Mathematical Modelling and Simulation of Periodontal Ligament Using COMSOL Multiphysics

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Abstract. This paper investigated the mathematical modelling and simulation of periodontal ligament using COMSOL Multiphysics. The behaviour of the periodontal ligament is studied. The periodontal ligament is sandwiched between two approached parallel rigid impervious plates. The governing equations and the specified boundary conditions are introduced to describe a rectangular domain. The approximate analytical solution of the problem is verified numerically by using COMSOL Multiphysics that is based on the finite element method. A 3D realistic geometry is constructed using scans of human teeth. A detailed analysis of the stress and displacement induced by a force is obtained.

Keywords: Tooth movement · Periodontal ligament · Finite element method · COMSOL Multiphysics

1 Introduction

The periodontal ligament (PDL) is a connective tissue that binds the tooth to the alveolar bone around it. The PDL is important for the distribution of physiological stresses on the alveolar bone and for preventing stress concentration during mastication and orthodontic therapy, in addition to providing tooth support. The PDL is also responsible for bone remodeling during orthodontic tooth movement [1]. Understanding the PDL via experimental, analytical, and computational methods has been an important topic in dental biomechanics for many years because of the PDL critical involvement in orthodontic tooth movement and bone remodeling. As a result, determining the PDL tissue's material qualities and behaviour is critical and a hotly debated topic. Identifying the qualities of the PDL can aid in the diagnosis of periodontal disease, the evaluation of PDL health following damage, and the consideration of orthodontic tooth movement [2].

The greatest advantage of the classical linear elasticity approach is the ability to visualize the stresses in complex structures, such as the periodontal ligament, and to

N. Wahi et al. (Eds.): ICMSS 2022, ACSR 98, pp. 267–277, 2023.
https://doi.org/10.2991/978-94-6463-014-5_25

observe the stress patterns in the elliptical paraboloid model, allowing the researcher to localize and quantify the stress magnitude. So that it will helps dentists to learn details about the elasticity of periodontal ligament by referring this study. More details about the modelling and simulation of tooth movement can be find in [3–17].

The COMSOL Multiphysics software is based on the finite element method (FEM). Studies using the FEM are becoming more common in order to better understand the mechanical and physiological model that regulates the force required to induce tooth movement. The FEM is a computer-aided mathematical method for studying stress, strain, and deformation of complicated geometries under diverse loading and boundary conditions. Its theory is built on breaking down complex structures into manageable elements that can be easily specified using differential equations. After that, a finite number of elements are put together to produce a rough mathematical model of the structure [7, 18, 19].

This paper will verify the approximate analytical solution of the periodontal ligament given in [4, 20] by using COMSOL Multiphysics software. A detailed analysis of stress and displacement induced by a force will be also investigated.

2 Mathematical Model

This paper investigates the deformation of the porous medium located within a narrow long gap between two approached parallel rigid impervious plates. The purpose is to determine stresses, strains, and displacements of the periodontal ligament solid matrix. The solution presented in this paper is numerical and describes some processes occurring in the periodontal ligament. The following model of partial differential equations will be considered which describe the poroelastic behavior of periodontal ligament [4, 20].

$$\begin{aligned}
&\nabla^2 u - \frac{1}{G}\frac{\partial p}{\partial x} + \frac{1}{1-2\nu}\frac{\partial e}{\partial x} = 0,\\
&\nabla^2 v - \frac{1}{G}\frac{\partial p}{\partial y} + \frac{1}{1-2\nu}\frac{\partial e}{\partial y} = 0,\\
&\nabla^2 p = 0,\\
&\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = e,
\end{aligned} \tag{1}$$

where, $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ and $G = \frac{E}{2(1+\nu)}$. The model (1) is explained in Table 1. The approximate analytical solution of the model (1) is given in [20].

The boundary value problem is presented graphically in Fig. 1. The periodontal ligament is assumed to be located between two plates compressed. Thus, the required solutions of model (1) are considered to meet the following boundary conditions

$$\begin{aligned}
&u(x,h) = 0 \quad \text{at } -l \le x \le l;\\
&u(x,-h) = 0 \text{ at } -l \le x \le l;\\
&v(x,h) = -\overline{u} \text{ at } -l \le x \le l;\\
&v(x,-h) = \overline{u} \text{ at } -l \le x \le l;\\
&p(\pm l, y) = 0 \text{ at } -h \le y \le h.
\end{aligned} \tag{2}$$

The mathematical expressions for the boundary conditions in Fig. 1 are given here demonstrating the corresponding Dirichlet boundary conditions.

Table 1. Description of model (1).

Symbol	Description
$u(x, y)$	the $x-$ component of the displacement of the periodontal ligament
$v(x, y)$	the $y-$ component of the displacement of the periodontal ligament
$p(x, y)$	the fluid pressure
e	the volume strain of the periodontal ligament
G	the shear modulus
ν	Poisson's ratio
E	Young's modulus.

