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Biomechanical time dependency of the periodontal ligament: a combined experimental and numerical approach

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SUMMARY The analysis of the non-linear and time-dependent viscoelasticity of the periodontal ligament (PDL) enables a better understanding of the biomechanical features of the key regulator tissue for tooth movement. This is of great significance in the field of orthodontics as targeted tooth movement remains still one of the main goals to accomplish. The investigation of biomechanical aspects of the PDL function, a difficult area of research, helps towards this direction. After analysing the time-dependent biomechanical properties of pig PDL specimens in an *in vitro* experimental study, it was possible to confirm that PDL has a viscoelastic anisotropic behaviour. Three-dimensional finite element models of mini-pig mandibular premolars with surrounding tissues were developed, based on micro-computed tomography (μCT) data of the experimental specimens. Tooth mobility was numerically analysed under the same force systems as used in the experiment. A bilinear material parameter set was assumed to simulate tooth displacements. The numerical force/displacement curves were fitted to the experimental curves by repeatedly calculating tooth displacements of 0.2 mm varying the loading velocities and the parameters, which describe the nonlinearity. The experimental results showed a good agreement with the numerical calculations. Mean values of Young's moduli E_1, E_2 and ultimate strain ε_{12} were derived for the elastic behaviour of the PDL for all loading velocities. E_1 and E_2 values increased with increasing the velocity, while ε_{12} remained relatively stable. A bilinear approximation of material properties of the PDL is a suitable description of measured force/displacement diagrams. The numerical results can be used to describe mechanical processes, especially stress–strain distributions in the PDL, accurately. Further development of suitable modelling assumptions for the response of PDL under load would be instrumental to orthodontists and engineers for designing more predictable orthodontic force systems and appliances.

Introduction

Orthodontic tooth movement occurs after the application of a force system. The predictability of orthodontic tooth movement after applying forces or moments is still a goal of orthodontic research to be achieved. The physiological mechanism that initiates tooth movement in response to force is the periodontal ligament (PDL; Proffit and Fields, 2000). Immediately after applying a force system on a tooth, initial tooth mobility occurs associated with an intra-alveolar tooth displacement, producing local stress and strain distributions in the desmodontium. At this initial phase, the deformation of the alveolar bone is reversible and of very low magnitude. Maintaining this state, the mechanical stress in the PDL triggers apposition and resorption of the alveolar bone, which is bone remodelling and results in a permanent change of the tooth position.

The degree of initial tooth displacement is related to the material properties of the different structures involved. It is regarded as primarily governed by PDL deformation as teeth are rigid and are connected *via* the PDL to an almost rigid alveolar bone (Bourauel *et al.*, 1999; Nishihira *et al.*, 2003). Much is known about the mechanical properties of teeth and alveolar bone but inconsistency exists with regard to the material properties of the PDL throughout the literature (Natali, 2003). It is the knowledge of the biomechanical behaviour of the PDL that will help us to understand the initial tooth mobility and consequently the biological response, which yet remains not well understood.

The PDL consists of 53–74 per cent collagen fibres and 1–2 per cent blood vessels and nerve endings embedded into an amorphous mucopolysaccharide matrix (Embery, 1990; Pietrzak *et al.*, 2002). It also harbours a variety of cell population that is able to stimulate periodontal regeneration, meaning the formation of new bone, cementum and connective tissue attachment (Berkovitz, 1990). This complex, fibre-reinforced substance responds to force in a viscoelastic and non-linear manner (Jónsdóttir *et al.*, 2006). The fibrous collagen phase resists tensile forces and the fluid phase is responsible for the PDL's viscoelastic properties and time-dependent behaviour under load (Carvalho *et al.*, 2006). The PDL's cellular response to mechanical loading leads in remodelling of the ground substance and fibrous tissue (Embery, 1990). Viscoelastic responses are the causes of strain energy dissipation, without which excessive energy would cause tissue breakage (Fung, 1981; Provenzano *et al.*, 2001; Sanctuary *et al.*, 2005; Sanctuary *et al.*, 2006; Shibata *et al.*, 2006; Komatsu *et al.*, 2007). Therefore, the viscoelastic response of the PDL, which still remains unclear, is important to be studied as it is important for the tooth support function (Komatsu *et al.*, 2004). Also, the determination of the stress levels in different areas of the PDL, which are the most important for orthodontic biomechanics, may lead to an objective correlation of the force application on a tooth and the tooth's response. However, functional adaptation phenomena still remain unclear because of the outstanding complexity and the difficulty in combining biomechanical and biochemical aspects in study designs.

