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Modeling and validation of a 3D premolar for finite element analysis

Modelagem e validação 3D de um premolar para análise de elementos finitos

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Resumo

Introdução: O desenvolvimento e validação de modelos matemáticos é uma importante etapa da metodologia de estudos de elementos finitos. **Objetivo:** Este estudo tem o objetivo descrever o desenvolvimento e validação de um modelo numérico tridimensional de um pré-molar superior para análise em elementos finitos. **Material e método:** Fotografias padronizadas de cortes sequenciais de um pré-molar hígido serviram de referência para o desenvolvimento do modelo 3D, que foi construído por meio do programa SolidWorks (Dassault, França). A fim de validar o modelo testes de compressão e simulação numérica foram realizados. Os gráficos de carga versus deslocamento de ambos os ensaios foram comparados visualmente, a percentagem de erro calculada e homogeneidade dos coeficientes de regressão testada. **Resultado:** Um modelo 3D preciso foi desenvolvido e validado, uma vez que os gráficos apresentavam-se visualmente semelhantes, o percentual de erro ficou dentro dos limites aceitáveis e as retas foram consideradas paralelas. **Conclusão:** Os procedimentos de modelagem e validação descritos permitem o desenvolvimento de modelos dentários 3D precisos com comportamento biomecânico semelhante aos dentes naturais. Os métodos podem ser aplicados no desenvolvimento e validação de novos modelos e estudos de simulações computacionais por meio do MEF.

Descritores: Simulação por computador; estudos de validação; análise de elementos finitos.

Abstract

Introduction: The development and validation of mathematical models is an important step of the methodology of finite element studies. **Objective:** This study aims to describe the development and validation of a three-dimensional numerical model of a maxillary premolar for finite element analysis. **Material and method:** The 3D model was based on standardized photographs of sequential slices of an intact premolar and generated with the use of SolidWorks Software (Dassault, France). In order to validate the model, compression and numerical tests were performed. The load versus displacement graphs of both tests were visually compared, the percentage of error calculated and homogeneity of regression coefficients tested. **Result:** An accurate 3D model was developed and validated since the graphs were visually similar, the percentage error was within acceptable limits, and the straight lines were considered parallel. **Conclusion:** The modeling procedures and validation described allows the development of accurate 3D dental models with biomechanical behavior similar to natural teeth. The methods may be applied in development and validation of new models and computer-aided simulations using FEM.

Descriptors: Computer simulation; validation studies; finite element analysis.

INTRODUCTION

The finite element method (FEM) was developed in the 1950s, initially for application in aerospace engineering. In Dentistry, the technique began to be studied in the 1970s[1]. The methodology has great versatility and analyzes the stresses produced in numerical models; it can be applied in research fields such as implantology[2], orthodontics[3], it can also simulate thermal[4] mechanical cycling[5], water sorption[6] and polymerization shrinkage[7] and can also be applied in cavity optimization[8] and cusp bending[9] studies.

One of the main advantages of finite element analysis (FEA) is its non-destructive and noninvasive nature[3], it can also access stress distribution in inaccessible areas[7]. It costs less than laboratory studies and it overcomes the ethical issues surrounding the use and collection of extracted teeth for research[10].

FEM offers a valid method for the analysis of complex situations in which the variables can be changed simulating various clinical conditions[3]. Improved computer and modeling techniques provide reliable and accurate approach in biomechanics[11]. Geometrically complex systems can be modeled and the accurate representation of each tissue is limited only by computational resources and modeling ability[12].

The development of a numerical model is a complex task, particularly in multicomponent biological structures such as teeth and supporting tissues. Accurate models should predict the behavior of the structure that is represented[13]. In order to make predictions the model has to be validated[14]. The validity of the 3D model depends on the geometric modeling techniques applied during the construction[15], correct geometry and assigned materials properties[16]. Furthermore, the accuracy of FE results is also dependent on element and node size, materials properties, boundary conditions and applied loads and validation against experimental data[16].

There are different ways to perform validation. Direct validation requires comparison of computer simulation with in vitro mechanical tests performed at either the same or a closely collaborating institution. In indirect validation, comparison is performed with laboratory tests or clinical studies published in the literature. The disadvantage of indirect validation is that the variables and test conditions cannot be controlled[17].

The validation can be done by the comparative analysis of the fracture patterns and stress patterns observed on the experimental and numerical models[10,18]. Furthermore, validation can also be performed by the comparison of strain-gauge studies[14] and cusp deflection in computer simulation[19,20].

The association between numerical simulation and traditional mechanical tests may be the best way to study materials and techniques used in Dentistry. When the results of mechanical tests are similar to those of the simulation, the validation of the model can be confirmed[10]. The aim of this study was to present and describe the modeling and the direct validation of a three-dimensional numerical model of an intact maxillary premolar. The hypothesis considered was that the 3D premolar numerical model and the real dental structure would have similar mechanical behavior under the same loading conditions.

