flow hindered. This process "injures the tissues" and promotes the release of inflammatory response mediators, which ultimately trigger the process of bone remodeling.[6,19]

Based on this information, which links the stress to the process of bone remodeling, a criterion was established to compare the axial stress obtained from the numerical model with capillary blood stress.

Axial stress and their comparison with capillary blood stress

Force on the crown = 0.39 N

The axial stress measured in the periodontal ligament fibers for a 0.39 N force applied to the bracket midpoint are illustrated in Figures 6 and 7A.

By observing the color scale and the magnitude of the axial stress along the periodontal fibers, the stress of greater magnitude clearly occurs in the cervical areas of the root. However, it is only in those cervical areas (labial and palatal) that stress magnitude exceeds capillary blood stress (0.0026 N/mm^2). It is therefore possible to assert that, in theory, it is only in those areas that the processes leading to bone remodeling occur.

On the other hand, stress of small magnitude, i.e., lower than capillary blood stress, occur in the apical root area along the periodontal fibers. Therefore, the magnitude of the applied force can be considered negligible in light of the desired tooth movement and it therefore does not trigger the process of bone remodeling in this area.

Classification of resulting tooth movement

The color scale indicates that in the apical area, the stress along the periodontal fibers are compressive stress (-) on the labial side and tensile stress (+) on the palatal side. The labial surface of the cervical area displays tensile stress (+) and compressive stress (-) on the palatal side. This fact, in conjunction with the observation of axial stress and tooth displacement, make it possible to classify the different types of tooth movements. We can thus note a non-controlled tipping movement, whereby the rotation center lies between the signal transition areas where the axial stress along the periodontal fibers are equal to zero, i.e., between the center of resistance and the root apex (Fig 7, A). This movement occurs when a force applied to the crown moves the root apex in the opposite direction of the applied force.

Marcotte[15] reports that in the center of rotation, stress are equal to zero. We can thus, with the aid of the axial stress, categorize the types of tooth movement in light of the forces applied to the dental crown and the location of the rotation center of the tooth.

Figure 7B shows the direction, magnitude and orientation of the displacement achieved by applying a force of 0.39 N, which further strengthened the reliability of the information obtained through the axial stress. This figure shows that the displacements around the root apex are oriented in the opposite direction of those found in the incisal edge.

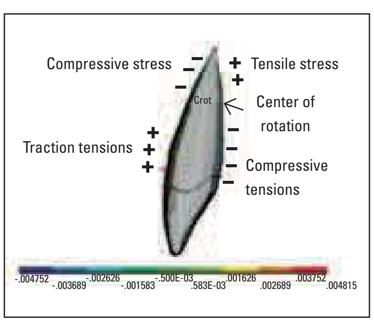

FIGURE 6 - Axial stress (N/mm²) resulting from a 0.39 N load.

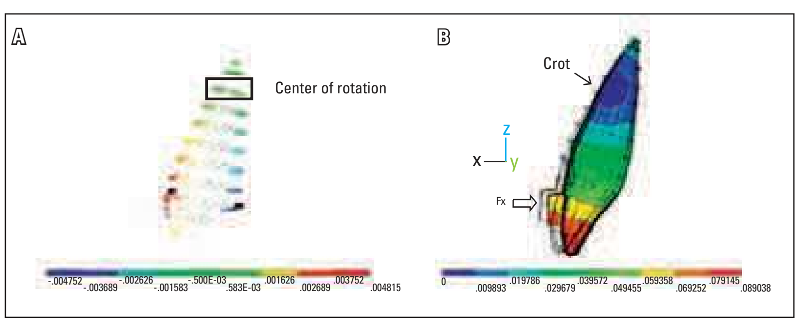

FIGURE 7 - View of the center of rotation under a 0.39 N load: **A**) axial stress, **B**) displacement.

Force on the crown = 0.70 N

A 0.39 N force was efficient enough to produce just a slight tipping movement in the upper central incisor, relative to the bone remodeling processes. In other words, this negligible force was capable of triggering the recruitment of remodeling cells in the cervical area only. Proffit and Fields[19] recommend forces between 0.30 N and 0.60 N to generate a tipping movement, while the magnitude of the force depends on the area of periodontal support. To identify the effects of excessive force, the magnitude of the applied force was increased to 0.70 N, a force considered to be above the force required for an efficient tipping movement of an upper central incisor.[19] Figures 8 and 9A show the axial stress resulting from a 0.70 N force.