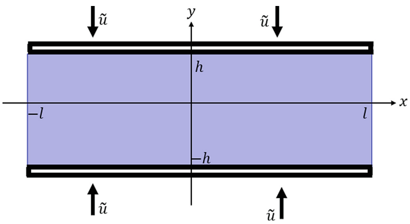

Fig. 1. Boundary value problem [20].

2.1 Numerical Results

The numerical treatment of the boundary value problem (1) is done with COMSOL Multiphysics. The model (1) is not available in finite element software like COMSOL Multiphysics, hence the boundary value problem could be implemented to use the software as a solver for the partial differential equations model. The model (1) can be written in COMSOL Multiphysics form as follows

$$-c\nabla^2\overline{u} - \alpha\nabla\overline{u} = f \tag{3}$$

with

$$\nabla = \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right], \overline{u} = \begin{bmatrix} u \\ v \\ p \\ e \end{bmatrix}, f = \begin{bmatrix} 0 \\ 0 \\ 0 \\ e \end{bmatrix}, c = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

$$\alpha = \begin{bmatrix} \frac{0}{0} & \frac{0}{0} & \frac{\frac{1}{G}}{0} & \frac{\frac{1}{2\nu-1}}{0} \\ \frac{0}{0} & \frac{0}{0} & \frac{0}{\frac{1}{G}} & \frac{0}{\frac{1}{2\nu-1}} \\ \frac{0}{0} & \frac{0}{0} & \frac{0}{0} & \frac{0}{0} \\ \frac{-1}{0} & \frac{0}{-1} & \frac{0}{0} & \frac{0}{0} \end{bmatrix}.$$

In COMSOL Multiphysics, the coefficients of the matrix Eq. (3) coefficients are inserted and the boundary conditions are specified using the software's built-in tools.

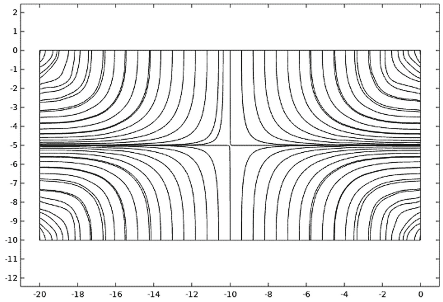

Fig. 2. The streamlines of u and v (COMSOL Multiphysics).

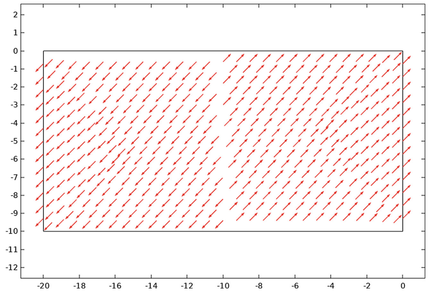

Fig. 3. Arrow surface of u and v (COMSOL Multiphysics).

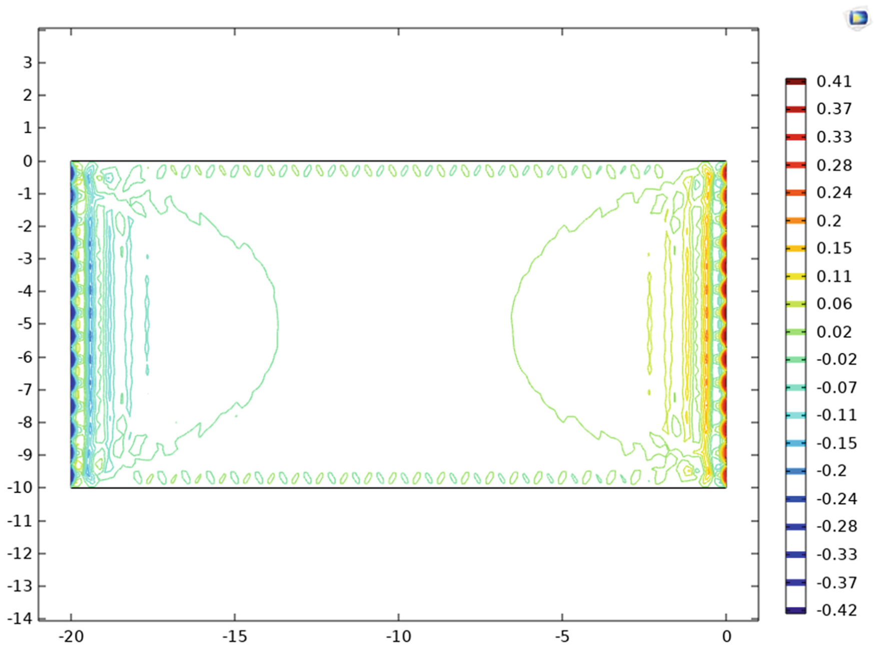

Fig. 4. Contour plot for the displacement u (COMSOL Multiphysics).