The aim of this study was to evaluate the biomechanical time-dependent behaviour of the PDL in relation to a given tooth displacement of 0.2 mm, simulating an uncontrolled tipping, which was achieved within 5, 10, 20, 30, 60, 120, 350, 450 and 600 seconds by using a combined experimental and numerical approach.

Materials and methods

For the experimental part of this study, initial tooth mobility for 0.1 and 0.2 mm displacement occurring in time spans of 5, 10, 20, 30, 60, 120, 300, 450 and 600 seconds was measured on a total of 18 deciduous premolars of 3- to 12-month-old mini-pigs (Papadopoulou *et al.*, 2011). The choice of the mini-pigs was based on their qualitative similarity to humans. They have a similar masticatory cycle and also go through a phase of primary teeth with a development similar to the human one (Weaver *et al.*, 1962; Herring, 1976; Rygh *et al.*, 1982). Therefore, they were considered to be suitable for the purpose of our study. Displacements with variable increasing loading time were applied to one premolar crown of each jaw segment into the linguobuccal direction through a force sensor provided by a specialised biomechanical set-up. The predefined displacement values to be achieved were 0.1 and 0.2 mm. Each of the given displacement increments was applied on the specimens with a linear displacement increase employing the following time spans: 5, 10, 20, 30, 60, 120, 300, 450 and 600 seconds. Force values were measured during load application in order to register force/displacement diagrams. After the maximum displacement was reached, force decay was monitored for a period of 600 seconds.

Due to the extreme force variations among specimens, errors of the means were found to be up to 50 per cent or even more. Possible factors to explain the high variations among specimens are the tooth anatomy, the root surface area and the extent of periodontal support and height (Cardaropoli and Gaveglio, 2007). In order to estimate the impact of the root volume and surface area on the presented results, the root surface and volume were calculated using an idealised paraboloid geometry formula (Bronstein *et al.*, 2007). The Spearman rank correlation test did not show any significant correlation of forces with root volumes or root surfaces.

We concluded that the initial force value deviations observed can be attributed to the biological tissue characteristics of the respective specimen and probably to the different morphology of the alveolar bone around the root of the teeth as well as the different states of dental development of the animals.

Development of the 3D finite element models

Following the completion of our experimental approach (Papadopoulou *et al.*, 2011), 13 specimens were selected based on the experimental results for the numerical analysis. Specimen geometries were obtained using micro-computed tomography (μCT) scans (SkyScan 1174, SKYSCAN, Belgium) with a resolution of 1024×1304. The number of slices in each scanned preparation ranged from 947 to 1011. As μCT scanning with the requested high resolution takes several hours to be completed, the specimens dry out because of the heat generated during scanning. Therefore, the samples were sent to μCT scanning after experimentation. A 3D surface reconstruction of the preparations including tooth, PDL and bone was conducted using the self-developed software ADOR-3D (Rahimi *et al.*, 2005; Figure 1a). Based on the μCT data, the bone was not differentiated into cortical and cancellous bone. Tooth structure was not differentiated into enamel, dentine, pulp and cementum because no substantial deformation of the dental hard tissue was to be expected (Nägerl and Kubein-Meesenburg, 1993; Haase, 1996). Consequently, an isotropic, homogenous and linear elastic model was assumed for the tooth with the elasticity parameters of dentine and for bone, which led to simplification of the calculations.

Improper visualisation problems that occurred were then further processed for all models and the five most suitable ones were selected for the finite element model (FEM) generation and the following finite element analysis (FEA). Criteria were the geometrical structure that would best apply to the following numerical calculations in combination with representative experimental results of the experimental study population. The reconstructed geometries of the five specimens were imported into the finite element (FE) package MSC.Marc/Mentat 2007r (MSC.Marc Mentat 2007r, MSC.Software Corporation, Santa Ana, CA, USA). Tetrahedral elements were used to create the volume