MATERIAL AND METHOD

Compression Test

For the compression test, 10 intact maxillary premolars were selected and embedded in cylinders with epoxy resin. A vertical load was applied until fracture, at speed of 1 mm/min by means of a 6-mm-diameter sphere placed on the occlusal surface of the specimen. Data were collected, mean values were obtained and a load versus displacement graphs was generated.

Computational Simulation

Numerical modeling

The three-dimensional model was based on a maxillary second premolar donated by the Department of Morphological Sciences, after approval by the Ethical Committee in Human Research of the Institution. The tooth was embedded in epoxy resin blocks and sliced into 1-mm thick sequential cross sections perpendicular to the long axis on a precision cutting machine.

The slices were photographed in a standardized manner and each photograph was transferred to SolidWorks Software (Waltham, Massachusetts, USA) The external contour of all slices, as well as the internal dentin and pulp contour, were outlined and subsequently assembled. The design of the cusps and occlusal anatomy were refined with the available software tools, generating individual three-dimensional solid models of the external anatomy of the premolar, pulp and coronary portion of the dentin. The superposition of the solid components and exclusion of common structures enabled the generation of the pulpal cavity and the internal and external contour of the enamel. The cementum was not modeled because of its small dimensions and difficulty in visualizing and delimiting boundaries. The components previously constructed were positioned, aligned, brought together, and assembled in an assembly workbench to generate a 3D model of a maxillary premolar composed of enamel, dentin, pulp cavity and pulp.

A cylinder measuring 20 mm height and 18 mm in internal diameter was built with the same program. Procedures of superposition and subtraction of the cylinder and the premolar model were applied to create a representative model of the epoxy cylinder, similar to the one obtained during the preparation of specimens for compressive testing. These files were brought together and assembled, generating the representative numerical model of the test specimens used in the compressive test. A 6-mm-diameter sphere, identical to the sphere used in mechanical testing, was constructed in the SolidWorks software. This sphere was placed on the occlusal surface of the numerical model to define the locations where the load would be applied.

Finite elements modeling

The mesh was composed of tetrahedral parabolic elements and the total number of node points and elements obtained were 222,915 and 145,659, respectively (Figure 1). The level of refinement of the mesh was defined by convergence studies in the ANSYS Workbench program (Swanson Analysis Inc., Houston, PA, USA).

Definition of mechanical properties

All constituents of the models were considered isotropic, elastic, and continuous. The elastic modulus and Poisson ratio of structures modeled were researched in the literature and are described in Table 1.

Definition of boundary and loading conditions

The model was constrained on the surrounding surfaces and at the base of the epoxy resin cylinder, assuming to be fixed in all directions. During computational simulation, a load of 1000 N was