The numerical solution is then carried out using the software's solver, with a sufficient number of triangular components achieving convergence.

Figures 2 and 3 show streamlines of u, v and vectors of u, v, respectively. Figure 2 indicated that the solution provides a qualitative description of some processes taking place in the periodontal ligament movement. This is coincided with the analytical solution given in [4, 20].

Figure 4 shows the contour plot for the internal field $u(x, y)$. The Dirichlet boundary conditions are satisfied.

3 Results

The COMSOL Multiphysics that based on finite element method gives us detailed information about the deformation, primary stress concentration (the kind of stress distribution, such as compressive or tensile stress), and Von Mises stress once an external force is applied. When the Von Mises stress of a material is compared to its ultimate tensile strength, it can be determined whether the material will fail under the load applied [21].

An analysis of the stress and displacements is presented in this section through images. Results in terms of stresses and displacements are studied to exclude any possibility of bone failure. Results obtained by FEM analysis are presented through colour maps applied on 3D renderings of the model. Colours are assigned so that there is a change of colour from maximum (red) to minimum (blue) values. Moreover, a colour scale shows the colour assigned to each value range on a colour map; a sample of the colours assigned to each level and the numerical value for each level are displayed [12]. These 3D images allow an overall qualitative view of the stress and displacement states.

3.1 Materials and Methods

A 3D realistic geometry is constructed using scans of human teeth as shown on Fig. 5. The material properties are given in Table 2. The material properties of the PDL are as follows [17]: Poisson's ratio: $\nu = 0.40$, Young's modulus: $E = 0.68$ and shear modulus: $G = 0.24$.

A horizontal concentrated force of 2 N is applied. Applying a horizontal force to the center of resistance, located on the tooth axis, will result in a pure translation in the direction of the force. The socket represents the outside boundary of the model, and the root represents the inside boundary of the model [17, 22]. Boundary conditions are defined to simulate how the model was constrained and to prevent it from free body motion.

3.2 Finite Element Model

Finite element method uses elements, nodes, and contour plots to provide a good visual impression. The basic concept of FEM is the subdivision of a body into many smaller elements as shown in Fig. 6. The mesh setting is given in Table 3.

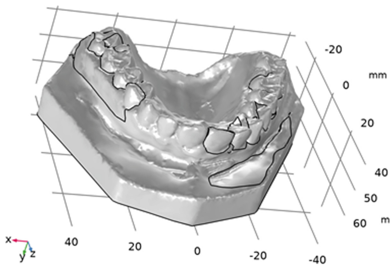

Fig. 5. Geometry. Units are millimeters.

Table 2. Material parameters (Bone) [10, 17].

Name	Value	Unit
Density	1908	kg/m^3
Young's modulus	2.03×10^7	KPa
Poisson's ratio	0.15	1

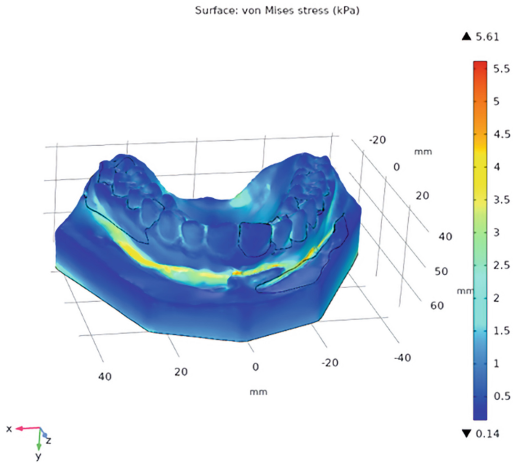

Fig. 6. Finite element model of teeth.

3.3 Stresses

The von Mises stress map allows a qualitative visualization of the amount of bone involved by the system and mechanically stressed [12]. Von Mises stress is reported as a colour map applied to the model as shown in Fig. 7 and Fig. 8. The red colour indicates higher stress values. The unit of Von Mises stres is kilopascal (kPa). The maximum Von Mises stress among teeth is 5.61 kPa as shown in Fig. 7. Figures 7 and 8 indicate that

Table 3. Mesh Settings.