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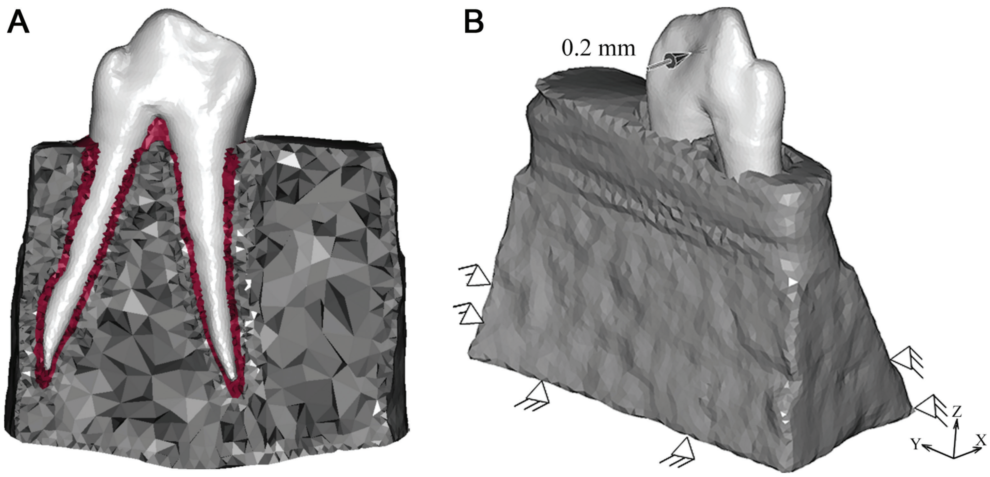

Figure 1 (A) Longitudinal section of a 3D finite element model (FEM) of the specimens after reconstruction of the geometry. (B) Boundary conditions used for the finite element analyses (FEA) according to the corresponding experimental data.

models. A particular attention was paid to developing the FEM at the furcation area in order to most accurately represent PDL, alveolae and the corresponding tooth root geometry in the furcation region (Figure 1a). Table 1 summarises the respective root length, diameter, surface and volume area for the calculation models.

Each numerical model consisted of tooth, bone, bone furcation, PDL and PDL furcation. The elements of PDL furcation were connected to those of PDL, excluding the interfaces in the horizontal level. The same was conducted with bone elements that were connected to bone furcation elements. In this way, PDL elements were created containing the furcation elements fitting perfectly the tooth–bone furcation region. Critical part was the connection of tooth and PDL elements and the connection between PDL elements to bone elements. For that, the tetrahedral meshing of bone elements was made in such way that bone elements became smaller and finer towards PDL elements to improve the accuracy of the interfaces and the outcome of the numerical calculations. Similarly, the outer surface of the tooth would conduct the PDL surface in the PDL–tooth interface. The models consisted of an average number of 47.235 nodes and 251.842 elements. The PDL structure consisted of 10.924 nodes and 64.743 elements in average for the five FEMs. Its maximum thickness was calculated in the FEM at 0.32 mm and its minimum at 0.12 mm in average. The PDL appeared to be thicker at the apex and at the furcation area as well as its cervical third area. The minimum thickness was noticed approximately at two-third of its length for each model. The mesh density of the models was thus within a region of stability determined in previous studies (Haase, 1996).

Table 1 Root length, diameter, surface and volume area for the calculation models used in this study.

Specimen	Intraosseous root length (mm)		Root diameter (mm)		Total root surface area (mm^2)	Total root volume area (mm^3)
	Mesial root	Distal root	Mesial root	Distal root		
Specimen 1	12	13	3	3	431	88
Specimen 2	16	10	3	4	313	119
Specimen 3	13	15	3	4	556	140
Specimen 4	16	14	3	4	338	115
Specimen 5	11	12	3	3	373	81

Tooth loading and boundary conditions were adjusted in order to resemble as accurately as possible the experimental tests for every corresponding specimen (Figure 1b). This involves the direction and point of force application, material and mechanical parameters. In the experimental probes, the point of force application was marked and measured with a calliper with respect to the occlusal, mesial and distal borders of the tooth crown. The transmission to the FEM followed with an accuracy better than 0.1 mm. The nodes at the position were chosen and exactly positioned according to the experiment. With the help of beam elements, the selected nodes were connected to the central node where the force was finally applied. Additionally, nodes localised at the lower third part of the bone model were fixed in all three degrees of freedom in order to represent the bone part embedded in the acrylic resin during experimentation.