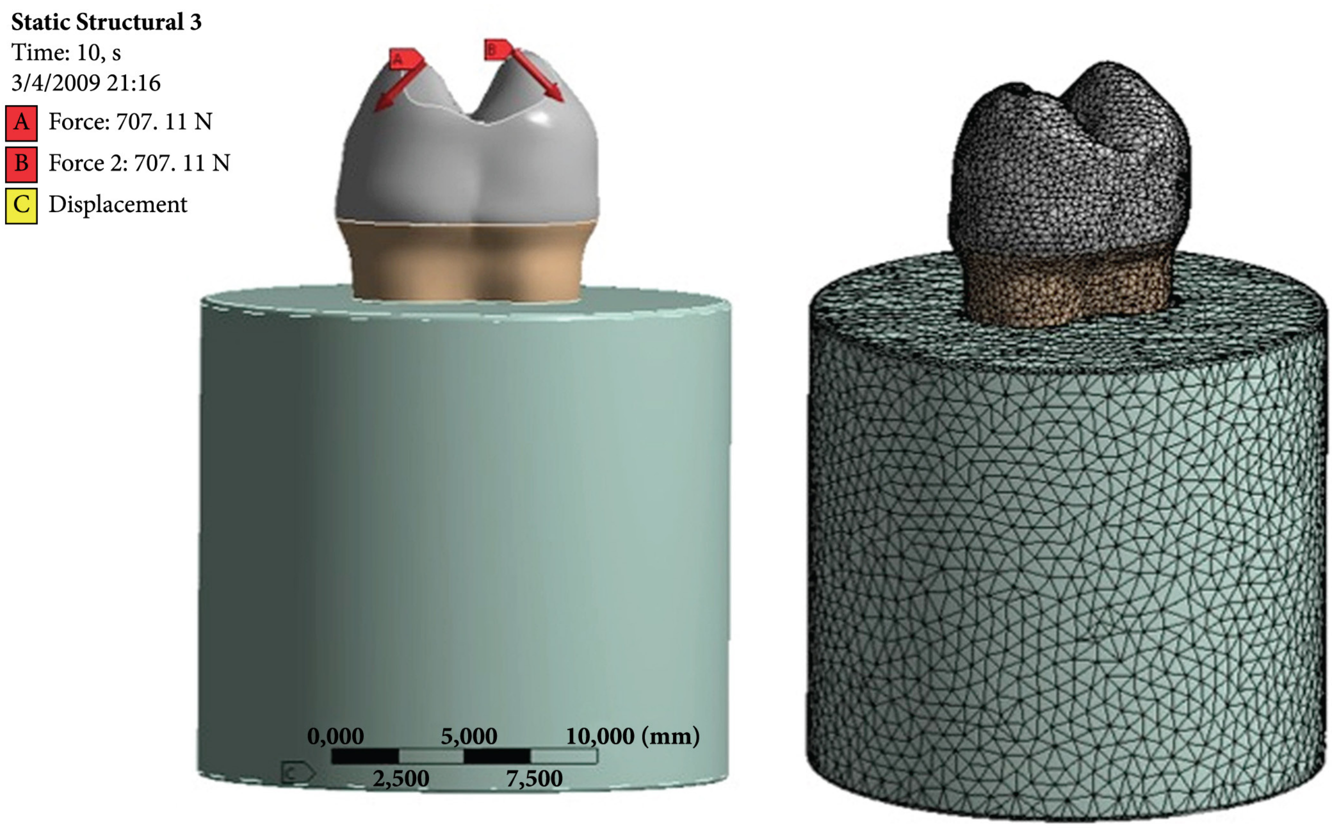

Figure 1. Discretization of model and boundary and loading conditions applied.

Table 1. Mechanical properties of the constituents of the numerical model

Tissue/Material	E	ν
Enamel	72.7 GPa	0.33
Dentin	18.6 GPa	0.31
Epoxy resin	270 GPa	0.35

applied on the occlusal surface. This load was distributed linearly into 10 stages to obtain the intermediate points of displacement, which allowed the construction of a load versus displacement graph of the numerical model. The value of 1000 N was chosen based on the mean data of fracture strength obtained in a previous compressive test.

Processing and post-processing

The processing stage was also performed in the ANSYS Workbench program (Swanson Analysis Inc., Houston, PA, USA). The results were visualized by color diagram for displacement obtained during simulation.

Validation

The validation of the numerical model was performed by: a) Visual analysis of the similarity between the load versus displacement graphs of the experimental test and numerical simulation; b) Calculation of the percentage error of the regression coefficients (slopes) of the numerical and experimental equations; and c) Regression slope homogeneity test (test of parallelism) of experimental and numerical trend lines. Regression trend lines were traced to determine the equation of the straight lines in both tests (numerical and experimental). Through the equations, it was possible to obtain the regression coefficients (slopes) of the lines and latter calculate the percentage of error and test the homogeneity of regression slops (test of parallelism).

RESULT

The mean values of load and displacement from compressive strength test and numerical simulation are shown in Table 2. Superposition of load/displacement data can be visualized in Figure 2. A similar behavior between numerical and experimental tests can be identified in the visual analysis.

Figure 3 shows the trend lines that determined the equation of the straight lines. The slopes of numerical and experimental equations were: a-num = 4082.8; and a-exp = 4279.3.

The percentage error of the regression coefficients (slopes) was 4.6%. According to Lin et al.[20], a percentage error of 10% is acceptable to validate numerical models. Therefore, the percentage error obtained in the present study is acceptable.

The result of the homogeneity of regression slopes (test of parallelism) show that the straight lines of experimental and numerical tests are considered parallel, which means that the numerical model and the real structure have similar behavior when subjected to the same loading conditions (Table 2).

Table 2. Mean load and displacement values of compressive strength test and load and displacement values of numerical simulation

Experimental		Numerical	
Displace-ment (mm)	Load (N)	Displace-ment (mm)	Load (N)
0.000	12.3	0.0000	0.0
0.025	56.0	0.0145	59.2
0.050	123.3	0.0290	118.4
0.075	209.1	0.0435	177.6
0.100	308.3	0.0580	236.8
0.125	415.9	0.0725	296.0
0.150	527.0	0.0870	355.2
0.175	636.3	0.1015	414.4
0.200	738.9	0.1160	473.6
0.225	829.8	0.1305	532.8
0.250	903.8	0.1450	592.0
0.275	955.9	0.1595	651.2
0.300	981.2	0.1740	710.4
		0.1885	769.6
		0.2030	828.8
		0.2175	888.0