By observing the color scale and the magnitude of the axial stress along the periodontal fibers it becomes clear that the stress of greater magnitude occur in the cervical area of the root, both in the tension and compression sides.

Unlike the previous case, however, the periodontal fibers that envelope almost the entire root area display stress levels which are higher than capillary blood stress (0.0026 N/mm^2) except in the area around the center of rotation (Fig 9, A).

Classification of resulting tooth movement

Similarly to the previous case, the color scale shows that along the periodontal fibers the compressive stress (-) are in the labial area of the root apex and the tensile stress (+) are on the palatal side. On the labial surface of the cervical area the tensile stress (+) are on the labial side and the compressive stress (-) are on the palatal side, which discloses a uncontrolled tipping movement.

Figure 9B shows the direction, magnitude and orientation of the displacement achieved by applying a 0.70 N force, which strengthen the reliability of the information obtained through the axial stress. This figure shows that the displacements around the root apex are also oriented in the opposite direction of those found in the incisal edge.

Force and moment of force on the crown

In cases of tooth movement with root movement control, it is advisable to apply to the bracket a force combined with a moment of force. With this procedure it is possible to generate different types of tooth movement, including uprighting, torque and translatory (bodily) movement. Control is exercised through a Moment/Force ratio[13,15,19] (M/F).

Thus, in order to obtain a translatory movement a 0.70 N force was applied, as in the previous case, and a 7.5 Nmm moment of force applied around the y axis. In this case, the M/F ratio which produced the translatory movement was 10.7:1. The moment of force acts as a root torque to be applied to the bracket by a supposed rectangular orthodontic archwire.

Figure 10 shows the boundary condition applied to achieve the translatory movement with the simultaneous loading of force and moment of force.

Figure 11 shows the axial stress obtained by simultaneously applying force and moment of force. By observing the color scale and the magnitude of the axial stress along the periodontal fibers it becomes clear that both exhibit nearly identical magnitude, distributed along the vertical axis of the root, on the labial and palatal surfaces. Several authors[1,6,13,15,19] claim that translatory movement entails a greater distribution of stress along the entire root length and that stress distribution along the root is relatively uniform.

In this case, nearly all of the root area surrounded by the periodontal fibers displays stress levels above capillary blood stress (0.0026 N/mm^2), confirming that in order to achieve the translatory movement of the central incisor the loads should be those recommended by Proffit and Fields[19], between 0.70 N and 1.20 N, depending on the periodontal area of the tooth while maintaining

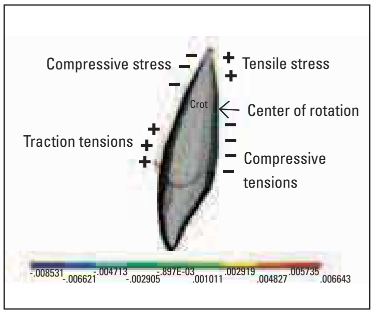

FIGURE 8 - Axial stress (N/mm²) resulting from a 0.70 N load.

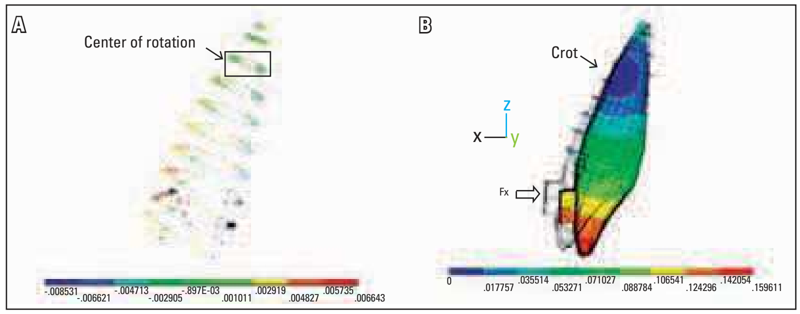

FIGURE 9 - View of the center of rotation under a 0.70 N load: **A**) axial stress, **B**) displacement.