Table 2 shows the Young's moduli used for bone and tooth structures, which were taken from early experiments by Spears *et al.* (1993). For the PDL, two different values for the initial Young's modulus were used and a value for the ultimate strain ε_{12} was specified to simulate their bilinear material characteristics.

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Table 2 Material parameters of tooth, bone and periodontal ligament (PDL) used in this study.

Material	Young's modulus (MPa)	Poisson's ratio (μ)
Tooth	20 000	0.30
Bone	2000	0.30
PDL	Bilinear	0.30

Values for tooth and bone are taken from Spears *et al.* (1993).

Comparison of the experimental and numerical results

Initially, a standard bilinear parameter set for the elasticity of the PDL was applied and then verified by comparing the load/displacement curves derived from the experimental and numerical results. When clear-cut discrepancies between the two curves appeared, the parameter set for the elastic properties of the PDL was varied accordingly, the calculation would be repeated and its results were compared once again with the measured results. This iterative procedure was continued until maximum correspondence was achieved for 0.2 mm displacement for the nine different velocities of the five specimens.

In the post-processing, the biomechanical responses of the PDL to initial tooth mobility were quantified by analysing and comparing the equivalent total strains and equivalent stresses.

Statistical analysis

Due to the small sample size, the data were regarded to be not normally distributed. The variability of the Young's moduli (E_1, E_2) and the ultimate strain (ε_{12}) of the PDL values according to the various time points was tested with Friedman's two-way analysis of variance (ANOVA) by ranks in IBM SPSS Statistics Version 20 (SPSS Inc., Chicago, IL, USA). A two-tailed $P \leq 0.05$ was considered statistically significant.

Results

The non-linear force/displacement behaviour could be described in a bilinear manner by means of two straight lines corresponding to two different Young's moduli. Most of the numerical fitted force/displacement curves showed good agreement with the experimental curves as illustrated in Figure 2a, b and 2c, which in turn assures the reliability of the determined Young's moduli (E_1 and E_2 values). Means and standard deviations for the elasticity parameters of PDL according to the numerical calculations were obtained (Figure 3). According to the statistical analysis, the data were found to vary statistically significant among the loading time spans between 5 and 600 seconds. Equivalent stress and strain values within the PDL were considered to present the numerical results. The stress reached its highest value