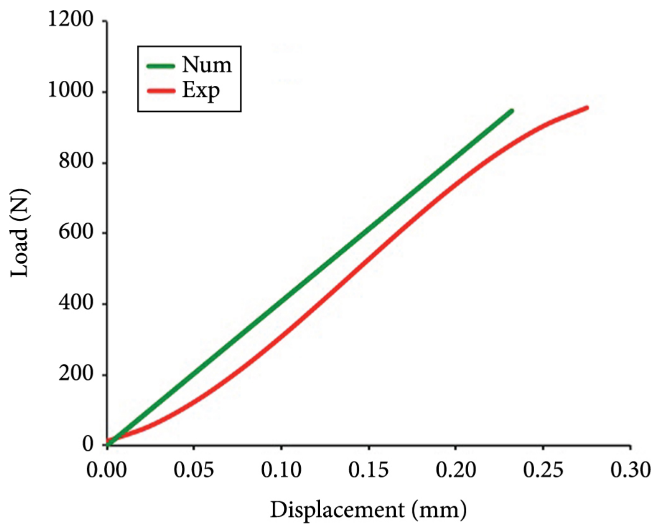

Figure 2. Load versus displacement graph of numerical simulation and experimental test.

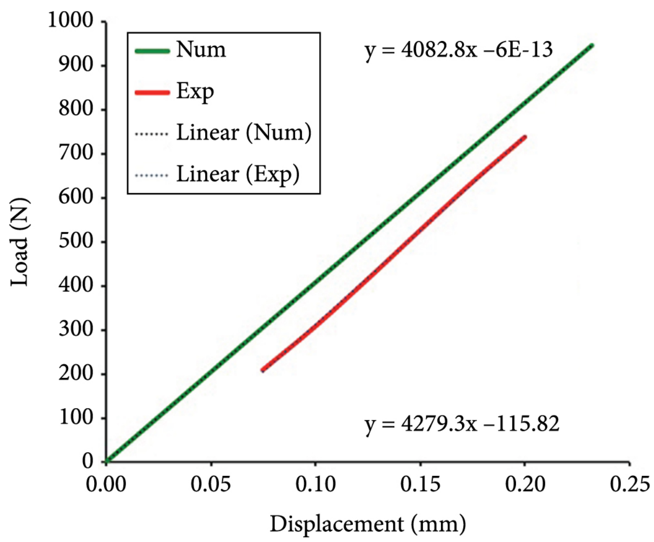

Figure 3. Regression trend lines of load versus displacement graph of numerical analysis and experimental test.

DISCUSSION

The reliability of studies applying finite element method is related to the quality of the numerical model, the boundary and loading conditions, and properties applied during the simulation[16]. The validation process is an important step of the methodology and the purpose is to demonstrate that the mathematical model has the same mechanical behavior as the real physical structure[17]. This process indicates that the results are reliable and accurate[14]. Although convergence studies indicates the reliability of the model, validation assures the accuracy of the results[16]. Once the model is constructed and validated, new analyses can be performed by alteration of properties and loading conditions.

Only few studies address validation of numerical models in dental literature. Recently, researchers from other fields have been attending to the need to validate models[12,21]. There is no standard methodology that describes the validation process. Some authors use compressive strength results for validation[22], while others use strain-gauges[14] and data from fatigue tests[10,14,18]. The studies that performed validation do not describe the methodology in detail, making it difficult to reproduce most of the procedures adopted.

The present study used three parameters to validate the maxillary premolar model: a) superposition and visual comparison of load versus displacement graphs of compressive strength tests and computer simulation; b) calculation of the percentage error of the regression coefficients of the straight lines; and c) application of the homogeneity test of regression coefficients that determines the existence of parallelism between straight lines. Besides validation against experimental data carried out by the authors, further validation can be performed by experimental data available in the literature[16].

The visual comparison of the graphs was performed in the studies of Ausiello et al.[22-24], The calculation of percentage error was conducted by Chang et al.[25] and Lin et al.[20]. The validation through parallelism analysis between the straight lines is less frequent. It is believed that this type of analysis is more objective because a statistical test is applied. Once parallelism is proven, the mathematical model is considered similar to the real physical structure regarding displacement when subjected to the same loading conditions.

Validation is a challenging step of FEM studies. However, the models cannot be completely validated since it is not possible to measure all the parameters that the model can predict. A limitation that should be highlighted is the fact that the validation was performed on a 3D model of a premolar embedded in epoxy resin, bone structures and periodontal ligament were not simulated. Hence validation must not be regarded as absolute proof, but an indication of the behavior of the model[17].

CONCLUSION

The modeling procedures and validation described in this study support the development of accurate 3D dental models with a biomechanical behavior similar to natural teeth. The methods may be applied on construction and validation of new models and FEM computer-aided simulations.

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CONFLICTS OF INTERESTS

The authors declare no conflicts of interest.

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