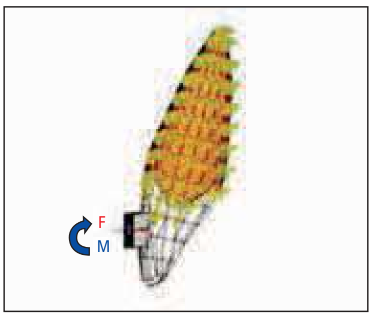

FIGURE 10 - Boundary conditions applied to the model: 0.70 N force and 7.5 Nmm moment of force onto the bracket and restrictions to alveolar movements.

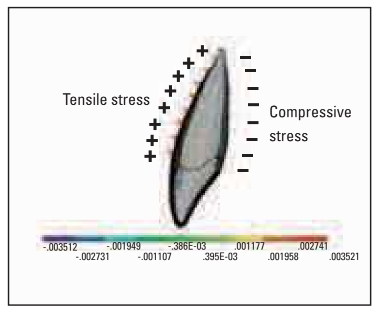

FIGURE 11 - Axial stress (N/mm²) resulting from simultaneously loading of force and moment of force.

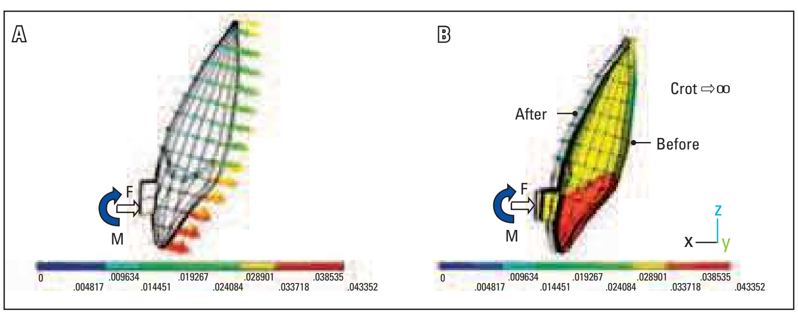

FIGURE 12 - Tooth displacement orientation resulting from the simultaneous loading of force and moment of force onto the bracket.

the same M/F ratio (10.7:1) which determines the direction of tooth movement.

Figure 11 also shows, regarding the long axis of the tooth, that along the periodontal fibers the compressive stress (-) are on the palatal side and the tensile stress (+) are on the labial side.

Classification of resulting tooth movement

Figure 12 shows the direction, magnitude and orientation of the displacement obtained as a result of force and moment of force application at a 10.7:1 ratio. The displacement occurs in parallel to the initial position, disclosing the

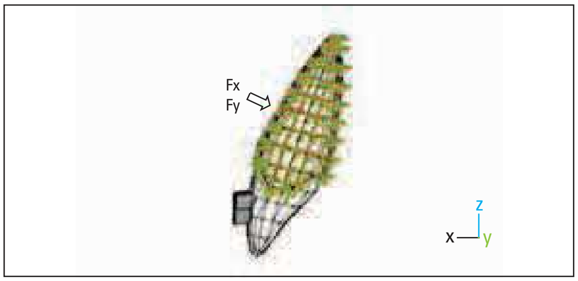

FIGURE 13 - Boundary conditions resulting from the application of force to the center of resistance (CRes).

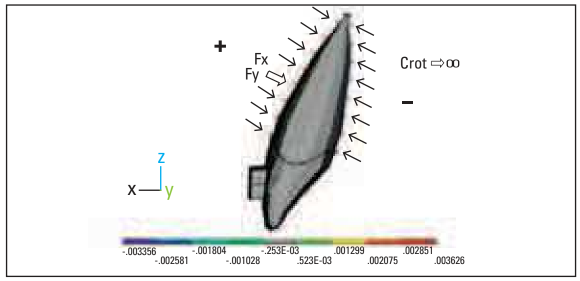

FIGURE 14 - Axial tensions (N/mm²) resulting from force applied to the center of resistance (CRes).

translatory movement in light of the forces applied while the center of rotation is located in an infinitely distant point from the tooth.