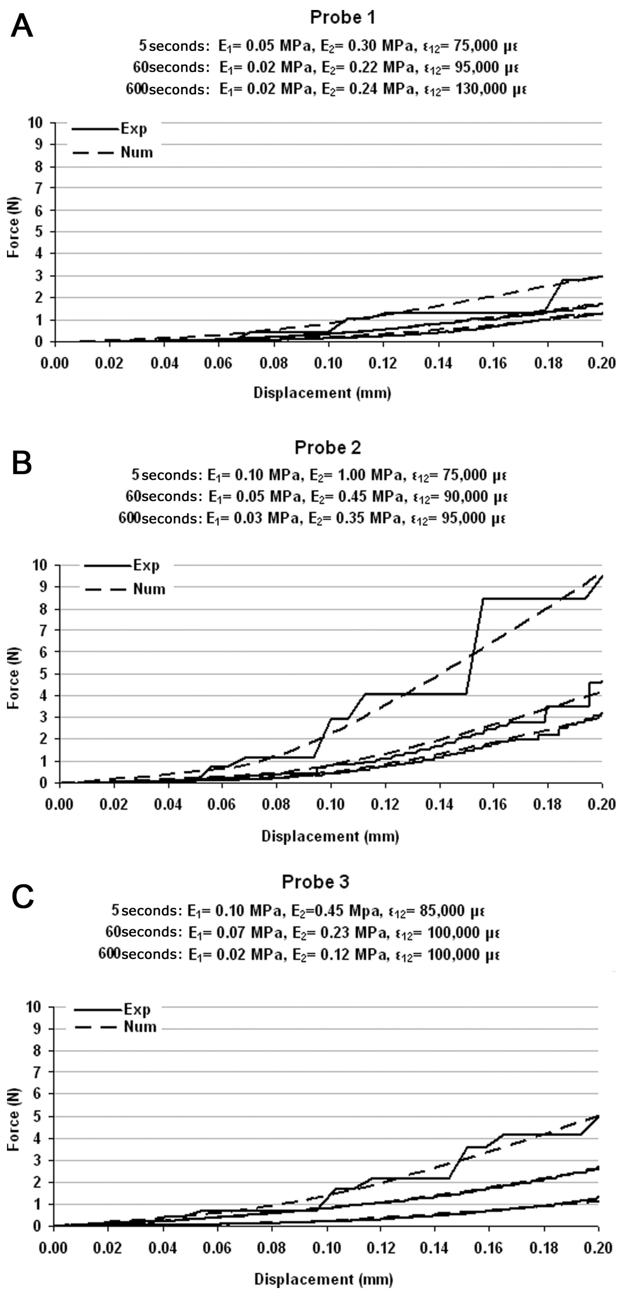

Figure 2 Approximation of the calculated curve to the measured force/displacement behaviour assuming a bilinear material behaviour of the periodontal ligament (PDL) for a loading time of 5, 60 and 600 seconds and total displacement of 0.2 mm of specimen 1 (2a), 2 (2b) and 3 (2c). The ultimate strain ε_{12} is the limit of the region with a low Young's modulus E_1 and the transition to a higher stiffness corresponding to modulus E_2.

of 2.2 MPa at 5 seconds (E_1 = 0.10 and E_2 = 0.45 MPa) and the lowest value of 0.17 MPa at 600 seconds (E_1 = 0.015 and E_2 = 0.072 MPa). The strain reached its highest value at 3.5 per cent for E_1 values, which range within 0.0150.03 MPa and E_2 values within a range of 0.100.04 MPa. Its lowest value is demonstrated at 1.3 per cent by a specimen whose E_1 values range within 0.020.15 MPa and E_2 values within

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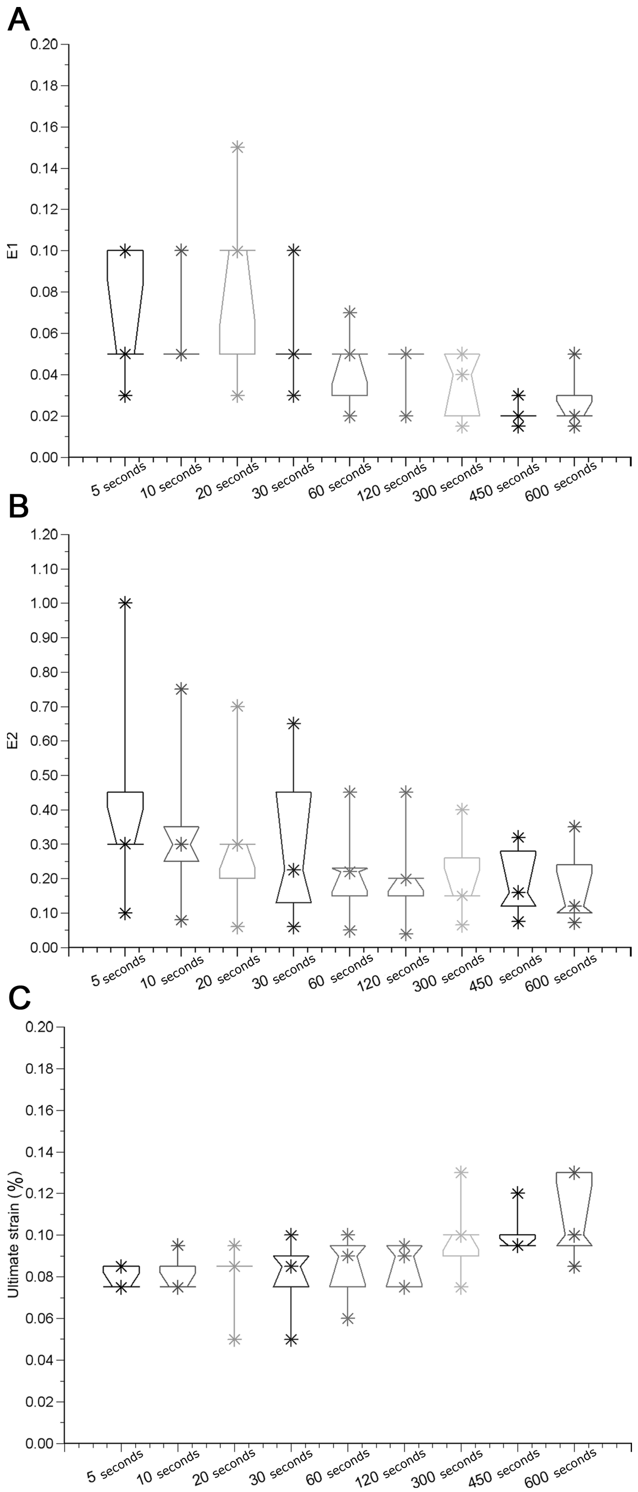

Figure 3 Box diagrams of the mean values of the bilinear set of parameters for the five probes for each loading velocity. (a) Mean values for E_1, (b) E_2 and (c) ultimate strain ε_{12}.