Description	Value
Maximum element size	8.58
Minimum element size	1.54
Curvature factor	0.6
Resolution of narrow regions	0.5
Maximum element growth rate	1.5

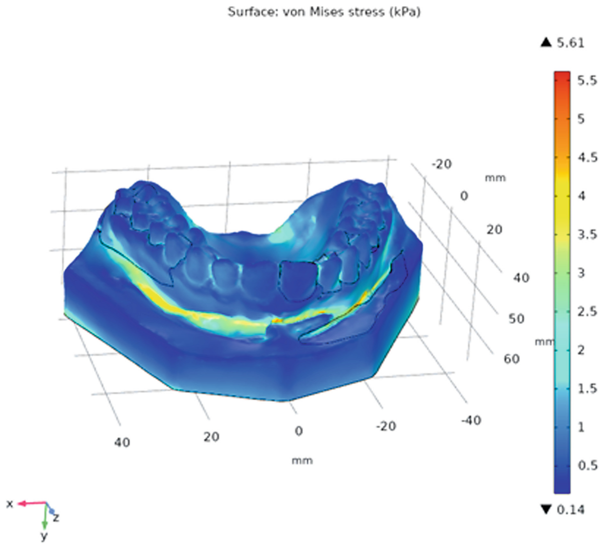

Fig. 7. Von Mises stress (kPa) without deformation.

under the loading conditions assumed for the simulation, the most stressed part is the enamel interface. Table 4 shows different values of stress.

3.4 Displacements

The maps of displacements are shown in Fig. 9. The displacement field attains its maximum of 4.87×10^{-6} mm as shown in Fig. 9. The red colour indicates higher displacements. It is observed that, the largest displacements are on the crown and the enamel. Table 5 shows different values of displacement.

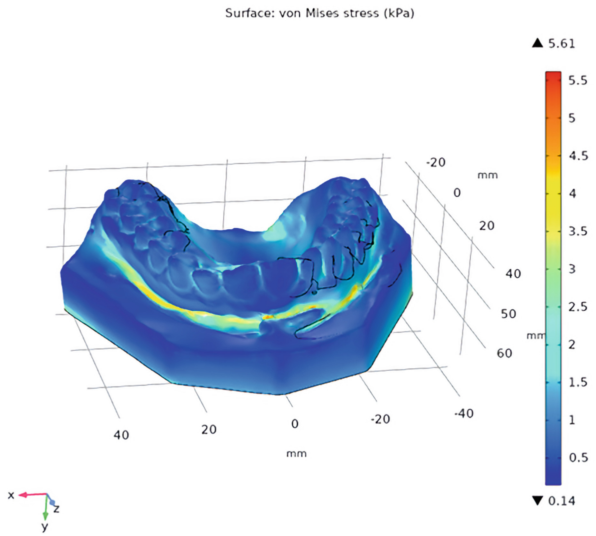

Fig. 8. Von Mises stress (kPa) with deformation.

Table 4. Interactive 3D values of stress.

x	y	z	Value of stress
7.8045	58.901	25.821	3.5301×10^{-7}
12.007	51.751	17.830	2.4733×10^{-6}
25.077	59.401	−1.9631	4.2269

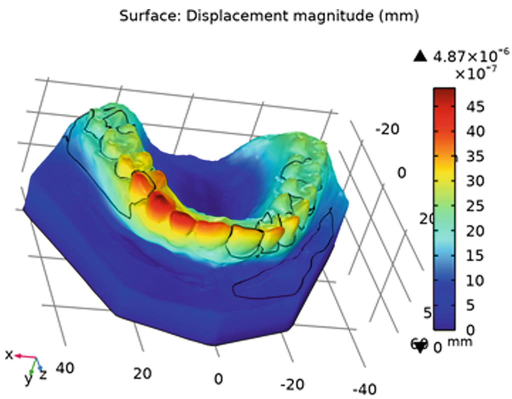

Fig. 9. Surface displacement map of the whole model (red, higher displacements). Units are millimeters.

Table 5. Interactive 3D values of displacement.

x	y	z	Value of Displacement
28.645	49.190	−7.6751	1.8992×10^{-6}
12.021	44.689	9.4545	2.9827×10^{-6}
19.673	40.288	14.137	4.8687×10^{-6}

4 Conclusion and Future Work

This paper investigated the mathematical modelling and simulation of periodontal ligament using COMSOL Multiphysics. The behavior of the periodontal ligament was studied. The periodontal ligament was sandwiched between two approached parallel rigid impervious plates. The governing equations and the specified boundary conditions were introduced to describe a rectangular domain. The approximate analytical solution of the problem was verified numerically by using COMSOL Multiphysics that is based on the finite element method. A 3D realistic geometry was constructed using scans of human teeth. A detailed analysis of the stress and displacement induced by a force was obtained. Next, we will try to find the safe force to use for orthodontic.

Acknowledgments. The authors would like to acknowledge the Ministry of Higher Education Malaysia, Research Management Centre-UTM, Universiti Teknologi Malaysia (UTM) and Dental Simulation and Virtual Learning Research Excellence Consortium for financial support through the Konsortium Kecemerlangan Pendidikan (KKP) grant with vote number 4L948.

Authors' Contributions. All authors read and approved the final manuscript.

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