Another way to achieve translatory movement is through the application of a force to the center of resistance. For this it is necessary to locate the center of resistance of the tooth.

Application of force to the center of resistance (CRes)

The orthodontic literature agrees that the application of a force to the center of resistance of a tooth promotes translatory movement[1,6,13,15,19]. For anatomical reasons, we do not apply, in conventional orthodontic treatment (force applied to the bracket), a force directly to the center of resistance, since the latter lies along the area of the root embedded in the alveolar bone. However, by means of lever mechanics (cantilever, power arm)[1,15] as well as in computer simulation it is possible to accomplish this movement.

The location of the center of resistance of the tooth was found to be at approximately 39.91% of the tooth height, measured from the alveolar crest. Burstone[1] and Marcotte[15] argue that the center of resistance of a single-rooted tooth is located around 40% of the root height, also measured from the alveolar crest. Some authors[6,17] assert that the center of resistance is located at 33% and others,[13,26] at 66% of the root height.

Figure 13 shows the new boundary condition applied to restrain all alveolar movements. The forces were applied perpendicularly to the long axis and directly to the center of resistance of the tooth.

To produce a translatory movement with a resultant force perpendicular to the longitudinal axis of the tooth at a force of 0.70 N in the horizontal direction (x), an additional 0.22 N force was added in the vertical direction (z).

Axial stress and capillary blood stress

Stress distribution appeared to be uniform along the root axis, as shown in Figure 14.

By observing the color scale and the magnitude of the axial stress along the periodontal fibers it is clear that the stress is distributed with virtually identical magnitude along the tooth axis. In this case, as in the previous case, the areas of the palatal and labial surfaces exhibit stress levels that exceed capillary blood stress. Observations of the color scale also revealed that, regarding axial tensions, the tensile stress (+) are on the labial surface and the compressive stress (-) are on the lingual surface.

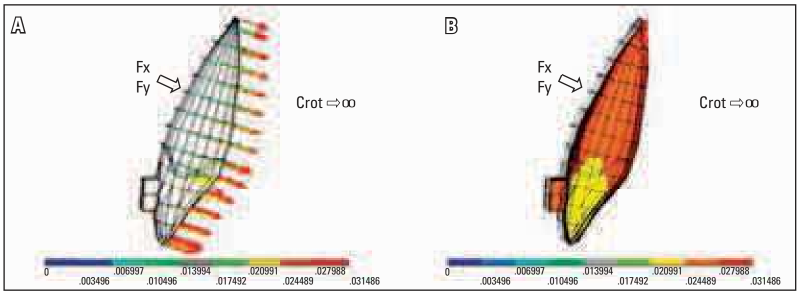

FIGURE 15 - Translatory movement resulting from the application of force to the center of resistance (CRes): **A**) resulting vectors, **B**) resulting displacement.

Classification of resulting tooth movement

Translatory movement, which occurred due to axial stress, was also confirmed by means of graphs showing the vectors and the total resulting displacement. Displacement occurred parallel to the tooth axis, evidencing the translatory movement (Figs 15, A and B), with the center of rotation located at infinity.

The methods used in the construction of this model served as the basis for building a complete model of a dental arch, which allows studies involving various orthodontic appliances.

CONCLUSIONS

1) To enable quantification of the parameters involved in studies of orthodontic mechanics a three-dimensional numerical model of a maxillary central incisor was validated.

2) The value of E=0.059 MPa (0.059 N/mm^2) assigned to the modulus of elasticity of the periodontal ligament fibers enabled the validation of the numerical model.

3) The axial stress measured in the model show consistent values and assist in setting an appropriate value for use in computer simulations, by FEM.

4) The definition of a criterion that compares axial stress with the stress exerted by the blood in the capillary vessel (0.0026 N/mm^2) made it possible to predict which areas are likely to trigger the onset of bone remodeling.

5) A computer model enables the visualization and quantification of root and crown movements as well as the positioning of the center of rotation and the center of resistance of the tooth, which is of primary importance in determining tooth movement type.

6) The model presented in this study enables changes in loading parameters (forces and moment of forces) and in boundary conditions, thereby allowing the creation of a complete model for a dental arch, to evaluation of different orthodontic mechanics alternatives.

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