0.100.30 MPa. Means and standard deviations for the PDL strains and stresses were additionally obtained for each loading velocity.

Discussion

Remodelling of the periodontal tissue after tooth loading with orthodontic forces has been the subject of extensive research. Factors such as tissue complexity and modelling assumptions (i.e. linear or non-linear, isotropic or anisotropic, elastic or viscoelastic) can explain the large inconsistency in values for PDL material properties. The PDL is known to be non-linear, anisotropic, non-homogeneous and viscoelastic (Andersen *et al.*, 1991). Most studies, however, use basic simplified models and analyse PDL as linear, elastic and isotropic, noting that this approach was sufficient for the purposes of their study (Tanne *et al.*, 1987; Andersen *et al.*, 1991; Clement *et al.*, 2004; Cattaneo *et al.*, 2005; Viecilli *et al.*, 2008; Kojima and Fukui, 2011). Few studies have assigned non-linear mechanical properties to the PDL (Middleton *et al.*, 1996; Durkee, 1997; Durkee *et al.*, 1998). Non-linear simulations of the PDL provide more accurate and reliable calculation for the stresses and strains over a wide range of different tooth movements (Pini *et al.*, 2004). Natali *et al.* (2011) proposed the development of a constitutive model with two viscous processes, with constant relaxation times, and a relative stiffness that depends on the strain by an exponential function. Their model gives an acceptable accuracy and limits the number of constitutive parameters for the case of describing the mechanical response of the PDL tissue under stress relaxation in tensile conditions. Numerical simulations often require additional experimental and/or clinical validations, which is of critical importance for ensuring the reliability of an analysis (Qian *et al.*, 2009). The present work was conducted in a combined experimental–numerical approach that allows identification of the time-dependent behaviour of the PDL by means of FEA.

Validity of the FEA results depends entirely on the ability to model the complexity of morphology and the tissues' material properties of the structures to be analysed (Cattaneo *et al.*, 2005). Constructing accurate and suitable FE meshes of tooth geometry is essential as FE simulation results are highly sensitive to geometric modelling assumptions (Hohmann *et al.*, 2011). In this study, 13 computerised models of the corresponding experimental specimens were reconstructed using an average number of 100 digitised cuts due to µCT scanning. The geometry of the resulting 3D models in combination with their corresponding experimental results was evaluated. The number of specimens that had achieved the most accurate geometrical characteristics while demonstrating a suitable geometry for the numerical calculations was listed. The specimens showing the most representative experimental results were also noted. Five of the models, which were included in both these groups, were considered as most suitable for the numerical approach. Additional attention was paid to the accurate and careful reconstruction of the PDL at the root furcation region. It is important to note that PDL width varies for each tooth as well as among specimens. Some authors provide 2D

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reconstruction of the experimental specimen (Middleton *et al.*, 1996; Rees and Jacobsen, 1997), whereas others consider a uniform PDL geometry (Toms *et al.*, 2002). The study of Toms and Eberhardt (2003) showed that predicted stresses using a uniform thickness of the PDL are substantially different from stresses predicted using a non-uniform thickness. Also, predicted stresses using non-linear mechanical properties are proved to be different from predicted stresses using linear ones (Toms and Eberhardt, 2003).

Apart from the benefits of FEA, the limitations of this method should also be considered. Problems might occur at every step during the generation of the 3D models due to improper position, insufficient rigid fixing in the scan or improper scanning parameters. During the 3D surface model and 3D FEM generation, problems can occur due to improper visualisation, identification of structures in the slices, number of slices discretised, smoothing factor, material and mechanical parameters and boundary conditions, which could cause unrealistic computerised transformation of the original experimental geometry.

Stress conditions in the periodontium can be expressed using complex mathematical equations—a constitutive model. Constitutive models help to establish a relationship between kinematic (strains) and static variables (stresses) (Curnier, 1994). The complexity of the constitutive laws increases even more with the inclusion of more behavioural parameters, such as the non-linearity and the viscoelasticity. Research in PDL biomechanics has focused on four specific types of structured constitutive modelling approaches: linear elastic, multi-phase, hyperelastic and viscoelastic models (Fill *et al.*, 2012). Most computational models assume bilinear elastic or non-linear hyperelastic PDL behaviour (Cattaneo *et al.*, 2005; Ziegler *et al.*, 2005), and few FE models exist that take the PDL's viscoelastic properties into account (Natali *et al.*, 2007; Pena *et al.*, 2007). In this study, the computational approximation of the mechanical behaviour of the PDL was carried out with a set of parameters that consisted of two different Young's moduli and an ultimate strain. The PDL was modelled as a bilinear material, whereas tooth and bone were modelled as isotropic and homogenous bodies. The obtained values of E_1 ranged from 0.015 to 0.15 MPa and those of E_2 from 0.04 to 1.00 MPa, showing agreement with the range found in the literature (Goel *et al.*, 1992; Pietrzak *et al.*, 2002). These studies used a simple linear model for the PDL with a mean Young's modulus over a stress/strain regime, typically showing non-linear behaviour. Our model is simple as well, considering the non-linearity by a bilinear approach for the same stress/strain regime. It is obvious that a mean Young's modulus for that regime should be in the same order of magnitude as the two moduli in our model. The disadvantage of the bilinear model though is that it cannot describe the continuous change of the Young's modulus with strain. The reported E_1 and E_2 values of this study give an idea of the hydrodynamic behaviour of the PDL and are meant to deliver start parameters for a more complex, biphasic, time-dependent and non-linear material model of the PDL, described in Favino *et al.* (2012).

Using FEA, the biomechanical response of the tooth and its surrounding structures can be readily interpreted through the visualisation of stress and strain distributions within the PDL. Melsen *et al.* (2007) postulated that it is the alteration of the stress and strain distributions of the periodontium and not any compression or tension forces that initiate a cascade of biological reactions, which in turn lead to tooth movement. In this study, we observed that stress values could be related to root geometry, and in fact, it seems that stresses concentrate in locations where the root morphology appears to be narrow, i.e. in furcation regions. Stress values were directly affected by the variations of E_1 and E_2. As they increase, stress values rise respectively. Equivalent of stress reached its highest value (2.2 MPa) at 5 seconds (E_1 = 0.10 MPa, E_2 = 0.45 MPa), whereas the stress was 0.65 MPa at 600 seconds (E_1 = 0.02 MPa, E_2 = 0.12 MPa) for the same specimen. The lowest level of equivalent stress among all specimens reached 0.17 MPa at 600 seconds (E_1 = 0.015 MPa, E_2 = 0.072 MPa). High strain concentrations occurred at the level of the cervix of the PDL near the furcation region too. The strain converged to certain values and remained stable for each model among the different loading velocities. The highest value of equivalent of total strain was 3.5 per cent, whereas the lowest equivalent of total strain was demonstrated at the value of 1.3 per cent.

The type of loading characterised from the loading direction and velocity, frequency and strain rate also contributes in the variety of the numerical results. The PDL may be loaded under a long-lasting, sustained force system (orthodontics) or under short-term, impact-type force applications (mastication). Viscoelastic properties are dependent on the magnitude and the frequency of the loads applied. Short-term tooth responses overestimate the material stiffness since initial fluid pressurisation occurs (van Driel *et al.*, 2000). In this study, we provided horizontal load of continuous forces for time spans ranging from 5 up to 600 seconds. The results showed that stiffness of the PDL increased with increasing loading velocity.

Conclusions

1. Numerical results showed a very good agreement with the experimental data implying that the FEM is a useful and reliable tool for investigating PDL biomechanics.
2. The Young's moduli and the ultimate strain of the PDL are affected by the loading time with a statistical significance, for a loading time of 5 seconds or more, i.e. the moduli decrease from shorter to longer loading times.
3. A model for orthodontic biomechanical characterisation with respect to realistic PDL digital reconstruction and with the least computational complexity would lead to

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better understanding and predicting orthodontic tooth movement.

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